



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:56 PM UTC

PDB ID : 8E1U / pdb_00008e1u
Title : Propionibacterium freudenreichii PPI-dependent PEPCK in complex with malate
Authors : McLeod, M.J.; Holyoak, T.
Deposited on : 2022-08-11
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

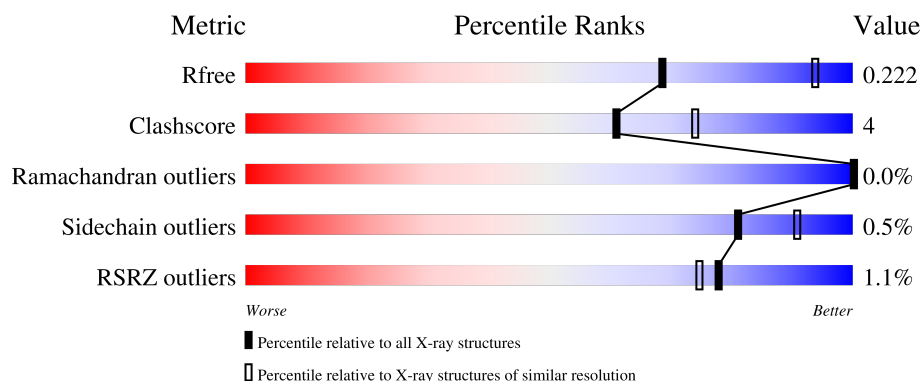
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	1131	
1	B	1131	
1	C	1131	
1	D	1131	
1	E	1131	

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Mol	Chain	Length	Quality of chain
1	F	1131	% 88% 11%
1	G	1131	2% 86% 12%
1	H	1131	% 88% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 72470 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 PPI-dependent PEPCK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1126	Total	C	N	O	S	0	0	0
			8928	5615	1574	1706	33			
1	B	1125	Total	C	N	O	S	0	0	0
			8921	5612	1573	1704	32			
1	C	1125	Total	C	N	O	S	0	0	0
			8922	5612	1573	1704	33			
1	D	1124	Total	C	N	O	S	0	0	0
			8914	5608	1572	1701	33			
1	E	1120	Total	C	N	O	S	0	0	0
			8881	5589	1567	1693	32			
1	F	1117	Total	C	N	O	S	0	0	0
			8868	5581	1564	1690	33			
1	G	1115	Total	C	N	O	S	0	0	0
			8859	5576	1562	1688	33			
1	H	1122	Total	C	N	O	S	0	0	0
			8895	5598	1567	1697	33			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

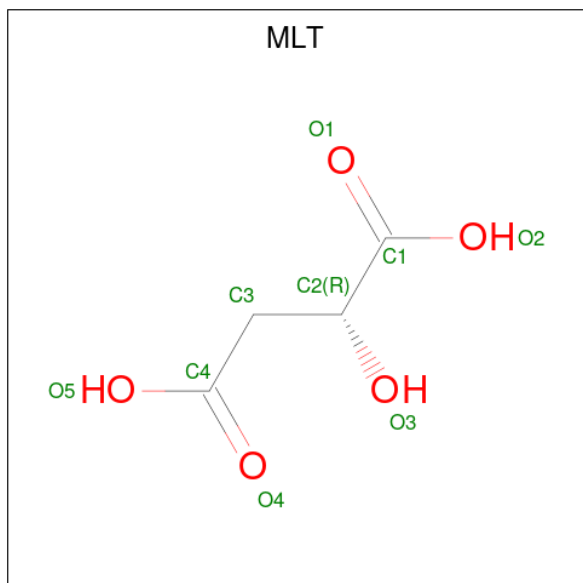
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		

- Molecule 3 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		

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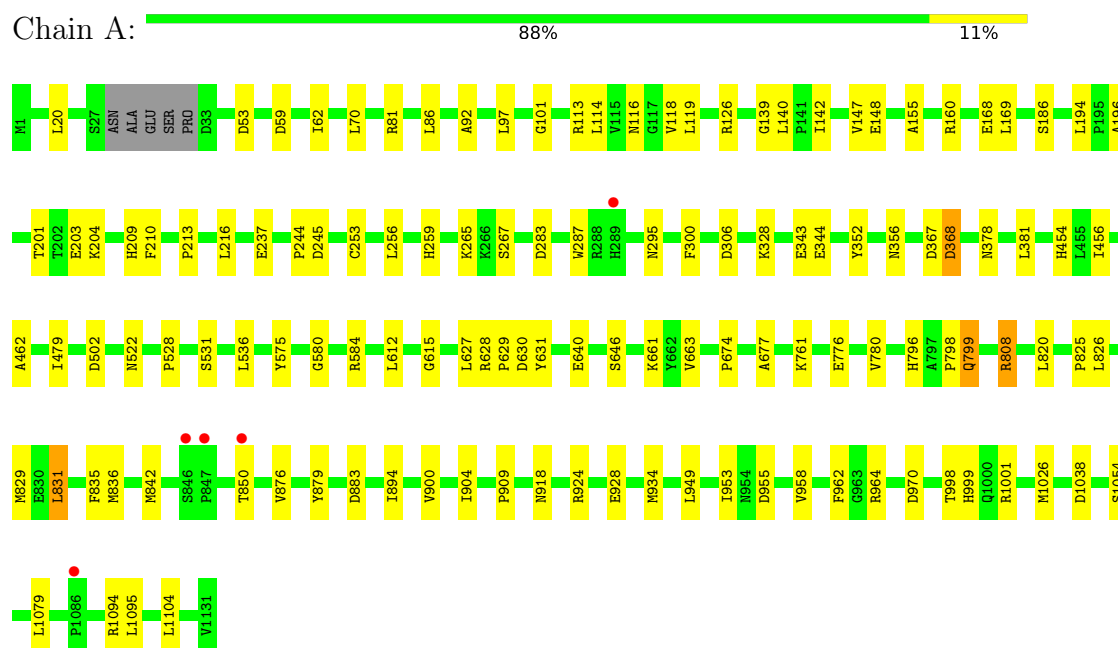
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	122	Total 122	O 122	0	0
4	C	141	Total 141	O 141	0	0
4	D	156	Total 156	O 156	0	0
4	E	144	Total 144	O 144	0	0
4	F	173	Total 173	O 173	0	0
4	G	137	Total 137	O 137	0	0
4	H	154	Total 154	O 154	0	0

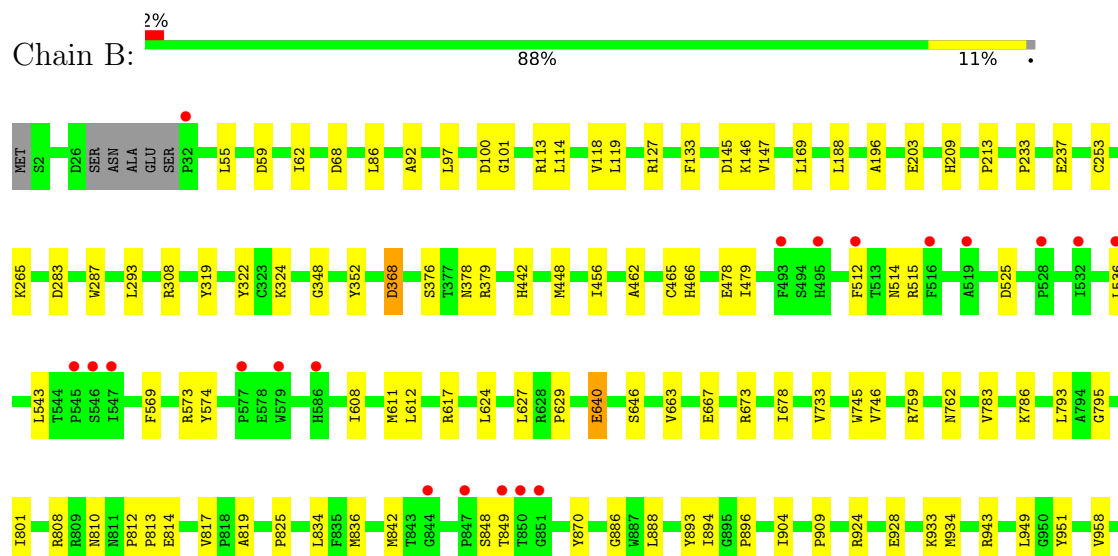
3 Residue-property plots

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: PPi-dependent PEPCK

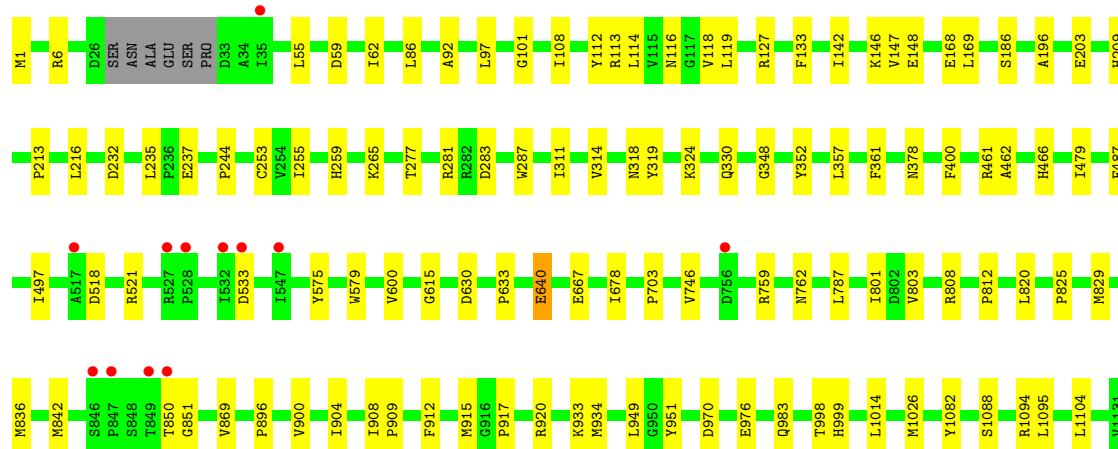
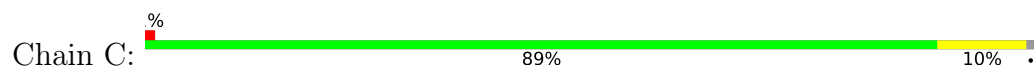


• Molecule 1: PPi-dependent PEPCK

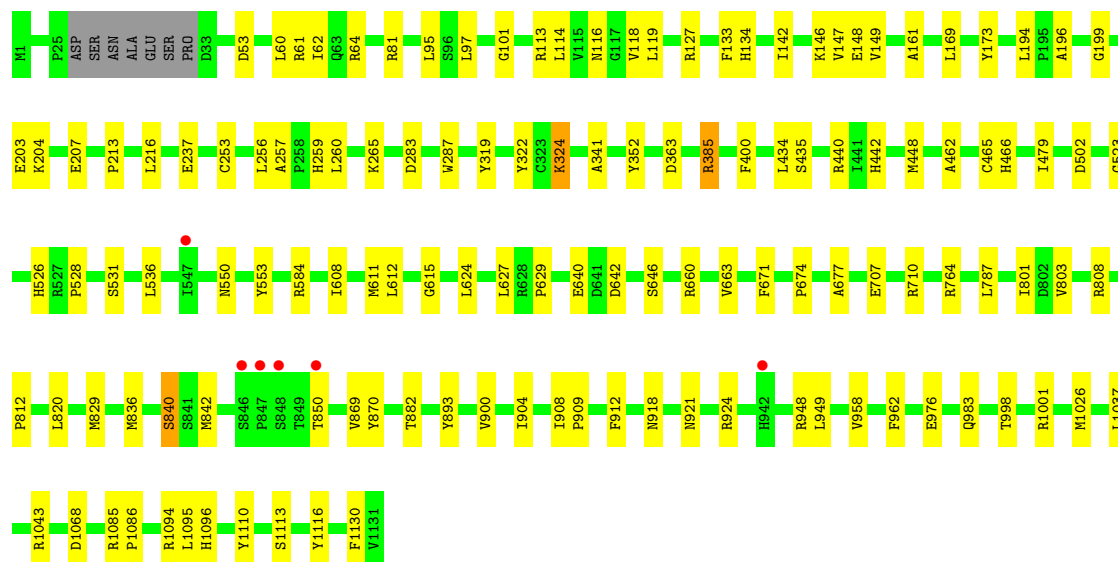
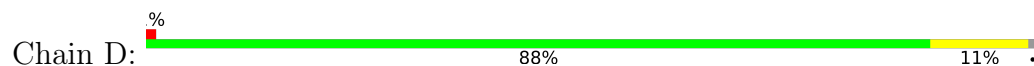




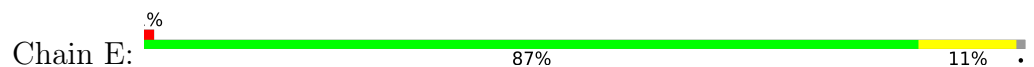
• Molecule 1: PPI-dependent PEPCK

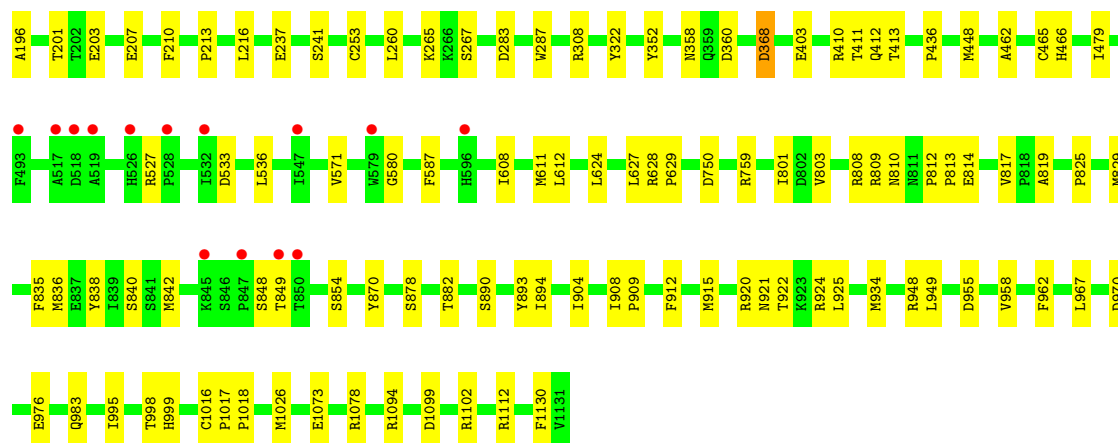


• Molecule 1: PPI-dependent PEPCK

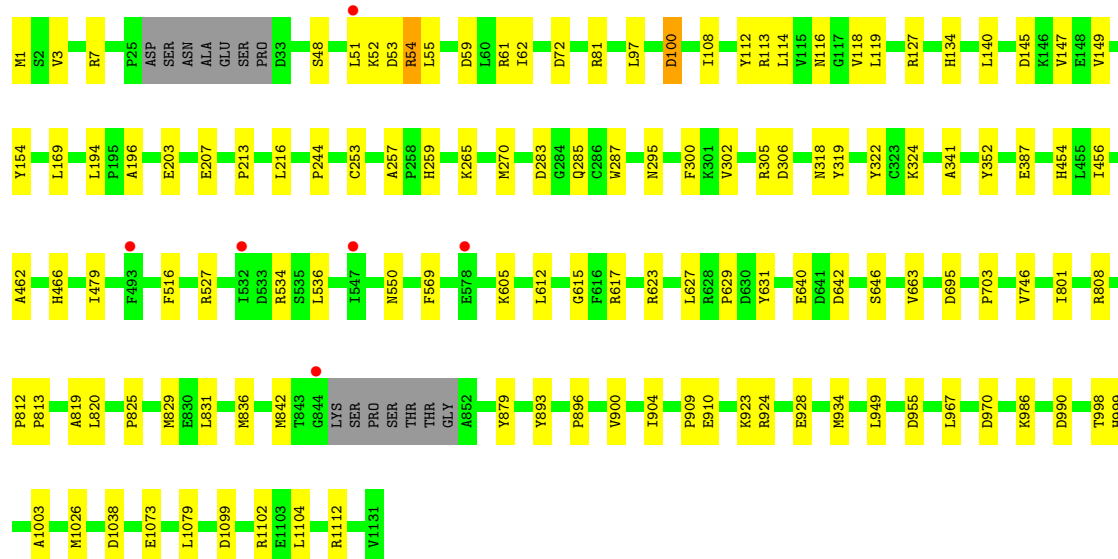
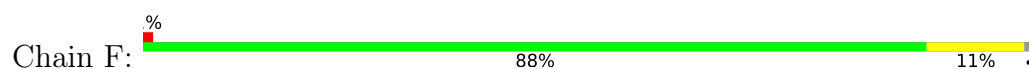


• Molecule 1: PPI-dependent PEPCK

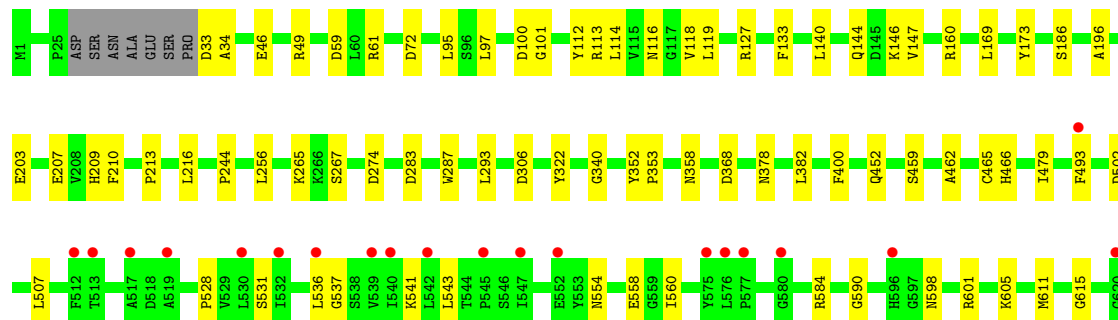
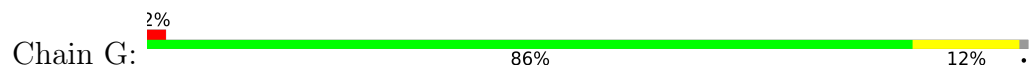


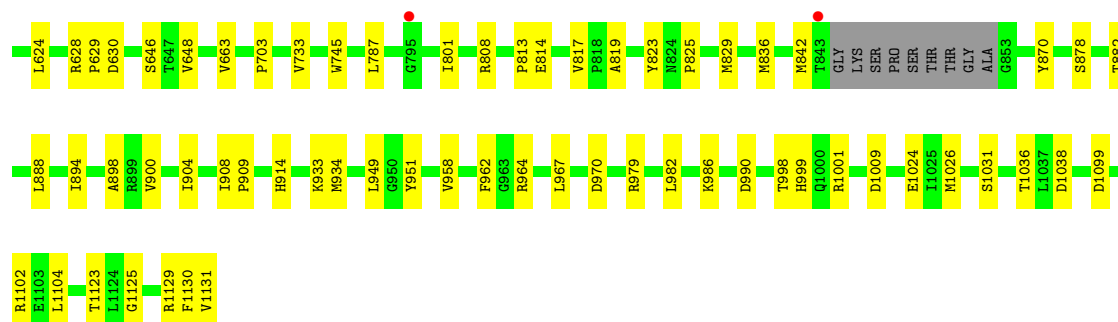


• Molecule 1: PPI-dependent PEPCK

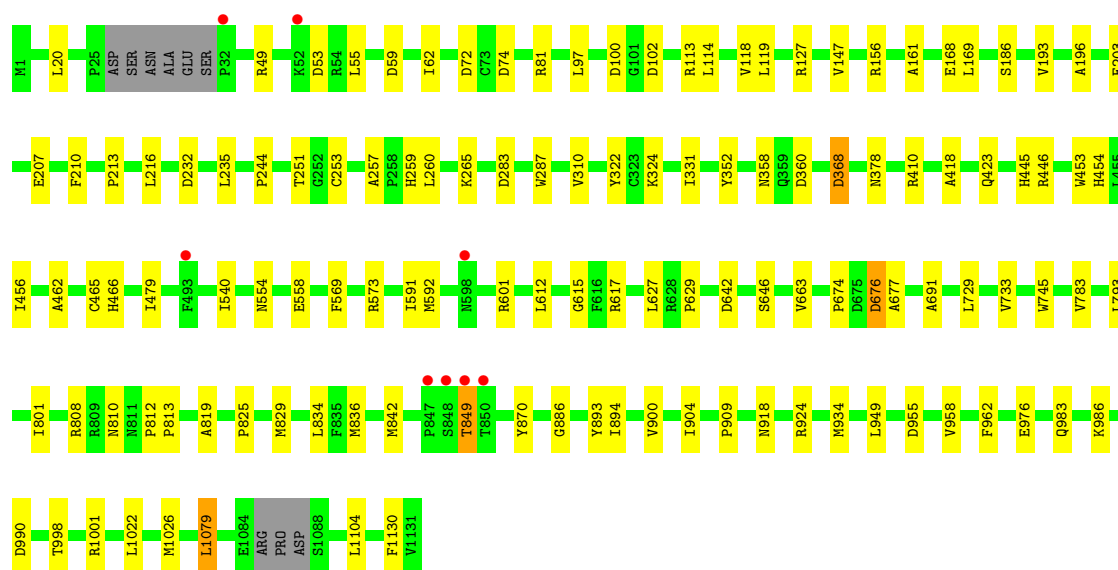
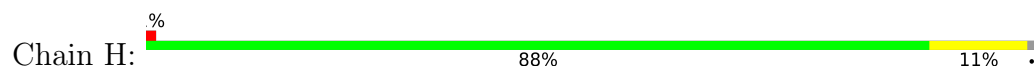


• Molecule 1: PPI-dependent PEPCK





● Molecule 1: PPI-dependent PEPCK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	134.13Å 146.95Å 151.09Å 82.70° 84.00° 70.80°	Depositor
Resolution (Å)	74.77 – 2.65 74.77 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.0 (74.77-2.65) 97.0 (74.77-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 8.0.006	Depositor
R, R_{free}	0.181 , 0.223 0.182 , 0.222	Depositor DCC
R_{free} test set	2000 reflections (0.64%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	72470	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.11	0/9149	0.27	0/12433
1	B	0.10	0/9143	0.26	0/12426
1	C	0.11	0/9143	0.27	0/12425
1	D	0.11	0/9135	0.27	0/12414
1	E	0.11	0/9101	0.27	1/12368 (0.0%)
1	F	0.11	0/9087	0.27	0/12347
1	G	0.11	0/9078	0.27	1/12335 (0.0%)
1	H	0.11	0/9115	0.27	0/12385
All	All	0.11	0/72951	0.27	2/99133 (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	E	358	ASN	CB-CA-C	-5.87	109.82	116.63
1	G	358	ASN	CB-CA-C	-5.50	110.25	116.63

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	8928	0	8656	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8921	0	8647	72	0
1	C	8922	0	8651	64	0
1	D	8914	0	8647	73	0
1	E	8881	0	8613	79	0
1	F	8868	0	8599	74	0
1	G	8859	0	8591	86	0
1	H	8895	0	8630	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	9	0	4	0	0
3	B	9	0	4	0	0
3	C	9	0	4	0	0
3	F	9	0	4	0	0
3	G	9	0	4	0	0
3	H	9	0	4	1	0
4	A	193	0	0	1	0
4	B	122	0	0	0	0
4	C	141	0	0	0	0
4	D	156	0	0	1	0
4	E	144	0	0	2	0
4	F	173	0	0	0	0
4	G	137	0	0	1	0
4	H	154	0	0	1	0
All	All	72470	0	69058	587	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 4.

All (587) 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:F:53:ASP:HA	1:F:81:ARG:HB3	1.67	0.76
1:H:53:ASP:HA	1:H:81:ARG:HB3	1.69	0.74
1:B:169:LEU:HD23	1:B:213:PRO:HB3	1.71	0.72
1:A:53:ASP:HA	1:A:81:ARG:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:ILE:HG13	1:D:909:PRO:HG3	1.72	0.71
1:G:466:HIS:HB2	1:G:801:ILE:HD12	1.73	0.70
1:G:836:MET:HE3	1:G:1026:MET:HG2	1.73	0.70
1:C:836:MET:HE3	1:C:1026:MET:HG2	1.74	0.70
1:H:147:VAL:HG13	1:H:283:ASP:HB3	1.74	0.70
1:E:147:VAL:HG13	1:E:283:ASP:HB3	1.74	0.69
1:C:265:LYS:HB2	1:C:287:TRP:HB3	1.73	0.69
1:A:237:GLU:OE2	1:A:1094:ARG:NH1	2.26	0.69
1:D:265:LYS:HB2	1:D:287:TRP:HB3	1.73	0.69
1:A:114:LEU:HD11	1:A:119:LEU:HB2	1.75	0.68
1:B:324:LYS:NZ	1:B:667:GLU:OE2	2.26	0.68
1:H:466:HIS:HB2	1:H:801:ILE:HD12	1.75	0.68
1:B:479:ILE:HG13	1:B:909:PRO:HG3	1.76	0.68
1:E:114:LEU:HD11	1:E:119:LEU:HB2	1.74	0.67
1:H:114:LEU:HD11	1:H:119:LEU:HB2	1.77	0.67
1:C:1094:ARG:HH21	1:H:49:ARG:HH12	1.42	0.67
1:A:836:MET:HE3	1:A:1026:MET:HG2	1.75	0.67
1:B:825:PRO:HB3	1:B:904:ILE:HD13	1.76	0.67
1:B:836:MET:HE3	1:B:1026:MET:HG2	1.77	0.67
1:G:479:ILE:HG13	1:G:909:PRO:HG3	1.75	0.67
1:A:367:ASP:OD2	1:D:1096:HIS:NE2	2.23	0.66
1:A:924:ARG:NH2	1:A:928:GLU:OE1	2.28	0.66
1:C:237:GLU:HG3	1:C:1095:LEU:HD21	1.78	0.66
1:B:536:LEU:HD21	1:B:629:PRO:HB2	1.77	0.65
1:A:479:ILE:HD12	1:A:909:PRO:HG3	1.77	0.65
1:F:114:LEU:HD11	1:F:119:LEU:HB2	1.78	0.65
1:G:536:LEU:HD21	1:G:629:PRO:HB2	1.78	0.65
1:D:836:MET:HE3	1:D:1026:MET:HG2	1.79	0.64
1:B:147:VAL:HG13	1:B:283:ASP:HB3	1.78	0.64
1:B:265:LYS:HB2	1:B:287:TRP:HB3	1.80	0.64
1:D:237:GLU:HG3	1:D:1095:LEU:HD21	1.80	0.64
1:G:169:LEU:HD23	1:G:213:PRO:HB3	1.80	0.64
1:C:466:HIS:HB2	1:C:801:ILE:HD12	1.80	0.63
1:H:324:LYS:NZ	1:H:642:ASP:OD2	2.31	0.63
1:C:101:GLY:O	1:C:113:ARG:NH1	2.30	0.63
1:E:127:ARG:HG3	1:E:322:TYR:CE1	2.33	0.63
1:F:479:ILE:HG13	1:F:909:PRO:HG3	1.80	0.63
1:B:196:ALA:HB2	1:B:203:GLU:HB2	1.80	0.63
1:F:536:LEU:HD21	1:F:629:PRO:HB2	1.79	0.63
1:F:924:ARG:NH1	1:F:928:GLU:OE1	2.32	0.62
1:D:836:MET:O	1:D:840:SER:OG	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1099:ASP:OD1	1:B:1102:ARG:NH2	2.32	0.62
1:C:147:VAL:HG13	1:C:283:ASP:HB3	1.82	0.62
1:F:1099:ASP:OD1	1:F:1102:ARG:NH2	2.32	0.62
1:H:265:LYS:HB2	1:H:287:TRP:HB3	1.81	0.62
1:D:842:MET:HG2	1:D:998:THR:HG21	1.82	0.62
1:H:842:MET:HG2	1:H:998:THR:HG21	1.81	0.62
1:A:169:LEU:HD23	1:A:213:PRO:HB3	1.83	0.61
1:B:237:GLU:HG3	1:B:1095:LEU:HD21	1.82	0.61
1:D:114:LEU:HD11	1:D:119:LEU:HB2	1.81	0.61
1:H:617:ARG:NH2	4:H:1302:HOH:O	2.33	0.61
1:B:114:LEU:HD11	1:B:119:LEU:HB2	1.81	0.60
1:B:466:HIS:HB2	1:B:801:ILE:HD12	1.81	0.60
1:F:808:ARG:NH1	1:F:842:MET:O	2.34	0.60
1:A:502:ASP:OD1	1:A:584:ARG:NH2	2.34	0.60
1:D:611:MET:HE2	1:D:624:LEU:HB3	1.82	0.60
1:E:101:GLY:O	1:E:113:ARG:NH1	2.34	0.60
1:E:466:HIS:HB2	1:E:801:ILE:HD12	1.82	0.60
1:E:810:ASN:OD1	1:E:890:SER:OG	2.19	0.60
1:F:100:ASP:OD1	1:F:100:ASP:N	2.34	0.60
1:A:213:PRO:HD2	1:A:216:LEU:HD12	1.84	0.60
1:B:934:MET:HE2	1:B:949:LEU:HD12	1.82	0.60
1:E:479:ILE:HG13	1:E:909:PRO:HG3	1.84	0.60
1:E:368:ASP:OD1	1:E:368:ASP:N	2.35	0.60
1:E:842:MET:HG2	1:E:998:THR:HG21	1.83	0.60
1:G:114:LEU:HD11	1:G:119:LEU:HB2	1.84	0.59
1:E:265:LYS:HB2	1:E:287:TRP:HB3	1.84	0.59
1:G:147:VAL:HG13	1:G:283:ASP:HB3	1.85	0.59
1:D:169:LEU:HD23	1:D:213:PRO:HB3	1.84	0.59
1:F:836:MET:HE3	1:F:1026:MET:HG2	1.85	0.59
1:H:213:PRO:HD2	1:H:216:LEU:HD13	1.85	0.59
1:B:808:ARG:HG3	1:B:888:LEU:HD11	1.84	0.59
1:F:169:LEU:HD23	1:F:213:PRO:HB3	1.85	0.58
1:A:147:VAL:HG13	1:A:283:ASP:HB3	1.85	0.58
1:C:324:LYS:NZ	1:C:667:GLU:OE2	2.33	0.58
1:C:518:ASP:HB3	1:C:521:ARG:HG2	1.85	0.58
1:D:196:ALA:HB2	1:D:203:GLU:HB2	1.86	0.58
1:G:196:ALA:HB2	1:G:203:GLU:HB2	1.84	0.58
1:A:528:PRO:HG2	1:A:531:SER:HB2	1.84	0.58
1:F:466:HIS:HB2	1:F:801:ILE:HD12	1.86	0.58
1:G:537:GLY:O	1:G:541:LYS:HG2	2.04	0.58
1:C:114:LEU:HD11	1:C:119:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:MET:HG2	1:A:998:THR:HG21	1.85	0.57
1:G:265:LYS:HB2	1:G:287:TRP:HB3	1.85	0.57
1:D:523:GLY:O	1:D:526:HIS:NE2	2.37	0.57
1:A:799:GLN:NE2	4:A:1307:HOH:O	2.38	0.57
1:F:527:ARG:HB2	1:F:534:ARG:HH11	1.69	0.57
1:H:62:ILE:HD13	1:H:253:CYS:HB2	1.87	0.57
1:H:196:ALA:HB2	1:H:203:GLU:HB2	1.87	0.57
1:B:68:ASP:OD2	1:B:308:ARG:NH1	2.38	0.57
1:E:611:MET:HE2	1:E:624:LEU:HB3	1.87	0.57
1:F:324:LYS:NZ	1:F:642:ASP:OD2	2.29	0.57
1:H:479:ILE:HG13	1:H:909:PRO:HG3	1.85	0.57
1:C:479:ILE:HG13	1:C:909:PRO:HG3	1.86	0.56
1:H:368:ASP:OD1	1:H:368:ASP:N	2.38	0.56
1:C:168:GLU:OE1	1:C:259:HIS:ND1	2.34	0.56
1:D:465:CYS:HB3	1:D:479:ILE:HD11	1.86	0.56
1:G:528:PRO:HG2	1:G:531:SER:HB2	1.87	0.56
1:H:169:LEU:HD23	1:H:213:PRO:HB3	1.87	0.56
1:E:915:MET:O	1:E:920:ARG:NH1	2.38	0.56
1:A:59:ASP:OD1	1:A:209:HIS:ND1	2.35	0.56
1:G:340:GLY:N	1:G:1125:GLY:O	2.38	0.56
1:A:101:GLY:O	1:A:113:ARG:NH1	2.37	0.56
1:C:169:LEU:HD23	1:C:213:PRO:HB3	1.88	0.56
1:C:829:MET:HE2	1:C:949:LEU:HA	1.88	0.56
1:F:147:VAL:HG13	1:F:283:ASP:HB3	1.87	0.56
1:F:615:GLY:HA2	1:F:900:VAL:HA	1.88	0.56
1:G:213:PRO:HD2	1:G:216:LEU:HD13	1.88	0.56
1:G:934:MET:HE2	1:G:949:LEU:HD12	1.88	0.56
1:A:160:ARG:HH22	1:A:267:SER:HB2	1.70	0.55
1:A:1079:LEU:HD12	1:A:1104:LEU:HD12	1.87	0.55
1:H:554:ASN:O	1:H:558:GLU:HG2	2.06	0.55
1:D:161:ALA:HB2	1:D:260:LEU:HD11	1.88	0.55
1:A:126:ARG:HH22	1:A:761:LYS:HB2	1.70	0.55
1:A:168:GLU:OE1	1:A:259:HIS:ND1	2.40	0.55
1:C:842:MET:HG2	1:C:998:THR:HG21	1.88	0.55
1:E:97:LEU:HD11	1:E:118:VAL:HG23	1.88	0.55
1:A:796:HIS:NE2	1:A:798:PRO:HG3	2.22	0.55
1:A:831:LEU:HD11	1:A:879:TYR:HB3	1.89	0.55
1:D:707:GLU:HG2	1:D:710:ARG:NH2	2.22	0.55
1:G:1099:ASP:OD1	1:G:1102:ARG:NH2	2.38	0.55
1:D:528:PRO:HG2	1:D:531:SER:HB2	1.87	0.55
1:E:196:ALA:HB2	1:E:203:GLU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:454:HIS:HE1	1:H:456:ILE:HD11	1.72	0.55
1:B:617:ARG:HD2	1:H:591:ILE:HD13	1.89	0.55
1:H:615:GLY:HA2	1:H:900:VAL:HA	1.88	0.55
1:A:265:LYS:HB2	1:A:287:TRP:HB3	1.89	0.54
1:F:454:HIS:HE1	1:F:456:ILE:HD11	1.71	0.54
1:G:646:SER:HB3	1:G:663:VAL:HG12	1.89	0.54
1:A:244:PRO:HG2	1:A:1104:LEU:HD21	1.88	0.54
1:D:466:HIS:HB2	1:D:801:ILE:HD12	1.88	0.54
1:A:836:MET:HE2	1:A:999:HIS:CD2	2.43	0.54
1:B:127:ARG:HG3	1:B:322:TYR:CE1	2.42	0.54
1:F:986:LYS:NZ	1:F:990:ASP:OD2	2.39	0.54
1:D:829:MET:HE2	1:D:949:LEU:HA	1.90	0.54
1:F:842:MET:HG2	1:F:998:THR:HG21	1.90	0.54
1:H:168:GLU:OE1	1:H:259:HIS:ND1	2.36	0.54
1:E:448:MET:HB2	1:E:608:ILE:HD13	1.90	0.54
1:E:360:ASP:OD2	1:E:410:ARG:NH2	2.40	0.54
1:G:934:MET:HG3	1:G:949:LEU:HB2	1.90	0.54
1:B:368:ASP:OD1	1:B:368:ASP:N	2.41	0.54
1:D:646:SER:HB3	1:D:663:VAL:HG12	1.90	0.54
1:G:133:PHE:HB3	1:G:146:LYS:HD2	1.90	0.54
1:B:100:ASP:OD1	1:B:100:ASP:N	2.36	0.53
1:A:368:ASP:OD1	1:A:368:ASP:N	2.37	0.53
1:C:97:LEU:HD11	1:C:118:VAL:HG23	1.90	0.53
1:E:169:LEU:HD23	1:E:213:PRO:HB3	1.91	0.53
1:G:611:MET:HE2	1:G:624:LEU:HB3	1.90	0.53
1:G:502:ASP:OD1	1:G:584:ARG:NH2	2.42	0.53
1:G:536:LEU:HD23	1:G:630:ASP:HB3	1.90	0.53
1:A:615:GLY:HA2	1:A:900:VAL:HA	1.91	0.53
1:G:894:ILE:HD11	1:G:904:ILE:HD12	1.90	0.53
1:H:74:ASP:OD2	1:H:156:ARG:NH2	2.42	0.53
1:D:127:ARG:HB2	1:D:319:TYR:CE2	2.44	0.53
1:E:133:PHE:HB3	1:E:146:LYS:HD2	1.91	0.53
1:H:986:LYS:NZ	1:H:990:ASP:OD2	2.41	0.53
1:B:834:LEU:HD22	1:B:886:GLY:HA3	1.90	0.53
1:B:934:MET:HG3	1:B:949:LEU:HB2	1.90	0.53
1:D:502:ASP:OD1	1:D:584:ARG:NH1	2.41	0.53
1:E:536:LEU:HD21	1:E:629:PRO:HD2	1.89	0.53
1:G:400:PHE:HE1	1:G:787:LEU:HD11	1.73	0.53
1:G:998:THR:HG23	1:G:1001:ARG:HH12	1.74	0.53
1:C:1082:TYR:O	1:C:1088:SER:OG	2.19	0.53
1:D:213:PRO:HD2	1:D:216:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:THR:O	1:A:1001:ARG:NH1	2.42	0.52
1:E:612:LEU:HG	1:E:627:LEU:HD11	1.92	0.52
1:D:536:LEU:HD21	1:D:629:PRO:HD2	1.91	0.52
1:C:97:LEU:HD13	1:C:113:ARG:HB2	1.90	0.52
1:F:1079:LEU:HD12	1:F:1104:LEU:HD12	1.92	0.52
1:B:870:TYR:OH	1:B:1130:PHE:O	2.26	0.52
1:H:783:VAL:HG13	1:H:793:LEU:HD22	1.92	0.52
1:B:188:LEU:HD22	1:B:233:PRO:HB3	1.90	0.52
1:E:836:MET:HE3	1:E:1026:MET:HG2	1.92	0.52
1:B:97:LEU:HD11	1:B:118:VAL:HG23	1.92	0.52
1:A:204:LYS:NZ	1:A:245:ASP:O	2.37	0.52
1:B:812:PRO:HB3	1:B:896:PRO:HA	1.91	0.52
1:D:60:LEU:HB3	1:D:64:ARG:NH1	2.24	0.52
1:B:848:SER:OG	1:B:849:THR:N	2.43	0.51
1:A:237:GLU:HG2	1:A:1095:LEU:HD21	1.92	0.51
1:D:101:GLY:O	1:D:113:ARG:NH1	2.43	0.51
1:F:265:LYS:HB2	1:F:287:TRP:HB3	1.91	0.51
1:C:213:PRO:HD2	1:C:216:LEU:HD13	1.92	0.51
1:B:970:ASP:N	1:B:970:ASP:OD1	2.41	0.51
1:H:592:MET:HE1	1:H:601:ARG:HH21	1.74	0.51
1:F:646:SER:HB3	1:F:663:VAL:HG12	1.91	0.51
1:B:924:ARG:NH2	1:B:961:TYR:OH	2.37	0.51
1:D:1068:ASP:OD2	1:D:1116:TYR:OH	2.28	0.51
1:F:134:HIS:HB3	1:F:149:VAL:HG21	1.91	0.51
1:C:133:PHE:HB3	1:C:146:LYS:HD2	1.93	0.51
1:D:133:PHE:HB3	1:D:146:LYS:HD2	1.92	0.51
1:D:324:LYS:NZ	1:D:642:ASP:OD2	2.44	0.51
1:G:829:MET:HE2	1:G:949:LEU:HA	1.92	0.51
1:H:569:PHE:HB3	1:H:629:PRO:HG2	1.93	0.51
1:G:878:SER:O	1:G:882:THR:OG1	2.24	0.51
1:B:814:GLU:HB2	1:B:817:VAL:HB	1.93	0.50
1:D:948:ARG:NH2	4:D:1305:HOH:O	2.41	0.50
1:H:955:ASP:OD1	1:H:955:ASP:N	2.44	0.50
1:B:646:SER:HB3	1:B:663:VAL:HG12	1.93	0.50
1:C:970:ASP:OD1	1:C:970:ASP:N	2.42	0.50
1:D:1037:LEU:O	1:D:1043:ARG:NH1	2.36	0.50
1:F:934:MET:HE2	1:F:949:LEU:HD12	1.92	0.50
1:D:142:ILE:HD12	1:D:148:GLU:HG3	1.94	0.50
1:E:970:ASP:OD1	1:E:970:ASP:N	2.45	0.50
1:G:507:LEU:HD21	1:G:543:LEU:HD21	1.94	0.50
1:H:825:PRO:HB3	1:H:904:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:HIS:HE1	1:A:456:ILE:HD11	1.76	0.50
1:F:1073:GLU:OE2	1:F:1112:ARG:NH2	2.36	0.50
1:E:160:ARG:HH22	1:E:267:SER:HB2	1.76	0.50
1:F:270:MET:HE3	1:F:285:GLN:HA	1.94	0.50
1:E:934:MET:HG3	1:E:949:LEU:HB2	1.94	0.49
1:E:825:PRO:HB3	1:E:904:ILE:HD13	1.93	0.49
1:F:1038:ASP:OD1	1:F:1038:ASP:N	2.40	0.49
1:G:116:ASN:OD1	1:G:116:ASN:N	2.44	0.49
1:G:842:MET:HG2	1:G:998:THR:HG21	1.94	0.49
1:G:813:PRO:HB3	1:G:819:ALA:HB2	1.93	0.49
1:F:213:PRO:HD2	1:F:216:LEU:HD13	1.93	0.49
1:G:160:ARG:HH22	1:G:267:SER:HB2	1.77	0.49
1:A:142:ILE:HD12	1:A:148:GLU:HG3	1.95	0.49
1:E:1099:ASP:OD1	1:E:1102:ARG:NH2	2.46	0.49
1:E:352:TYR:CE2	1:E:462:ALA:HB2	2.48	0.49
1:E:412:GLN:OE1	4:E:1301:HOH:O	2.20	0.49
1:H:360:ASP:OD2	1:H:410:ARG:NH1	2.45	0.49
1:A:352:TYR:CE2	1:A:462:ALA:HB2	2.48	0.49
1:B:842:MET:HG2	1:B:998:THR:HG21	1.93	0.49
1:E:922:THR:HA	1:E:925:LEU:HB2	1.94	0.49
1:F:97:LEU:HD13	1:F:113:ARG:HB2	1.95	0.49
1:F:194:LEU:HD13	1:F:341:ALA:HB2	1.93	0.49
1:H:193:VAL:HG22	1:H:331:ILE:HG23	1.94	0.49
1:H:646:SER:HB3	1:H:663:VAL:HG12	1.95	0.49
1:H:934:MET:HG3	1:H:949:LEU:HB2	1.93	0.49
1:D:803:VAL:HG11	1:D:912:PHE:CD2	2.48	0.49
1:C:934:MET:HE2	1:C:949:LEU:HD12	1.95	0.48
1:D:921:ASN:HB3	1:D:924:ARG:HG2	1.94	0.48
1:G:615:GLY:HA2	1:G:900:VAL:HA	1.95	0.48
1:H:612:LEU:HD12	1:H:627:LEU:HD21	1.96	0.48
1:B:673:ARG:HD3	1:B:762:ASN:OD1	2.13	0.48
1:H:352:TYR:CE2	1:H:462:ALA:HB2	2.48	0.48
1:B:1068:ASP:OD2	1:B:1116:TYR:OH	2.31	0.48
1:F:127:ARG:HG3	1:F:322:TYR:CE1	2.48	0.48
1:F:516:PHE:O	1:F:550:ASN:ND2	2.46	0.48
1:F:831:LEU:HD11	1:F:879:TYR:HB3	1.95	0.48
1:A:850:THR:OG1	1:A:1001:ARG:HD3	2.13	0.48
1:G:825:PRO:HB3	1:G:904:ILE:HD13	1.96	0.48
1:D:352:TYR:CE2	1:D:462:ALA:HB2	2.48	0.48
1:E:97:LEU:HD13	1:E:113:ARG:HB2	1.96	0.48
1:F:836:MET:HE2	1:F:999:HIS:ND1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1036:THR:OG1	1:G:1038:ASP:OD1	2.27	0.48
1:A:628:ARG:HH11	1:A:964:ARG:HA	1.78	0.48
1:E:403:GLU:HB3	1:E:436:PRO:HG2	1.96	0.48
1:F:295:ASN:ND2	1:F:300:PHE:HB3	2.29	0.48
1:F:352:TYR:CE2	1:F:462:ALA:HB2	2.49	0.48
1:G:986:LYS:NZ	1:G:990:ASP:OD2	2.47	0.48
1:F:48:SER:O	1:F:52:LYS:N	2.47	0.48
1:C:55:LEU:HB3	1:C:59:ASP:HB2	1.95	0.48
1:C:86:LEU:HD13	1:C:92:ALA:HB2	1.96	0.48
1:F:1:MET:N	1:F:695:ASP:OD1	2.38	0.48
1:C:825:PRO:HB3	1:C:904:ILE:HD13	1.95	0.47
1:H:934:MET:HE2	1:H:949:LEU:HD12	1.95	0.47
1:B:813:PRO:HB3	1:B:819:ALA:HB2	1.96	0.47
1:D:97:LEU:HD11	1:D:118:VAL:HG23	1.96	0.47
1:F:97:LEU:HD11	1:F:118:VAL:HG23	1.95	0.47
1:H:358:ASN:OD1	1:H:573:ARG:NH1	2.47	0.47
1:F:116:ASN:OD1	1:F:116:ASN:N	2.47	0.47
1:F:454:HIS:CE1	1:F:456:ILE:HD11	2.50	0.47
1:F:617:ARG:NH1	1:F:623:ARG:HE	2.11	0.47
1:G:101:GLY:O	1:G:113:ARG:NH1	2.46	0.47
1:C:311:ILE:HD13	1:C:330:GLN:HG2	1.97	0.47
1:D:400:PHE:HE1	1:D:787:LEU:HD11	1.80	0.47
1:G:33:ASP:OD1	1:G:34:ALA:N	2.47	0.47
1:H:808:ARG:HE	1:H:810:ASN:HD21	1.63	0.47
1:E:808:ARG:HE	1:E:810:ASN:HD21	1.62	0.47
1:H:127:ARG:HG3	1:H:322:TYR:CE1	2.49	0.47
1:H:1079:LEU:HD22	1:H:1104:LEU:HD12	1.97	0.47
1:E:213:PRO:HG2	1:E:216:LEU:HD13	1.97	0.47
1:G:100:ASP:OD1	1:G:101:GLY:N	2.46	0.47
1:G:216:LEU:HD22	1:G:256:LEU:HB3	1.97	0.47
1:G:265:LYS:HE3	1:G:293:LEU:O	2.15	0.47
1:H:454:HIS:CE1	1:H:456:ILE:HD11	2.50	0.47
1:B:611:MET:HE2	1:B:624:LEU:HB3	1.97	0.47
1:E:527:ARG:NH1	1:E:533:ASP:O	2.45	0.47
1:G:368:ASP:OD1	1:G:368:ASP:N	2.46	0.47
1:A:62:ILE:HD13	1:A:253:CYS:HB2	1.96	0.47
1:A:356:ASN:HB3	1:A:630:ASP:HA	1.96	0.47
1:A:955:ASP:OD1	1:A:955:ASP:N	2.47	0.47
1:F:55:LEU:HB3	1:F:59:ASP:HB2	1.97	0.47
1:F:808:ARG:HH22	1:F:820:LEU:HD13	1.80	0.47
1:G:808:ARG:HG2	1:G:888:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:PRO:HB3	1:A:904:ILE:HD13	1.97	0.47
1:E:814:GLU:HB2	1:E:817:VAL:HB	1.96	0.47
1:H:418:ALA:HB3	1:H:423:GLN:HG3	1.97	0.47
1:E:836:MET:HE2	1:E:999:HIS:CD2	2.50	0.46
1:B:825:PRO:HD3	1:B:894:ILE:HD13	1.96	0.46
1:C:232:ASP:HB3	1:C:235:LEU:HG	1.96	0.46
1:D:660:ARG:NH2	1:D:882:THR:O	2.48	0.46
1:D:976:GLU:HB3	1:D:983:GLN:HG2	1.98	0.46
1:E:161:ALA:HB2	1:E:260:LEU:HD11	1.97	0.46
1:E:976:GLU:HB3	1:E:983:GLN:HG2	1.97	0.46
1:F:812:PRO:HD3	1:F:893:TYR:CG	2.49	0.46
1:B:376:SER:HA	1:B:379:ARG:HG3	1.97	0.46
1:E:628:ARG:HA	1:E:967:LEU:HD13	1.97	0.46
1:F:140:LEU:HG	1:F:306:ASP:HA	1.96	0.46
1:G:95:LEU:HA	1:G:173:TYR:HB2	1.96	0.46
1:H:918:ASN:O	1:H:924:ARG:HD3	2.16	0.46
1:B:986:LYS:NZ	1:B:990:ASP:OD2	2.47	0.46
1:H:870:TYR:OH	1:H:1130:PHE:O	2.32	0.46
1:C:933:LYS:HB2	1:C:951:TYR:CE2	2.51	0.46
1:E:186:SER:HA	1:E:210:PHE:O	2.16	0.46
1:G:46:GLU:OE1	1:G:49:ARG:NH2	2.48	0.46
1:G:814:GLU:HB2	1:G:817:VAL:HB	1.97	0.46
1:B:145:ASP:HB3	1:B:1005:MET:HE1	1.97	0.46
1:C:127:ARG:HG3	1:C:319:TYR:HE2	1.81	0.46
1:C:812:PRO:HB3	1:C:896:PRO:HA	1.97	0.46
1:D:612:LEU:HD12	1:D:627:LEU:HD21	1.98	0.46
1:F:108:ILE:HG22	1:F:318:ASN:CG	2.40	0.46
1:F:127:ARG:HB2	1:F:319:TYR:CE2	2.51	0.46
1:G:452:GLN:HE21	1:G:605:LYS:HD3	1.81	0.46
1:A:295:ASN:ND2	1:A:300:PHE:HB3	2.30	0.46
1:B:133:PHE:HB3	1:B:146:LYS:HD2	1.98	0.46
1:B:448:MET:HB2	1:B:608:ILE:HD13	1.97	0.46
1:F:61:ARG:NE	1:F:207:GLU:OE2	2.44	0.46
1:G:59:ASP:OD1	1:G:209:HIS:ND1	2.48	0.46
1:C:400:PHE:HE1	1:C:787:LEU:HD11	1.81	0.46
1:C:487:PHE:CZ	1:C:633:PRO:HG3	2.51	0.46
1:C:116:ASN:OD1	1:C:116:ASN:N	2.45	0.45
1:C:127:ARG:HG3	1:C:319:TYR:CE2	2.51	0.45
1:F:569:PHE:CD2	1:F:967:LEU:HD11	2.51	0.45
1:A:970:ASP:OD1	1:A:970:ASP:N	2.48	0.45
1:D:440:ARG:HH21	1:D:442:HIS:CE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:MET:HB2	1:D:608:ILE:HD13	1.98	0.45
1:E:809:ARG:NH2	4:E:1313:HOH:O	2.44	0.45
1:F:51:LEU:O	1:F:54:ARG:HB2	2.15	0.45
1:G:541:LYS:NZ	1:G:628:ARG:HH12	2.13	0.45
1:A:116:ASN:OD1	1:A:116:ASN:N	2.46	0.45
1:F:527:ARG:HB2	1:F:534:ARG:NH1	2.30	0.45
1:H:836:MET:HE3	1:H:1026:MET:HG2	1.98	0.45
1:A:575:TYR:OH	1:A:580:GLY:O	2.22	0.45
1:B:352:TYR:CE2	1:B:462:ALA:HB2	2.52	0.45
1:C:976:GLU:HB3	1:C:983:GLN:HG2	1.99	0.45
1:E:870:TYR:OH	1:E:1130:PHE:O	2.33	0.45
1:F:825:PRO:HB3	1:F:904:ILE:HD13	1.98	0.45
1:G:72:ASP:OD1	1:G:72:ASP:N	2.49	0.45
1:B:836:MET:HE2	1:B:999:HIS:ND1	2.31	0.45
1:D:918:ASN:O	1:D:924:ARG:HD3	2.17	0.45
1:G:958:VAL:HA	1:G:962:PHE:HD2	1.82	0.45
1:A:196:ALA:HB2	1:A:203:GLU:HB2	1.99	0.45
1:B:512:PHE:O	1:B:515:ARG:HG2	2.17	0.45
1:C:112:TYR:CZ	1:C:703:PRO:HG3	2.52	0.45
1:C:803:VAL:HG11	1:C:912:PHE:CD2	2.52	0.45
1:E:955:ASP:N	1:E:955:ASP:OD1	2.49	0.45
1:E:958:VAL:O	1:E:962:PHE:HB2	2.15	0.45
1:G:836:MET:HE2	1:G:999:HIS:ND1	2.31	0.45
1:A:97:LEU:HD11	1:A:118:VAL:HG23	1.98	0.45
1:A:627:LEU:HD13	1:A:631:TYR:CD2	2.52	0.45
1:D:127:ARG:HG3	1:D:322:TYR:CE1	2.51	0.45
1:G:808:ARG:NH1	1:G:842:MET:O	2.47	0.45
1:H:465:CYS:HB3	1:H:479:ILE:HD11	1.98	0.45
1:H:674:PRO:HB2	1:H:677:ALA:HB2	1.99	0.45
1:B:1079:LEU:HD12	1:B:1104:LEU:HD12	1.99	0.45
1:E:894:ILE:HD11	1:E:904:ILE:HD12	1.98	0.45
1:H:102:ASP:HB3	1:H:113:ARG:HB3	1.99	0.45
1:H:257:ALA:HB1	1:H:259:HIS:CE1	2.52	0.45
1:A:646:SER:HB3	1:A:663:VAL:HG12	1.99	0.45
1:B:478:GLU:OE1	1:B:478:GLU:N	2.50	0.45
1:C:904:ILE:O	1:C:908:ILE:HG12	2.17	0.45
1:D:671:PHE:CE1	1:D:764:ARG:HB3	2.52	0.45
1:B:612:LEU:HG	1:B:627:LEU:HD11	2.00	0.44
1:C:237:GLU:OE2	1:C:1094:ARG:NH1	2.50	0.44
1:F:145:ASP:OD1	1:F:145:ASP:N	2.49	0.44
1:B:62:ILE:HD13	1:B:253:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:813:PRO:HB3	1:E:819:ALA:HB2	1.99	0.44
1:F:244:PRO:HG2	1:F:1104:LEU:HD11	1.98	0.44
1:G:933:LYS:HB2	1:G:951:TYR:CE2	2.51	0.44
1:A:216:LEU:HD13	1:A:256:LEU:HB2	2.00	0.44
1:D:958:VAL:O	1:D:962:PHE:HB2	2.17	0.44
1:B:265:LYS:HE3	1:B:293:LEU:O	2.17	0.44
1:D:870:TYR:OH	1:D:1130:PHE:O	2.30	0.44
1:E:878:SER:O	1:E:882:THR:OG1	2.32	0.44
1:F:134:HIS:HB3	1:F:149:VAL:CG2	2.48	0.44
1:G:507:LEU:HD11	1:G:560:ILE:HD13	1.98	0.44
1:C:142:ILE:HD12	1:C:148:GLU:HG3	2.00	0.44
1:F:154:TYR:HD1	1:F:302:VAL:HG22	1.81	0.44
1:G:186:SER:HA	1:G:210:PHE:O	2.18	0.44
1:F:257:ALA:HB1	1:F:259:HIS:CE1	2.53	0.44
1:H:186:SER:HA	1:H:210:PHE:O	2.18	0.44
1:H:244:PRO:HG2	1:H:1104:LEU:HD21	1.98	0.44
1:A:454:HIS:CE1	1:A:456:ILE:HD11	2.53	0.44
1:C:1:MET:HE3	1:C:6:ARG:HG3	2.00	0.44
1:D:194:LEU:HB3	1:D:204:LYS:HB2	2.00	0.44
1:D:237:GLU:CD	1:D:1094:ARG:HH12	2.26	0.44
1:E:1073:GLU:OE2	1:E:1112:ARG:NH2	2.46	0.44
1:F:829:MET:HE2	1:F:949:LEU:HA	1.99	0.44
1:G:870:TYR:OH	1:G:1130:PHE:O	2.34	0.44
1:H:834:LEU:HD22	1:H:886:GLY:HA3	1.98	0.44
1:D:1110:TYR:O	1:D:1113:SER:OG	2.29	0.44
1:F:62:ILE:HD13	1:F:253:CYS:HB2	2.00	0.44
1:G:144:GLN:HB2	1:G:1009:ASP:HB3	2.00	0.44
1:G:914:HIS:O	1:G:964:ARG:NH1	2.44	0.44
1:B:808:ARG:HE	1:B:810:ASN:HD21	1.65	0.44
1:C:196:ALA:HB2	1:C:203:GLU:HB2	1.99	0.44
1:C:357:LEU:HD13	1:C:361:PHE:CD1	2.53	0.44
1:D:53:ASP:HA	1:D:81:ARG:HB3	2.00	0.44
1:D:674:PRO:HB2	1:D:677:ALA:HB2	2.00	0.44
1:E:934:MET:HE2	1:E:949:LEU:HD12	2.00	0.44
1:H:958:VAL:O	1:H:962:PHE:HB2	2.18	0.44
1:C:352:TYR:CE2	1:C:462:ALA:HB2	2.53	0.43
1:E:116:ASN:OD1	1:E:116:ASN:N	2.50	0.43
1:E:958:VAL:HA	1:E:962:PHE:HD2	1.83	0.43
1:G:97:LEU:HD11	1:G:118:VAL:HG23	2.00	0.43
1:H:207:GLU:HG3	1:H:251:THR:HG23	1.99	0.43
1:H:976:GLU:HB3	1:H:983:GLN:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:813:PRO:HB3	1:H:819:ALA:HB2	1.99	0.43
1:H:894:ILE:HD11	1:H:904:ILE:HD12	2.00	0.43
1:A:522:ASN:O	1:D:199:GLY:HA2	2.18	0.43
1:B:812:PRO:HD3	1:B:893:TYR:CG	2.53	0.43
1:G:127:ARG:HG3	1:G:322:TYR:CE1	2.54	0.43
1:C:348:GLY:N	1:C:640:GLU:HG3	2.34	0.43
1:E:61:ARG:NE	1:E:207:GLU:OE2	2.46	0.43
1:C:277:THR:O	1:C:281:ARG:HG3	2.19	0.43
1:E:62:ILE:HD13	1:E:253:CYS:HB2	2.00	0.43
1:G:554:ASN:O	1:G:558:GLU:HG2	2.18	0.43
1:G:733:VAL:HG11	1:G:745:TRP:CD1	2.53	0.43
1:B:101:GLY:O	1:B:113:ARG:NH1	2.52	0.43
1:G:465:CYS:HB3	1:G:479:ILE:HD11	1.99	0.43
1:H:446:ARG:NE	3:H:1202:MLT:O5	2.49	0.43
1:B:733:VAL:HG11	1:B:745:TRP:CD1	2.53	0.43
1:C:915:MET:O	1:C:920:ARG:NH1	2.52	0.43
1:D:97:LEU:HD13	1:D:113:ARG:HB2	2.00	0.43
1:D:812:PRO:HD3	1:D:893:TYR:CD1	2.53	0.43
1:F:112:TYR:CZ	1:F:703:PRO:HG3	2.54	0.43
1:A:918:ASN:O	1:A:924:ARG:HD3	2.19	0.43
1:C:615:GLY:HA2	1:C:900:VAL:HA	2.00	0.43
1:E:100:ASP:OD1	1:E:100:ASP:N	2.48	0.43
1:H:676:ASP:N	1:H:676:ASP:OD1	2.52	0.43
1:B:442:HIS:CE1	1:B:456:ILE:HB	2.54	0.43
1:B:465:CYS:HB3	1:B:479:ILE:HD11	2.00	0.43
1:C:319:TYR:OH	1:C:762:ASN:ND2	2.42	0.43
1:H:161:ALA:HB2	1:H:260:LEU:HD11	2.01	0.43
1:A:140:LEU:HG	1:A:306:ASP:HA	2.01	0.43
1:A:776:GLU:O	1:A:780:VAL:HG23	2.19	0.43
1:D:257:ALA:HB1	1:D:259:HIS:CE1	2.53	0.43
1:D:850:THR:OG1	1:D:1001:ARG:HD3	2.19	0.43
1:G:244:PRO:HG2	1:G:1104:LEU:HD21	2.00	0.43
1:A:612:LEU:HD12	1:A:627:LEU:HD21	2.01	0.42
1:A:958:VAL:O	1:A:962:PHE:HB2	2.18	0.42
1:D:707:GLU:HG2	1:D:710:ARG:HH22	1.83	0.42
1:D:1085:ARG:HG3	1:D:1086:PRO:HD2	2.01	0.42
1:E:68:ASP:CG	1:E:308:ARG:HH12	2.25	0.42
1:E:241:SER:HB2	1:E:1078:ARG:HH11	1.84	0.42
1:F:812:PRO:HB3	1:F:896:PRO:HA	2.01	0.42
1:E:812:PRO:HD3	1:E:893:TYR:CD1	2.54	0.42
1:E:921:ASN:HB3	1:E:924:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:ALA:HB2	1:F:203:GLU:HB2	2.00	0.42
1:F:631:TYR:OH	1:F:910:GLU:OE1	2.36	0.42
1:D:134:HIS:HB3	1:D:149:VAL:CG2	2.50	0.42
1:E:35:ILE:HD12	1:E:35:ILE:H	1.84	0.42
1:G:979:ARG:CZ	1:G:982:LEU:HD11	2.50	0.42
1:A:344:GLU:OE2	1:A:661:LYS:NZ	2.41	0.42
1:E:571:VAL:HG12	1:E:587:PHE:CE2	2.55	0.42
1:E:750:ASP:HA	1:E:759:ARG:NH1	2.35	0.42
1:F:970:ASP:OD1	1:F:970:ASP:N	2.45	0.42
1:H:72:ASP:OD1	1:H:72:ASP:N	2.50	0.42
1:A:934:MET:HG3	1:A:949:LEU:HB2	2.01	0.42
1:D:363:ASP:OD2	1:D:435:SER:OG	2.22	0.42
1:D:385:ARG:HD2	1:D:385:ARG:HA	1.79	0.42
1:G:590:GLY:H	1:G:601:ARG:NH1	2.17	0.42
1:A:139:GLY:O	1:F:72:ASP:HB3	2.20	0.42
1:A:194:LEU:HD21	1:A:201:THR:HB	2.01	0.42
1:A:536:LEU:HD21	1:A:629:PRO:HB2	2.00	0.42
1:F:305:ARG:HD3	1:F:305:ARG:N	2.34	0.42
1:G:112:TYR:CZ	1:G:703:PRO:HG3	2.55	0.42
1:G:842:MET:HE3	1:G:842:MET:HB2	1.99	0.42
1:B:958:VAL:O	1:B:962:PHE:HB2	2.20	0.42
1:D:147:VAL:HG13	1:D:283:ASP:HB3	2.02	0.42
1:E:237:GLU:CD	1:E:1094:ARG:HH12	2.28	0.42
1:E:465:CYS:HB3	1:E:479:ILE:HD11	2.00	0.42
1:E:848:SER:OG	1:E:849:THR:N	2.53	0.42
1:H:232:ASP:HB3	1:H:235:LEU:HG	2.00	0.42
1:H:445:HIS:HB3	1:H:453:TRP:CE2	2.55	0.42
1:H:733:VAL:HG11	1:H:745:TRP:CD1	2.55	0.42
1:B:783:VAL:HG13	1:B:793:LEU:HD22	2.01	0.42
1:C:255:ILE:HB	1:C:314:VAL:HG22	2.00	0.42
1:C:678:ILE:HD11	1:C:759:ARG:HH21	1.85	0.42
1:C:808:ARG:HH22	1:C:820:LEU:HD13	1.85	0.42
1:D:95:LEU:HA	1:D:173:TYR:HB2	2.02	0.42
1:D:550:ASN:HB2	1:D:553:TYR:H	1.85	0.42
1:E:803:VAL:HG11	1:E:912:PHE:CD2	2.55	0.42
1:E:835:PHE:HA	1:E:838:TYR:HB2	2.02	0.42
1:F:813:PRO:HB3	1:F:819:ALA:HB2	2.01	0.42
1:B:573:ARG:HD3	1:B:574:TYR:CE2	2.55	0.42
1:B:924:ARG:NH1	1:B:928:GLU:OE1	2.53	0.42
1:C:186:SER:HB2	1:C:209:HIS:CE1	2.55	0.42
1:D:116:ASN:OD1	1:D:116:ASN:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LEU:HD22	1:D:256:LEU:HB3	2.02	0.42
1:G:72:ASP:OD2	4:G:1301:HOH:O	2.22	0.42
1:B:678:ILE:HD11	1:B:759:ARG:HH21	1.85	0.41
1:D:904:ILE:O	1:D:908:ILE:HG12	2.19	0.41
1:F:3:VAL:O	1:F:7:ARG:HG3	2.20	0.41
1:C:850:THR:OG1	1:C:851:GLY:N	2.45	0.41
1:E:72:ASP:OD1	1:E:72:ASP:N	2.52	0.41
1:F:612:LEU:HG	1:F:627:LEU:HD11	2.02	0.41
1:H:97:LEU:HD11	1:H:118:VAL:HG23	2.02	0.41
1:A:70:LEU:HD22	1:A:155:ALA:HB2	2.02	0.41
1:A:826:LEU:HB3	1:A:953:ILE:HD13	2.02	0.41
1:B:86:LEU:HD13	1:B:92:ALA:HB2	2.02	0.41
1:D:61:ARG:NE	1:D:207:GLU:OE2	2.42	0.41
1:A:86:LEU:HD13	1:A:92:ALA:HB2	2.03	0.41
1:C:244:PRO:HG2	1:C:1104:LEU:HD11	2.01	0.41
1:C:575:TYR:HA	1:C:579:TRP:CZ3	2.55	0.41
1:D:62:ILE:HD13	1:D:253:CYS:HB2	2.03	0.41
1:D:434:LEU:HD12	1:D:440:ARG:HG3	2.01	0.41
1:D:808:ARG:HH21	1:D:820:LEU:HD22	1.85	0.41
1:E:829:MET:HE2	1:E:949:LEU:HA	2.02	0.41
1:H:808:ARG:HE	1:H:810:ASN:ND2	2.17	0.41
1:C:62:ILE:HD13	1:C:253:CYS:HB2	2.03	0.41
1:C:497:ILE:HD12	1:C:600:VAL:HG22	2.02	0.41
1:E:842:MET:HE3	1:E:842:MET:HB2	1.98	0.41
1:F:605:LYS:HD2	1:F:605:LYS:N	2.36	0.41
1:F:955:ASP:OD1	1:F:955:ASP:N	2.54	0.41
1:A:829:MET:HE2	1:A:949:LEU:HA	2.02	0.41
1:A:894:ILE:HD11	1:A:904:ILE:HD12	2.03	0.41
1:B:55:LEU:HB3	1:B:59:ASP:HB2	2.03	0.41
1:C:1094:ARG:NH2	1:H:49:ARG:HH12	2.13	0.41
1:E:836:MET:HE1	1:E:948:ARG:HD3	2.02	0.41
1:E:904:ILE:O	1:E:908:ILE:HG12	2.20	0.41
1:G:352:TYR:CE2	1:G:462:ALA:HB2	2.55	0.41
1:G:493:PHE:CE1	1:G:598:ASN:HB3	2.55	0.41
1:G:648:VAL:O	1:G:1123:THR:HA	2.20	0.41
1:G:958:VAL:O	1:G:962:PHE:HB2	2.20	0.41
1:G:1024:GLU:HB3	1:G:1031:SER:HA	2.02	0.41
1:H:540:ILE:HA	1:H:569:PHE:CZ	2.55	0.41
1:H:1022:LEU:O	1:H:1026:MET:HG3	2.21	0.41
1:A:186:SER:HA	1:A:210:PHE:O	2.20	0.41
1:A:894:ILE:HD11	1:A:904:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ILE:O	1:C:318:ASN:ND2	2.47	0.41
1:C:461:ARG:HH21	1:C:917:PRO:HG3	1.86	0.41
1:C:869:VAL:HG21	1:C:1014:LEU:HB2	2.03	0.41
1:D:194:LEU:HD13	1:D:341:ALA:HB2	2.03	0.41
1:G:823:TYR:CE2	1:G:949:LEU:HD22	2.55	0.41
1:G:894:ILE:O	1:G:898:ALA:HB3	2.21	0.41
1:H:812:PRO:HD3	1:H:893:TYR:CD1	2.56	0.41
1:A:835:PHE:CZ	1:A:876:VAL:HA	2.55	0.41
1:B:127:ARG:HB2	1:B:319:TYR:CE2	2.55	0.41
1:B:543:LEU:HD12	1:B:569:PHE:CE1	2.55	0.41
1:C:630:ASP:OD1	1:C:630:ASP:N	2.53	0.41
1:E:840:SER:O	1:E:854:SER:OG	2.36	0.41
1:G:140:LEU:HG	1:G:306:ASP:HA	2.03	0.41
1:H:829:MET:HE2	1:H:949:LEU:HA	2.01	0.41
1:A:328:LYS:NZ	1:A:343:GLU:OE2	2.48	0.41
1:A:674:PRO:HB2	1:A:677:ALA:HB2	2.03	0.41
1:A:808:ARG:NH2	1:A:820:LEU:HD13	2.36	0.41
1:B:59:ASP:OD1	1:B:209:HIS:ND1	2.40	0.41
1:B:842:MET:HE1	1:B:995:ILE:HG23	2.02	0.41
1:C:836:MET:HE2	1:C:999:HIS:ND1	2.36	0.41
1:E:842:MET:SD	1:E:995:ILE:HA	2.61	0.41
1:F:387:GLU:OE1	1:F:387:GLU:N	2.54	0.41
1:F:923:LYS:HD3	1:F:923:LYS:HA	1.88	0.41
1:G:628:ARG:HA	1:G:967:LEU:HD13	2.02	0.41
1:G:904:ILE:O	1:G:908:ILE:HG12	2.21	0.41
1:E:411:THR:O	1:E:413:THR:HG23	2.21	0.41
1:E:1017:PRO:HD3	1:G:1129:ARG:NH2	2.36	0.41
1:G:61:ARG:NE	1:G:207:GLU:OE2	2.47	0.41
1:G:970:ASP:OD1	1:G:970:ASP:N	2.54	0.41
1:H:998:THR:HG23	1:H:1001:ARG:HH12	1.86	0.41
1:B:97:LEU:HD13	1:B:113:ARG:HB2	2.03	0.40
1:D:615:GLY:HA2	1:D:900:VAL:HA	2.02	0.40
1:H:592:MET:HE1	1:H:601:ARG:NH2	2.35	0.40
1:H:691:ALA:HA	1:H:729:LEU:HD22	2.03	0.40
1:H:55:LEU:HD22	1:H:59:ASP:HB3	2.03	0.40
1:B:933:LYS:HB2	1:B:951:TYR:CE2	2.57	0.40
1:E:194:LEU:HD21	1:E:201:THR:HB	2.03	0.40
1:F:1003:ALA:HB2	1:F:1026:MET:HE2	2.04	0.40
1:G:353:PRO:HG2	1:G:459:SER:HB3	2.02	0.40
1:G:378:ASN:O	1:G:382:LEU:HG	2.22	0.40
1:G:400:PHE:CE1	1:G:787:LEU:HD11	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:251:THR:O	1:H:310:VAL:HA	2.21	0.40
1:B:348:GLY:N	1:B:640:GLU:HG3	2.37	0.40
1:B:786:LYS:NZ	1:B:795:GLY:O	2.37	0.40
1:G:629:PRO:HD3	1:G:967:LEU:HD13	2.04	0.40
1:A:160:ARG:HH22	1:A:267:SER:CB	2.34	0.40
1:B:515:ARG:NH2	1:B:525:ASP:OD2	2.54	0.40
1:E:104:PHE:HB3	1:E:111:SER:HB2	2.04	0.40
1:E:812:PRO:HD3	1:E:893:TYR:CG	2.57	0.40
1:E:1016:CYS:SG	1:E:1018:PRO:HD2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1122/1131 (99%)	1094 (98%)	28 (2%)	0	100	100
1	B	1121/1131 (99%)	1075 (96%)	46 (4%)	0	100	100
1	C	1121/1131 (99%)	1090 (97%)	31 (3%)	0	100	100
1	D	1120/1131 (99%)	1084 (97%)	36 (3%)	0	100	100
1	E	1114/1131 (98%)	1084 (97%)	29 (3%)	1 (0%)	48	66
1	F	1111/1131 (98%)	1073 (97%)	38 (3%)	0	100	100
1	G	1109/1131 (98%)	1075 (97%)	34 (3%)	0	100	100
1	H	1116/1131 (99%)	1086 (97%)	29 (3%)	1 (0%)	48	66
All	All	8934/9048 (99%)	8661 (97%)	271 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	849	THR

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Mol	Chain	Res	Type
1	E	580	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	964/968 (100%)	953 (99%)	11 (1%)	65	80
1	B	963/968 (100%)	956 (99%)	7 (1%)	76	86
1	C	963/968 (100%)	959 (100%)	4 (0%)	84	93
1	D	962/968 (99%)	957 (100%)	5 (0%)	81	91
1	E	958/968 (99%)	957 (100%)	1 (0%)	88	95
1	F	956/968 (99%)	952 (100%)	4 (0%)	84	93
1	G	956/968 (99%)	954 (100%)	2 (0%)	87	95
1	H	960/968 (99%)	953 (99%)	7 (1%)	76	86
All	All	7682/7744 (99%)	7641 (100%)	41 (0%)	81	91

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	368	ASP
1	A	378	ASN
1	A	381	LEU
1	A	640	GLU
1	A	799	GLN
1	A	808	ARG
1	A	831	LEU
1	A	883	ASP
1	A	1038	ASP
1	A	1054	SER
1	B	368	ASP
1	B	378	ASN
1	B	514	ASN

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Mol	Chain	Res	Type
1	B	640	GLU
1	B	746	VAL
1	B	943	ARG
1	B	975	GLU
1	C	378	ASN
1	C	533	ASP
1	C	640	GLU
1	C	746	VAL
1	D	324	LYS
1	D	385	ARG
1	D	640	GLU
1	D	840	SER
1	D	869	VAL
1	E	368	ASP
1	F	54	ARG
1	F	100	ASP
1	F	640	GLU
1	F	746	VAL
1	G	274	ASP
1	G	1131	VAL
1	H	20	LEU
1	H	100	ASP
1	H	368	ASP
1	H	378	ASN
1	H	676	ASP
1	H	849	THR
1	H	1079	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	219	ASN
1	A	295	ASN
1	A	454	HIS
1	A	548	GLN
1	A	586	HIS
1	A	598	ASN
1	B	14	ASN
1	B	285	GLN
1	B	419	HIS
1	B	442	HIS

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Mol	Chain	Res	Type
1	B	706	HIS
1	C	124	HIS
1	C	219	ASN
1	C	289	HIS
1	C	419	HIS
1	C	610	ASN
1	C	679	HIS
1	C	1004	GLN
1	D	44	GLN
1	D	219	ASN
1	D	295	ASN
1	D	596	HIS
1	D	679	HIS
1	D	717	GLN
1	D	1004	GLN
1	D	1028	HIS
1	E	24	HIS
1	E	280	GLN
1	E	336	ASN
1	E	359	GLN
1	F	182	HIS
1	F	550	ASN
1	F	717	GLN
1	G	596	HIS
1	G	717	GLN
1	G	767	GLN
1	G	918	ASN
1	H	24	HIS
1	H	419	HIS
1	H	505	GLN
1	H	796	HIS
1	H	799	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MLT	C	1202	-	8,8,8	1.08	0	10,10,10	1.62	1 (10%)
3	MLT	F	1202	-	8,8,8	1.09	0	10,10,10	1.58	3 (30%)
3	MLT	G	1202	-	8,8,8	1.07	0	10,10,10	1.72	2 (20%)
3	MLT	B	1202	-	8,8,8	1.09	0	10,10,10	1.58	2 (20%)
3	MLT	A	1202	-	8,8,8	1.07	0	10,10,10	1.65	2 (20%)
3	MLT	H	1202	-	8,8,8	1.09	0	10,10,10	1.69	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	MLT	C	1202	-	-	6/8/8/8	-
3	MLT	F	1202	-	-	4/8/8/8	-
3	MLT	G	1202	-	-	2/8/8/8	-
3	MLT	B	1202	-	-	4/8/8/8	-
3	MLT	A	1202	-	-	6/8/8/8	-
3	MLT	H	1202	-	-	5/8/8/8	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1202	MLT	O2-C1-C2	3.78	120.73	112.74
3	G	1202	MLT	O2-C1-C2	3.73	120.62	112.74
3	C	1202	MLT	O2-C1-C2	3.60	120.36	112.74
3	A	1202	MLT	O2-C1-C2	3.44	120.01	112.74
3	F	1202	MLT	O2-C1-C2	3.29	119.69	112.74
3	B	1202	MLT	O2-C1-C2	3.28	119.68	112.74
3	B	1202	MLT	O5-C4-C3	2.26	121.02	114.00
3	A	1202	MLT	O5-C4-C3	2.18	120.77	114.00
3	G	1202	MLT	O5-C4-C3	2.17	120.75	114.00
3	F	1202	MLT	O2-C1-O1	-2.08	119.35	124.08
3	F	1202	MLT	O5-C4-C3	2.05	120.38	114.00

There are no chirality outliers.

All (27) torsion outliers are listed below:

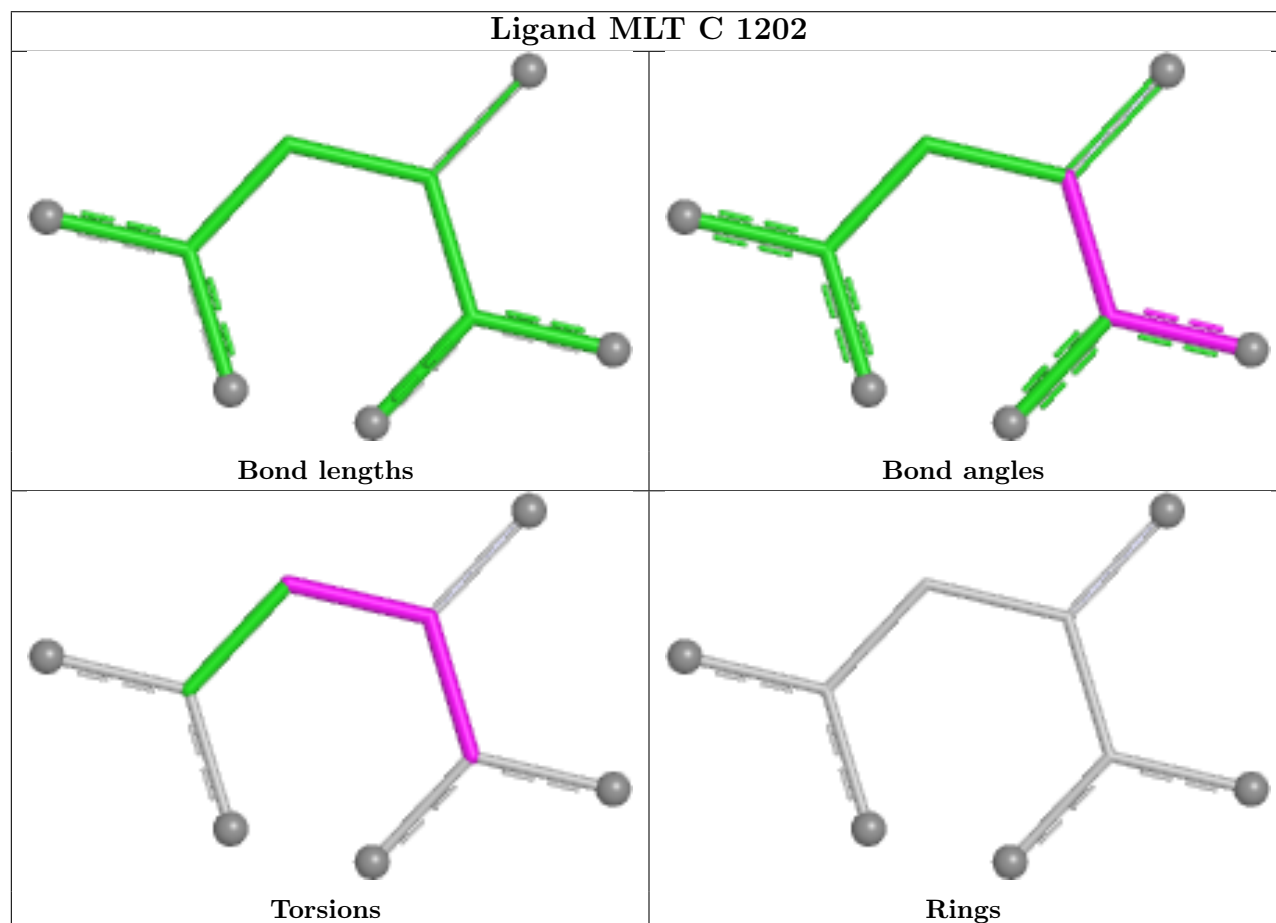
Mol	Chain	Res	Type	Atoms
3	B	1202	MLT	O3-C2-C3-C4
3	C	1202	MLT	O1-C1-C2-O3
3	C	1202	MLT	O2-C1-C2-O3
3	F	1202	MLT	O1-C1-C2-O3
3	F	1202	MLT	O2-C1-C2-O3
3	G	1202	MLT	O1-C1-C2-O3
3	G	1202	MLT	O2-C1-C2-O3
3	H	1202	MLT	O1-C1-C2-O3
3	H	1202	MLT	O2-C1-C2-O3
3	H	1202	MLT	O3-C2-C3-C4
3	H	1202	MLT	C1-C2-C3-C4
3	B	1202	MLT	C1-C2-C3-C4
3	A	1202	MLT	O1-C1-C2-O3
3	A	1202	MLT	O2-C1-C2-O3
3	A	1202	MLT	O1-C1-C2-C3
3	A	1202	MLT	O2-C1-C2-C3
3	F	1202	MLT	O2-C1-C2-C3
3	A	1202	MLT	C2-C3-C4-O5
3	H	1202	MLT	C2-C3-C4-O5
3	A	1202	MLT	C2-C3-C4-O4
3	C	1202	MLT	O3-C2-C3-C4
3	C	1202	MLT	C1-C2-C3-C4
3	B	1202	MLT	O2-C1-C2-C3
3	C	1202	MLT	O1-C1-C2-C3
3	C	1202	MLT	O2-C1-C2-C3
3	F	1202	MLT	O1-C1-C2-C3
3	B	1202	MLT	C2-C3-C4-O5

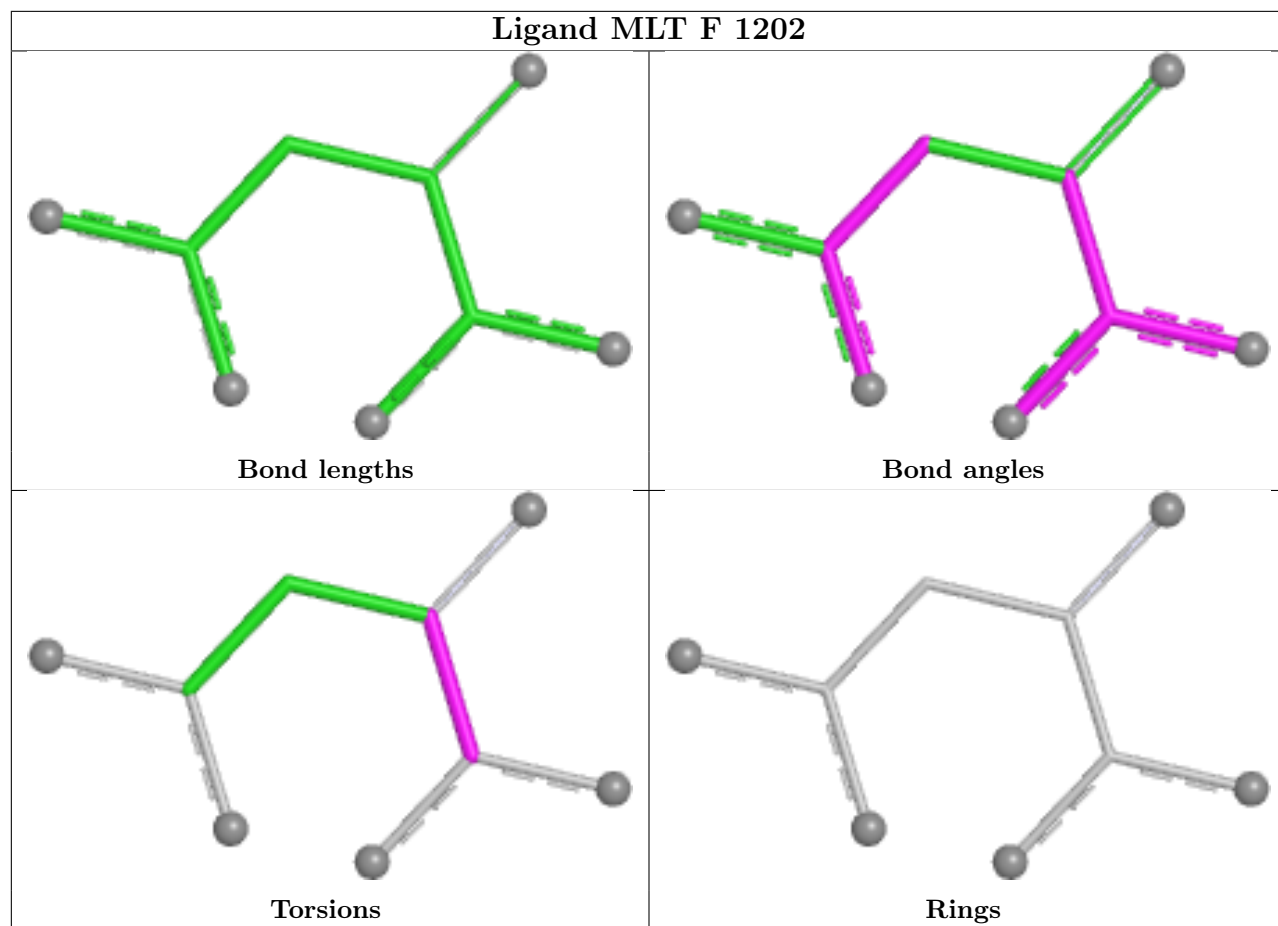
There are no ring outliers.

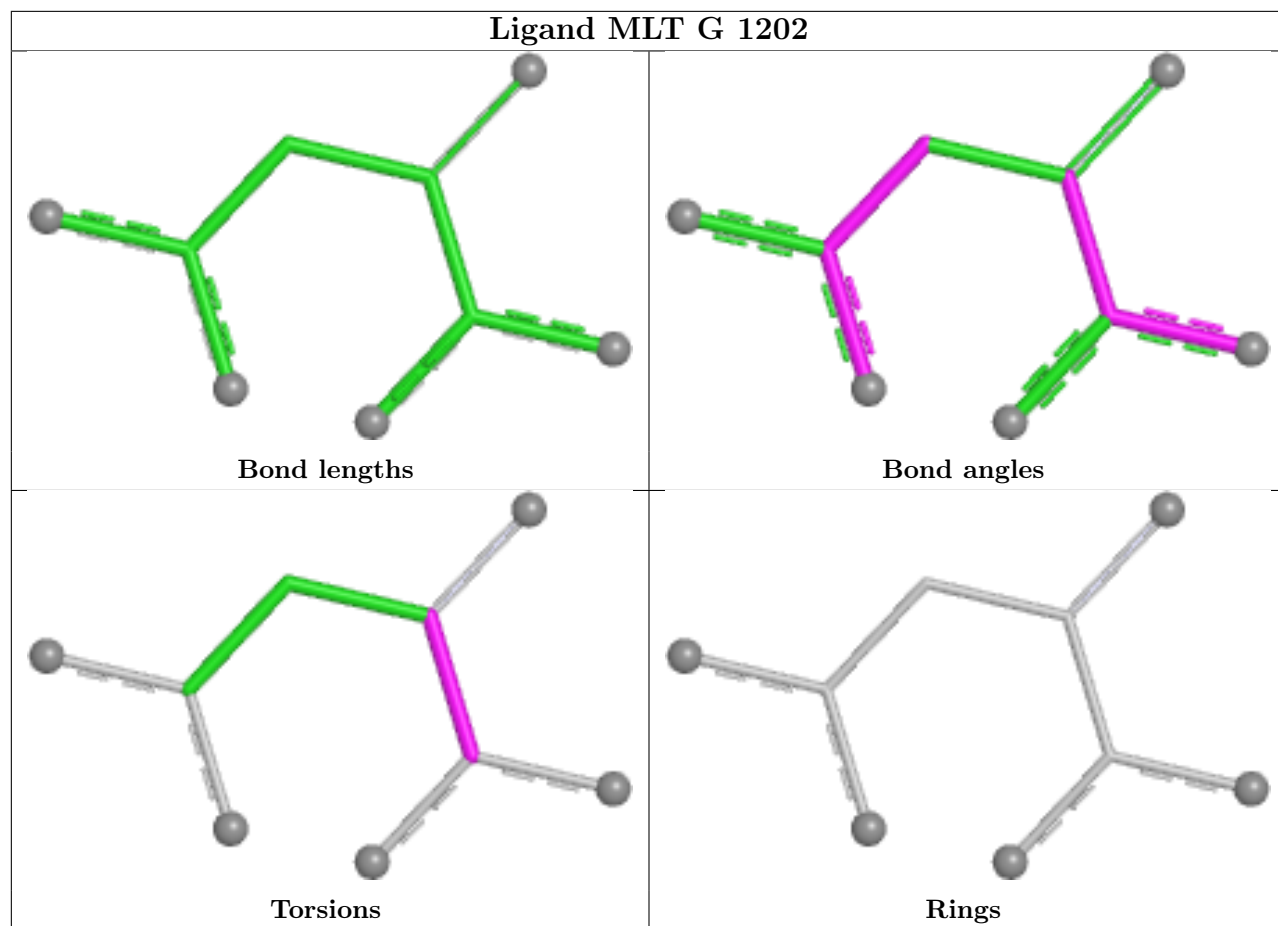
1 monomer is involved in 1 short contact:

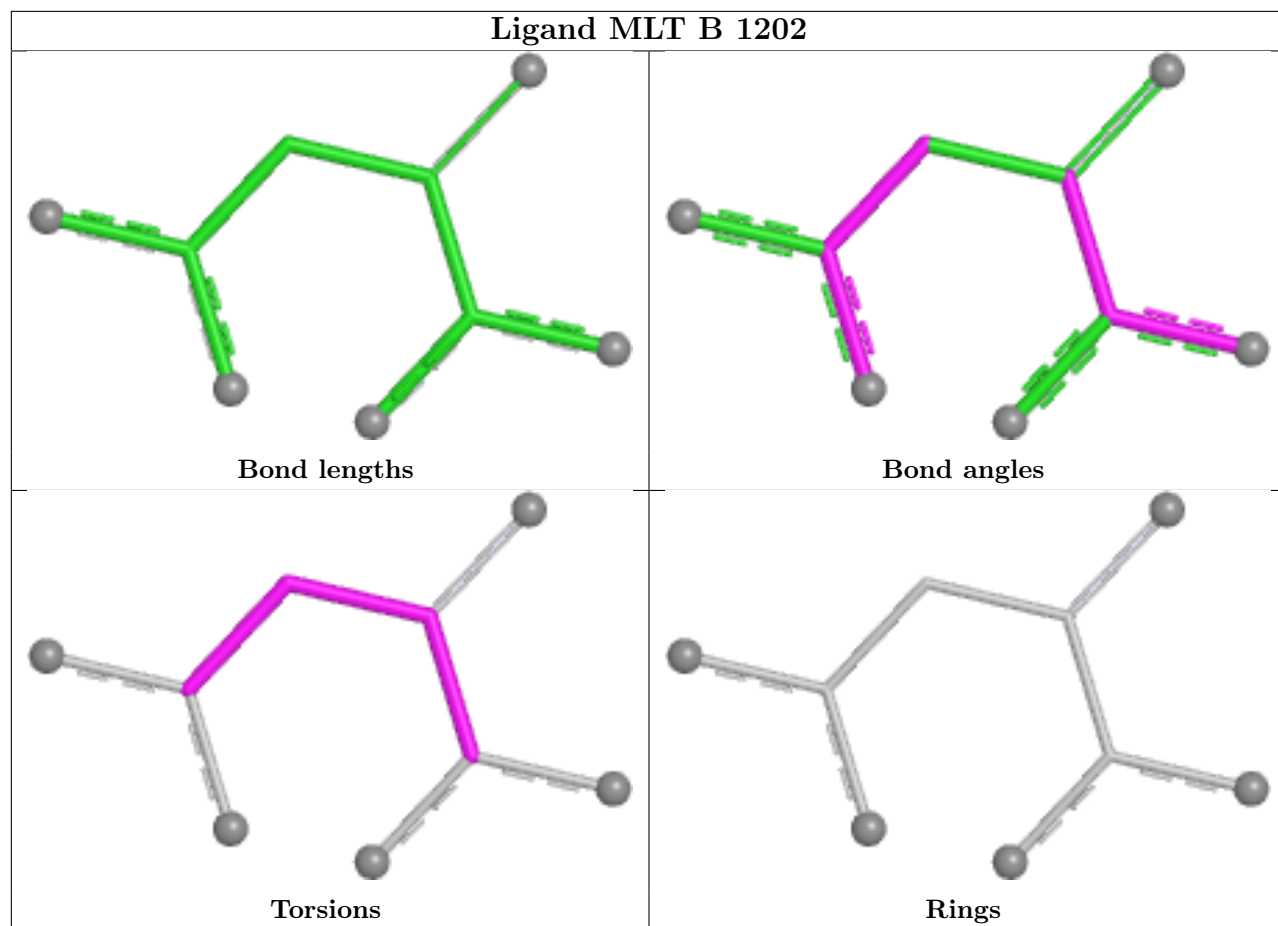
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1202	MLT	1	0

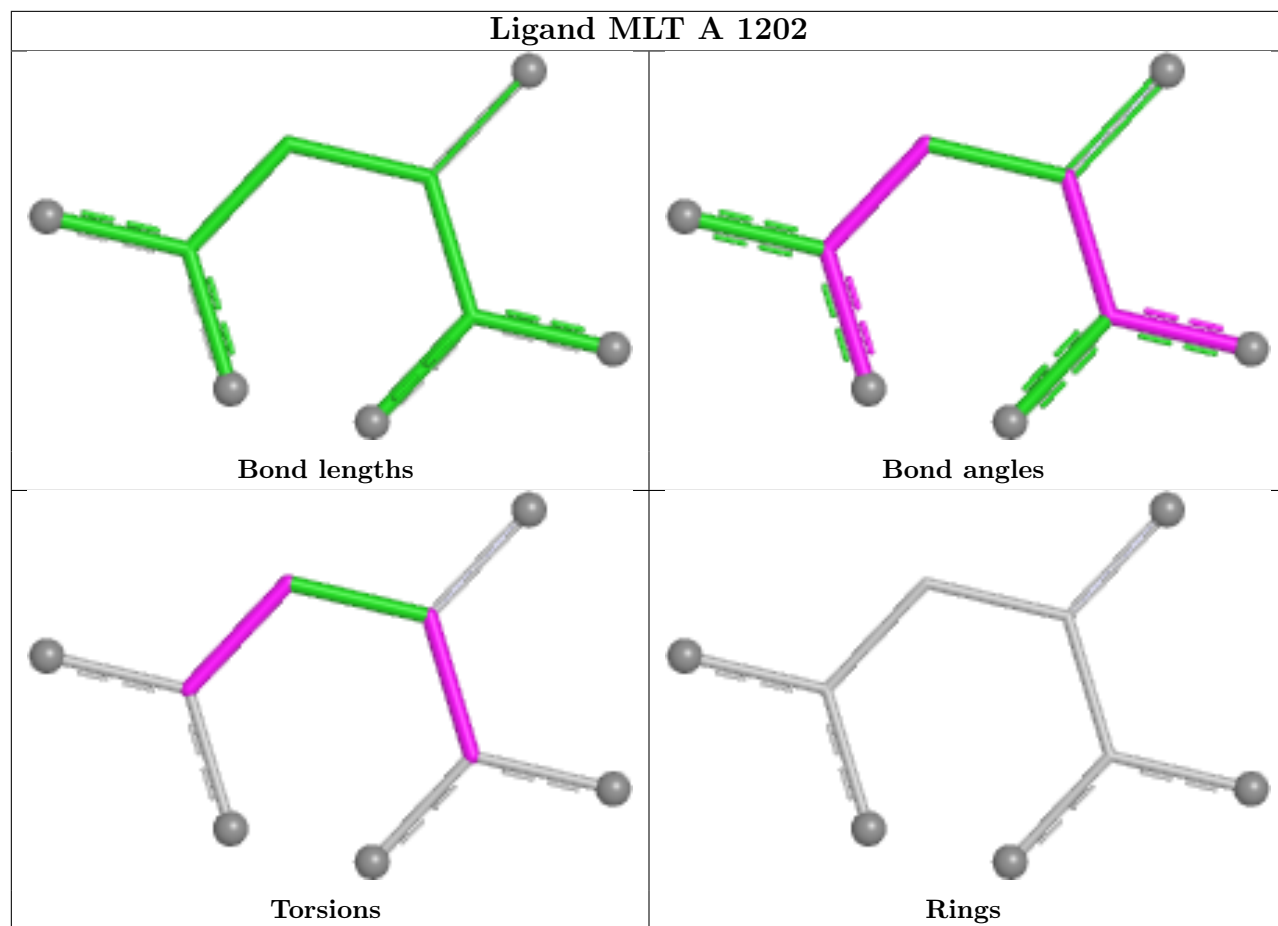
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

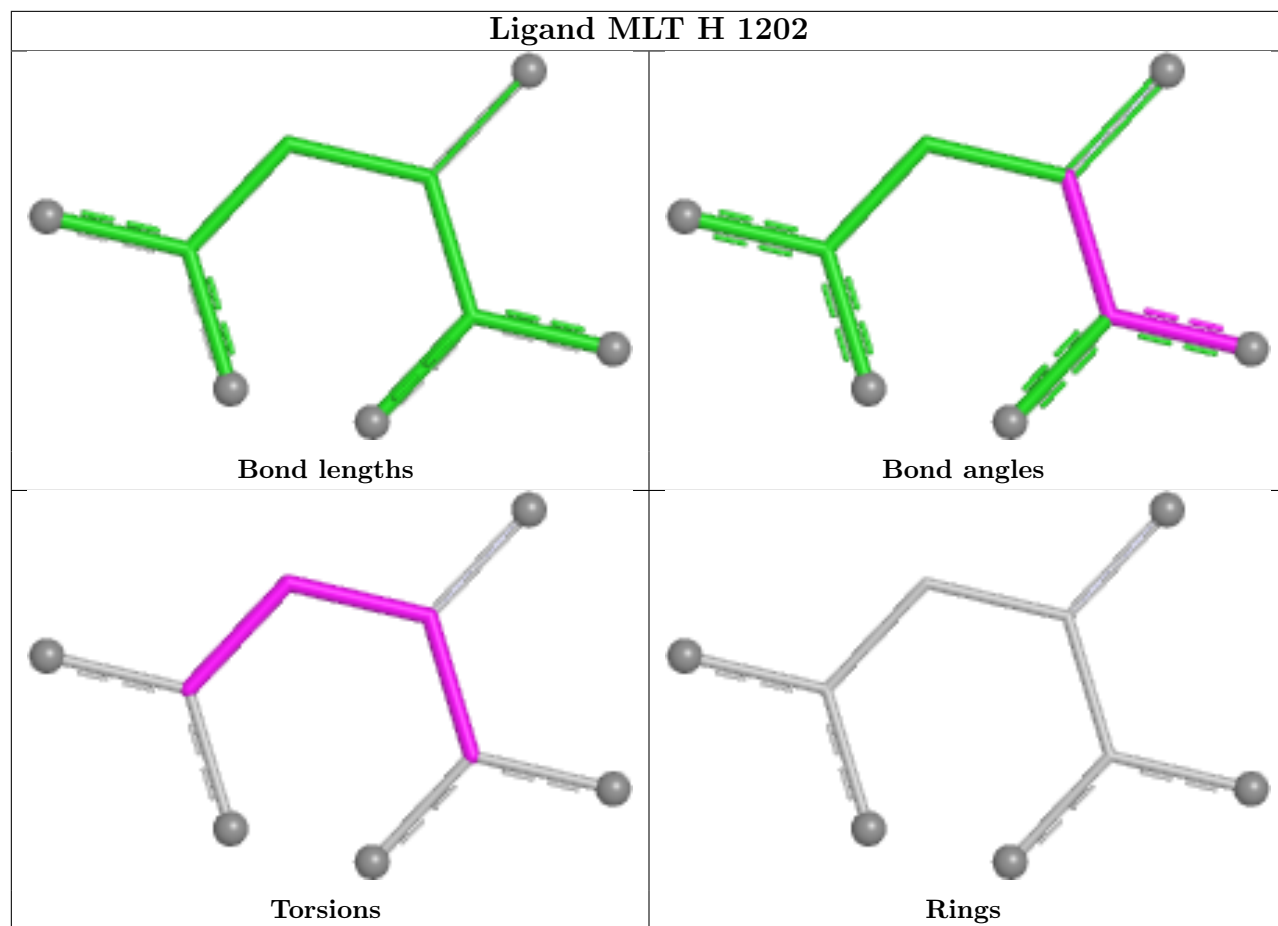












5.7 Other polymers [i](#)

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	1126/1131 (99%)	-0.30	5 (0%) 88 87	31, 49, 78, 145	0
1	B	1125/1131 (99%)	-0.09	20 (1%) 67 63	33, 53, 121, 185	0
1	C	1125/1131 (99%)	-0.21	12 (1%) 78 75	31, 49, 94, 161	0
1	D	1124/1131 (99%)	-0.25	6 (0%) 87 85	32, 48, 86, 138	0
1	E	1120/1131 (99%)	-0.18	16 (1%) 73 69	30, 52, 101, 175	0
1	F	1117/1131 (98%)	-0.21	6 (0%) 87 85	28, 52, 78, 145	0
1	G	1115/1131 (98%)	-0.10	22 (1%) 65 59	32, 54, 84, 121	0
1	H	1122/1131 (99%)	-0.29	8 (0%) 84 82	34, 48, 78, 141	0
All	All	8974/9048 (99%)	-0.20	95 (1%) 78 75	28, 51, 88, 185	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	532	ILE	4.4
1	B	32	PRO	4.3
1	G	519	ALA	3.9
1	B	547	ILE	3.6
1	D	547	ILE	3.5
1	B	847	PRO	3.5
1	H	849	THR	3.4
1	D	850	THR	3.4
1	B	850	THR	3.3
1	G	596	HIS	3.3
1	H	850	THR	3.3
1	E	579	TRP	3.2
1	D	847	PRO	3.2
1	B	577	PRO	3.2
1	G	580	GLY	3.2
1	A	850	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	532	ILE	3.0
1	B	528	PRO	3.0
1	E	517	ALA	3.0
1	B	579	TRP	2.9
1	H	32	PRO	2.9
1	C	533	ASP	2.9
1	E	847	PRO	2.9
1	C	850	THR	2.9
1	G	539	VAL	2.9
1	E	519	ALA	2.9
1	G	536	LEU	2.9
1	C	547	ILE	2.8
1	B	536	LEU	2.8
1	B	493	PHE	2.8
1	C	527	ARG	2.8
1	B	519	ALA	2.8
1	G	542	LEU	2.7
1	D	848	SER	2.7
1	E	34	ALA	2.7
1	H	847	PRO	2.7
1	F	493	PHE	2.7
1	E	547	ILE	2.6
1	F	547	ILE	2.6
1	B	512	PHE	2.6
1	A	846	SER	2.6
1	E	526	HIS	2.6
1	G	513	THR	2.6
1	F	51	LEU	2.6
1	E	528	PRO	2.6
1	G	517	ALA	2.6
1	C	517	ALA	2.5
1	E	849	THR	2.5
1	C	532	ILE	2.5
1	H	52	LYS	2.5
1	B	586	HIS	2.5
1	C	756	ASP	2.5
1	E	596	HIS	2.5
1	G	576	LEU	2.4
1	H	848	SER	2.4
1	B	851	GLY	2.4
1	A	289	HIS	2.4
1	C	847	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	493	PHE	2.4
1	B	532	ILE	2.4
1	C	846	SER	2.4
1	E	493	PHE	2.4
1	G	843	THR	2.3
1	G	547	ILE	2.3
1	B	849	THR	2.3
1	G	577	PRO	2.3
1	B	516	PHE	2.3
1	G	512	PHE	2.3
1	B	495	HIS	2.3
1	A	847	PRO	2.3
1	C	528	PRO	2.2
1	G	795	GLY	2.2
1	G	530	LEU	2.2
1	C	35	ILE	2.2
1	E	850	THR	2.2
1	G	552	GLU	2.2
1	F	532	ILE	2.2
1	F	844	GLY	2.2
1	B	546	SER	2.2
1	F	578	GLU	2.1
1	B	545	PRO	2.1
1	B	844	GLY	2.1
1	E	518	ASP	2.1
1	A	1086	PRO	2.1
1	E	845	LYS	2.1
1	G	493	PHE	2.1
1	C	849	THR	2.1
1	D	942	HIS	2.1
1	G	540	ILE	2.1
1	D	846	SER	2.1
1	H	598	ASN	2.1
1	G	575	TYR	2.1
1	G	545	PRO	2.0
1	E	35	ILE	2.0
1	G	620	GLY	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

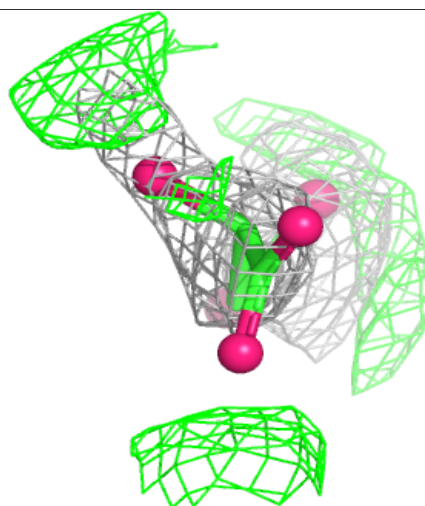
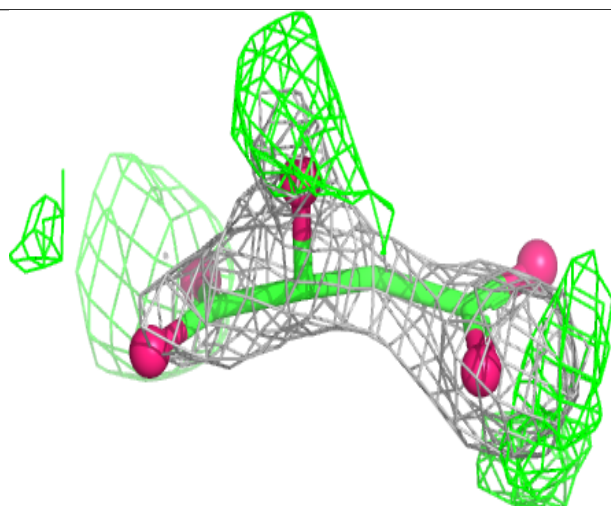
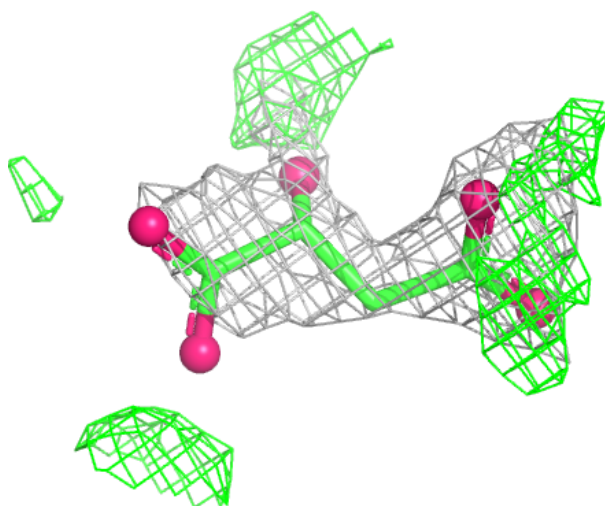
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MLT	C	1202	9/9	0.63	0.23	43,48,54,56	9
3	MLT	B	1202	9/9	0.83	0.15	52,54,56,56	9
3	MLT	G	1202	9/9	0.84	0.18	43,48,50,51	9
3	MLT	F	1202	9/9	0.88	0.16	35,38,40,42	9
3	MLT	A	1202	9/9	0.88	0.16	37,41,42,42	9
3	MLT	H	1202	9/9	0.88	0.13	42,43,46,46	9
2	MG	C	1201	1/1	0.99	0.19	42,42,42,42	0
2	MG	F	1201	1/1	0.99	0.07	32,32,32,32	0
2	MG	A	1201	1/1	1.00	0.08	31,31,31,31	0
2	MG	D	1201	1/1	1.00	0.09	33,33,33,33	0
2	MG	E	1201	1/1	1.00	0.09	29,29,29,29	0
2	MG	B	1201	1/1	1.00	0.08	33,33,33,33	0
2	MG	G	1201	1/1	1.00	0.12	31,31,31,31	0
2	MG	H	1201	1/1	1.00	0.12	32,32,32,32	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.

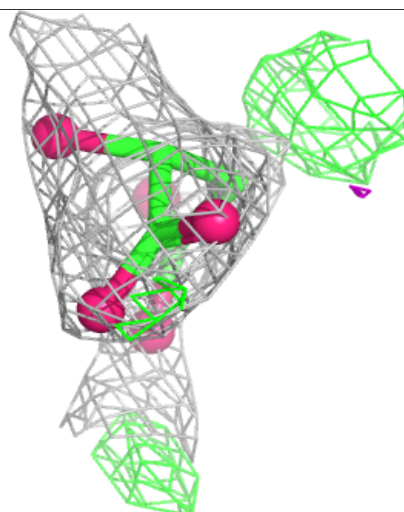
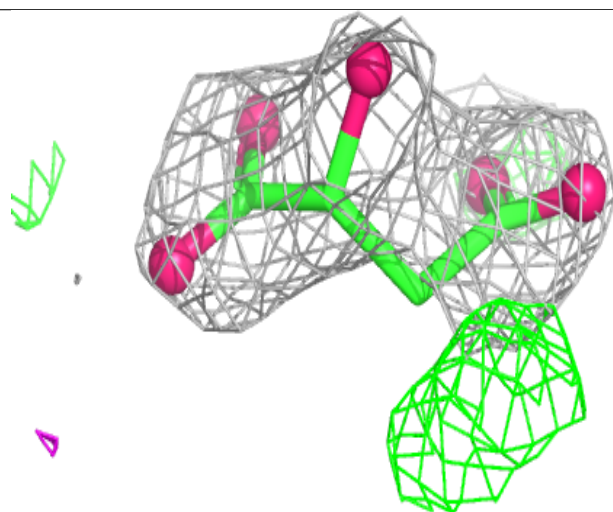
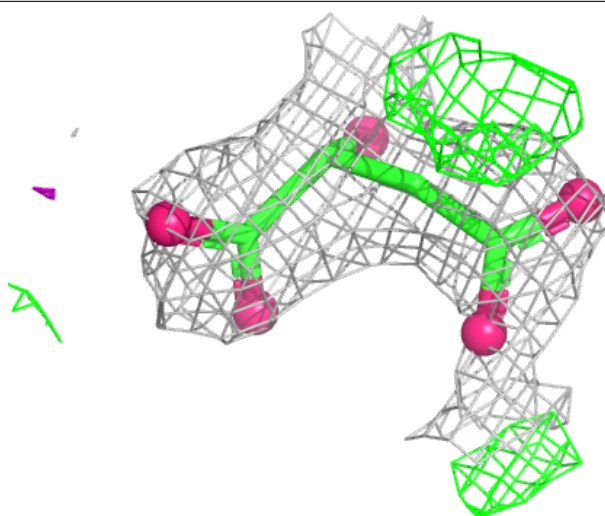
Electron density around MLT C 1202:

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



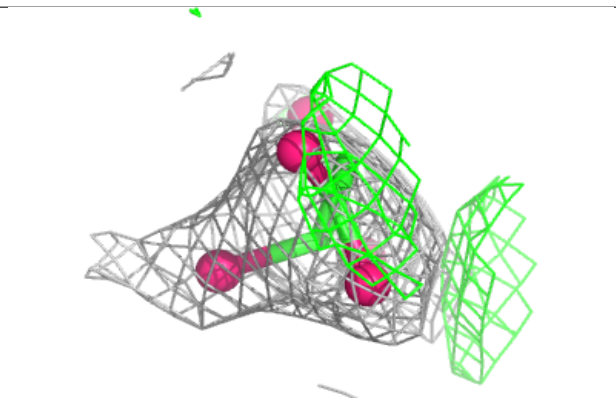
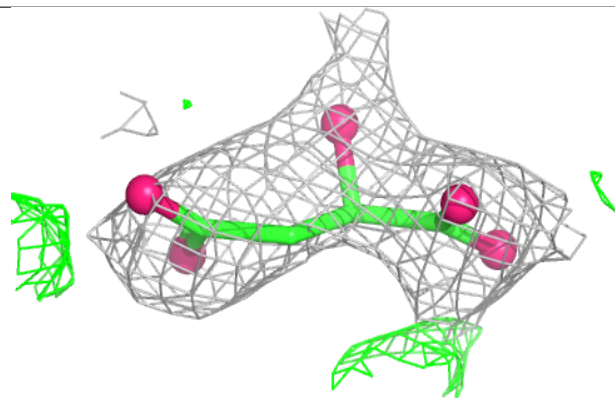
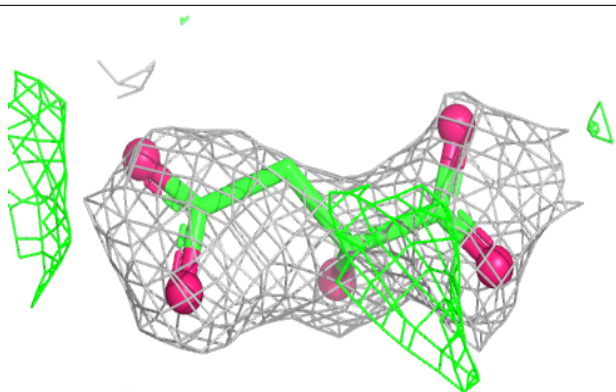
Electron density around MLT B 1202:

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

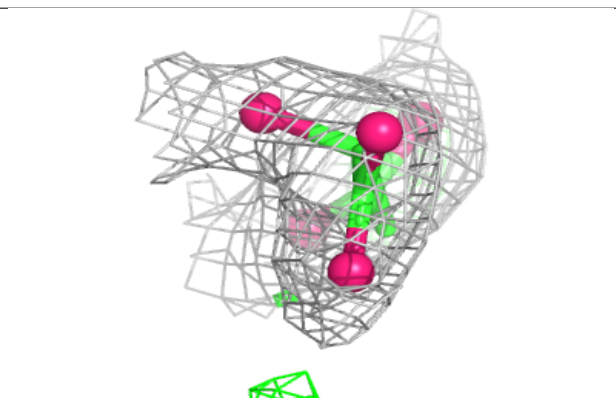
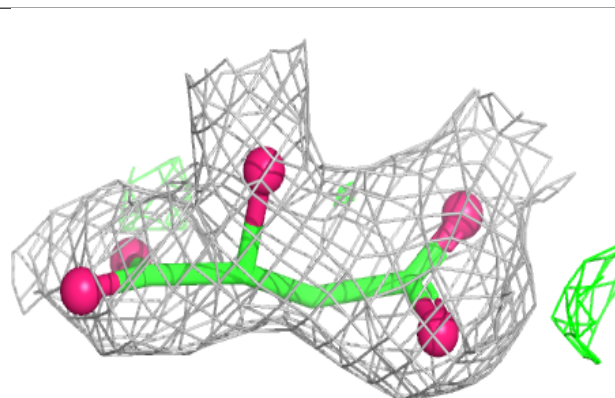
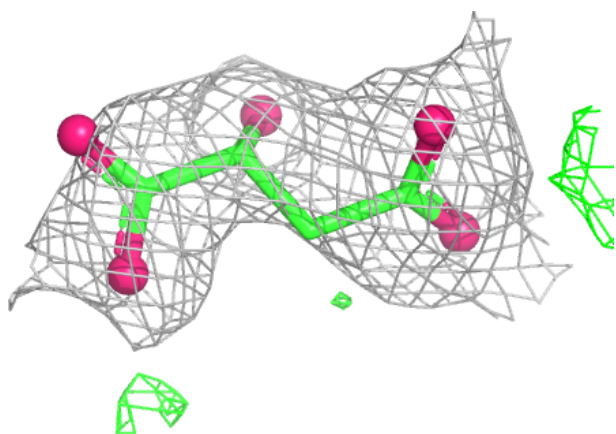


Electron density around MLT G 1202:

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

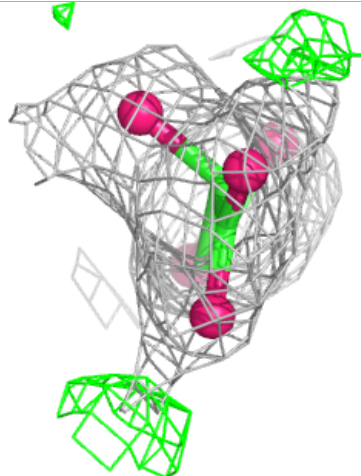
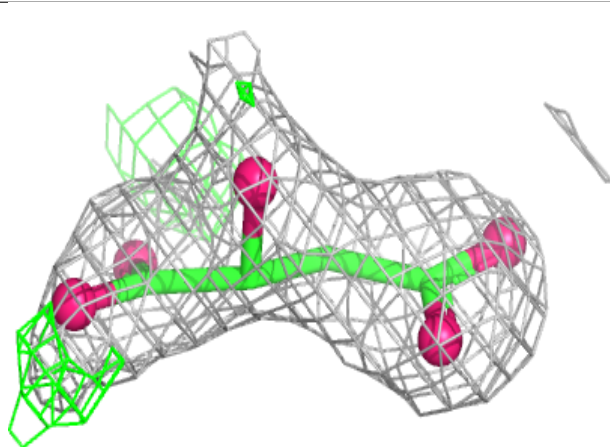
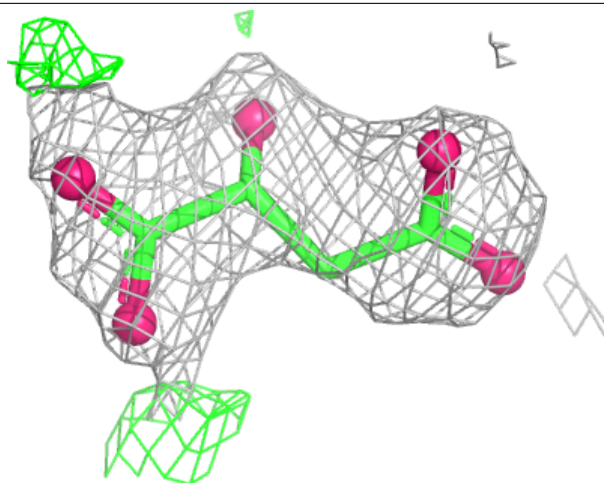
**Electron density around MLT F 1202:**

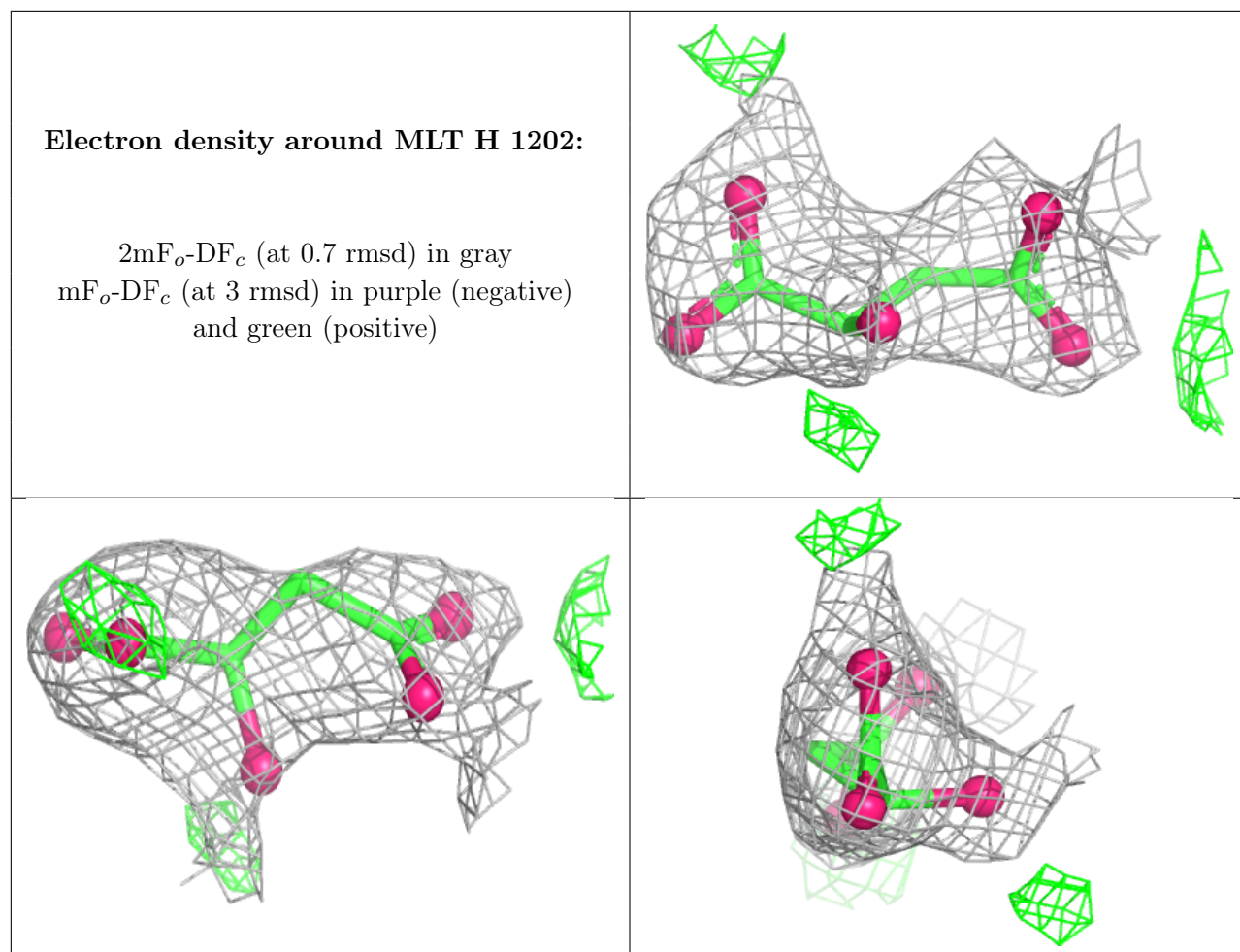
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MLT A 1202:

$2mF_o-DF_c$ (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.