



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:18 PM UTC

PDB ID : 6I35 / pdb_00006i35
Title : Crystal structure of human glycine decarboxylase (P-protein) bound with pyridoxyl-glycine-5'-monophosphate
Authors : Van Laer, B.; Kapp, U.; Leonard, G.; Mueller-Dieckmann, C.
Deposited on : 2018-11-05
Resolution : 2.00 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:

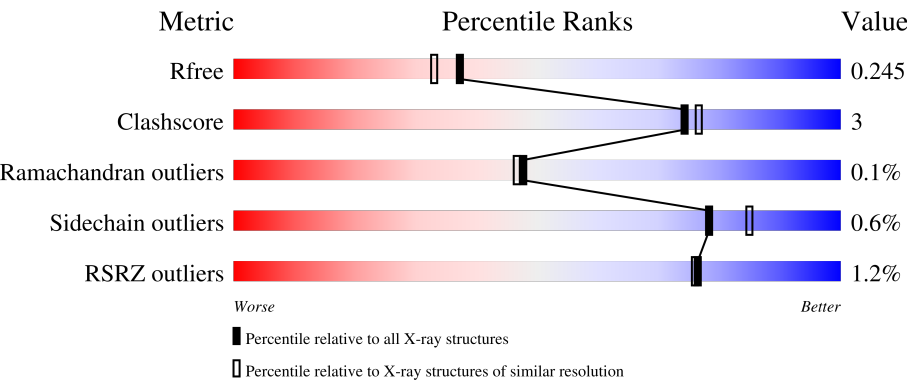
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	984	% 88%8% .
1	B	984	2% 89%8% ..
1	C	984	% 89%8% .
1	D	984	% 89%8% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30932 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 Glycine dehydrogenase (decarboxylating), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	0
			7433	4684	1317	1378	54			
1	B	954	Total	C	N	O	S	0	0	0
			7442	4688	1318	1382	54			
1	C	953	Total	C	N	O	S	0	0	0
			7433	4684	1317	1378	54			
1	D	954	Total	C	N	O	S	0	0	0
			7442	4688	1318	1382	54			

There are 32 discrepancies between the modelled and reference sequences:

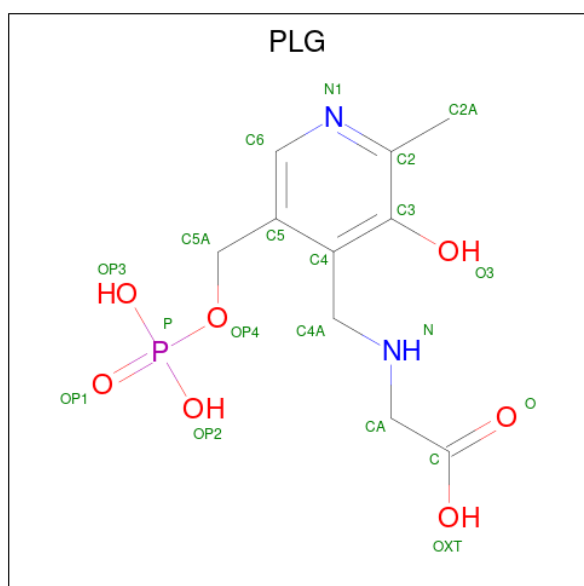
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP P23378
A	1021	GLY	-	expression tag	UNP P23378
A	1022	HIS	-	expression tag	UNP P23378
A	1023	HIS	-	expression tag	UNP P23378
A	1024	HIS	-	expression tag	UNP P23378
A	1025	HIS	-	expression tag	UNP P23378
A	1026	HIS	-	expression tag	UNP P23378
A	1027	HIS	-	expression tag	UNP P23378
B	44	MET	-	initiating methionine	UNP P23378
B	1021	GLY	-	expression tag	UNP P23378
B	1022	HIS	-	expression tag	UNP P23378
B	1023	HIS	-	expression tag	UNP P23378
B	1024	HIS	-	expression tag	UNP P23378
B	1025	HIS	-	expression tag	UNP P23378
B	1026	HIS	-	expression tag	UNP P23378
B	1027	HIS	-	expression tag	UNP P23378
C	44	MET	-	initiating methionine	UNP P23378
C	1021	GLY	-	expression tag	UNP P23378
C	1022	HIS	-	expression tag	UNP P23378
C	1023	HIS	-	expression tag	UNP P23378
C	1024	HIS	-	expression tag	UNP P23378

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1025	HIS	-	expression tag	UNP P23378
C	1026	HIS	-	expression tag	UNP P23378
C	1027	HIS	-	expression tag	UNP P23378
D	44	MET	-	initiating methionine	UNP P23378
D	1021	GLY	-	expression tag	UNP P23378
D	1022	HIS	-	expression tag	UNP P23378
D	1023	HIS	-	expression tag	UNP P23378
D	1024	HIS	-	expression tag	UNP P23378
D	1025	HIS	-	expression tag	UNP P23378
D	1026	HIS	-	expression tag	UNP P23378
D	1027	HIS	-	expression tag	UNP P23378

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (CCD ID: PLG) (formula: C₁₀H₁₅N₂O₇P) (labeled as "Ligand of Interest" by depositor).



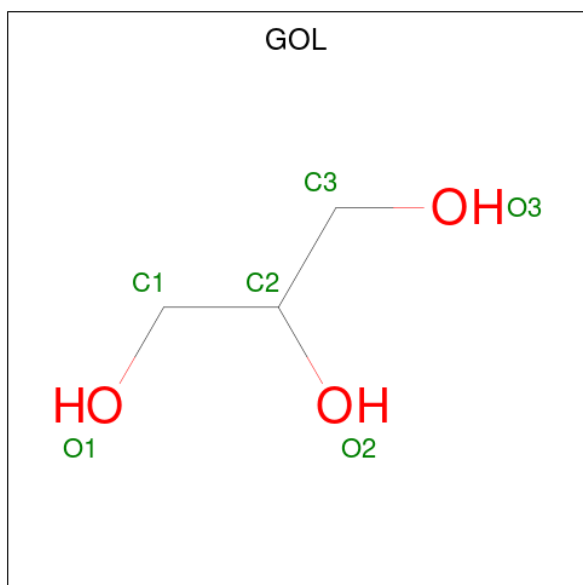
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



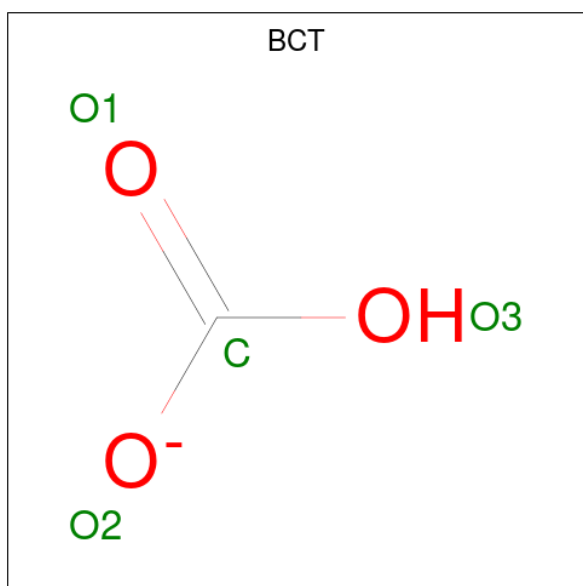
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



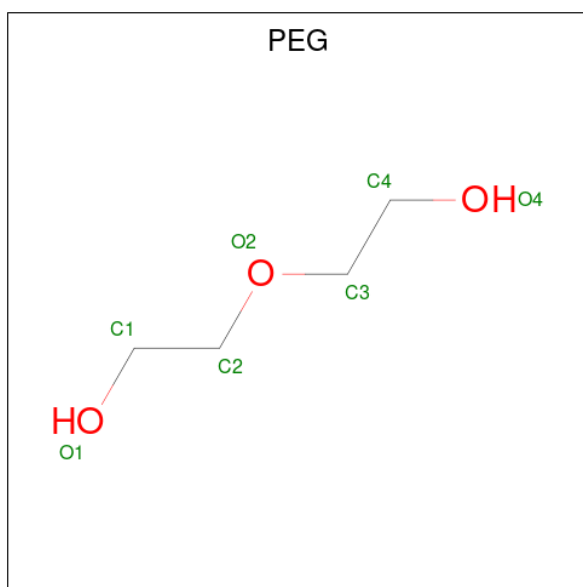
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



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

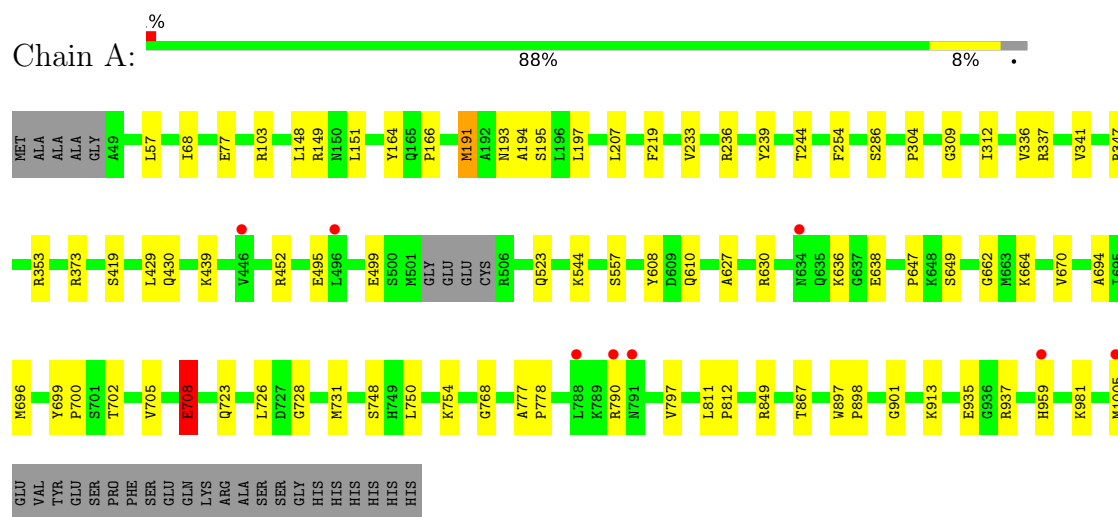
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	318	Total	O	0	0
			318	318		
7	B	192	Total	O	0	0
			192	192		
7	C	314	Total	O	0	0
			314	314		
7	D	200	Total	O	0	0
			200	200		

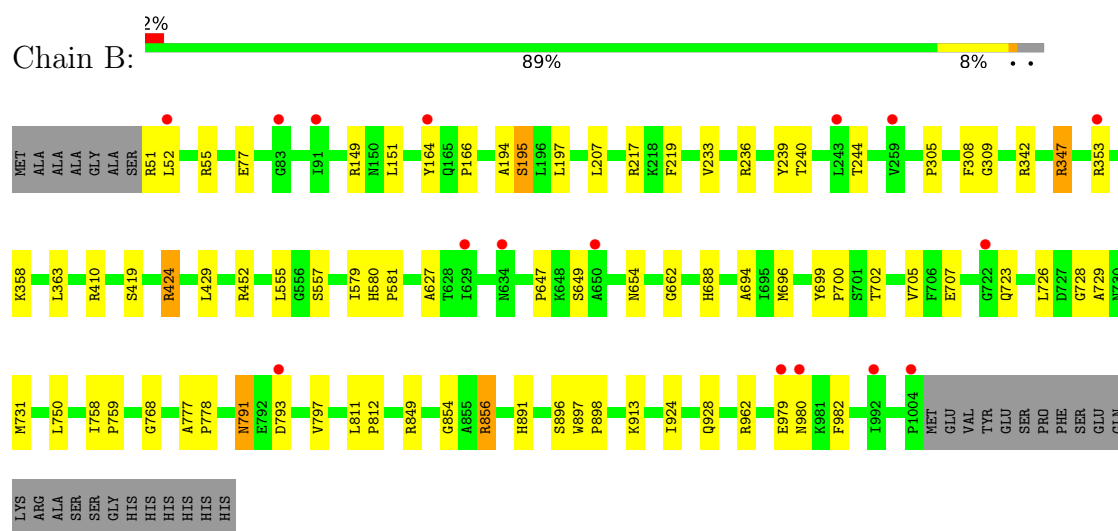
3 Residue-property plots [i](#)

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.

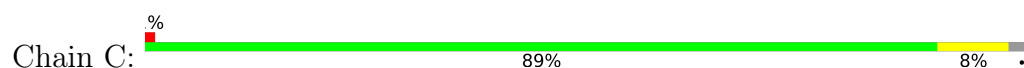
- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial

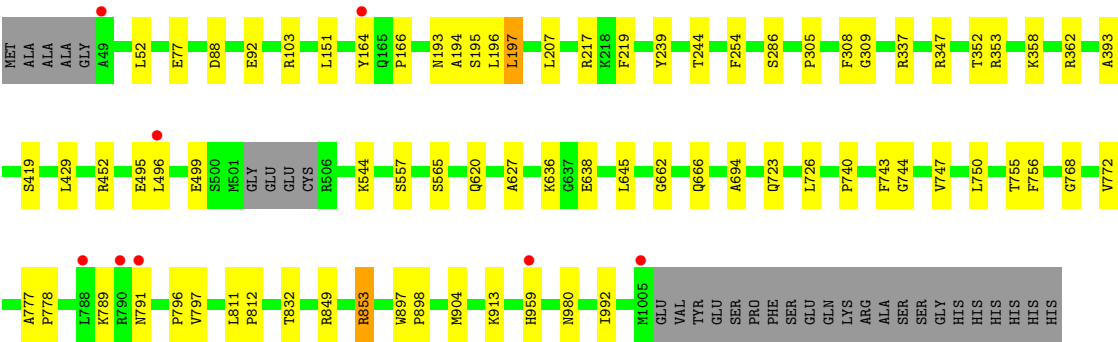


- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial

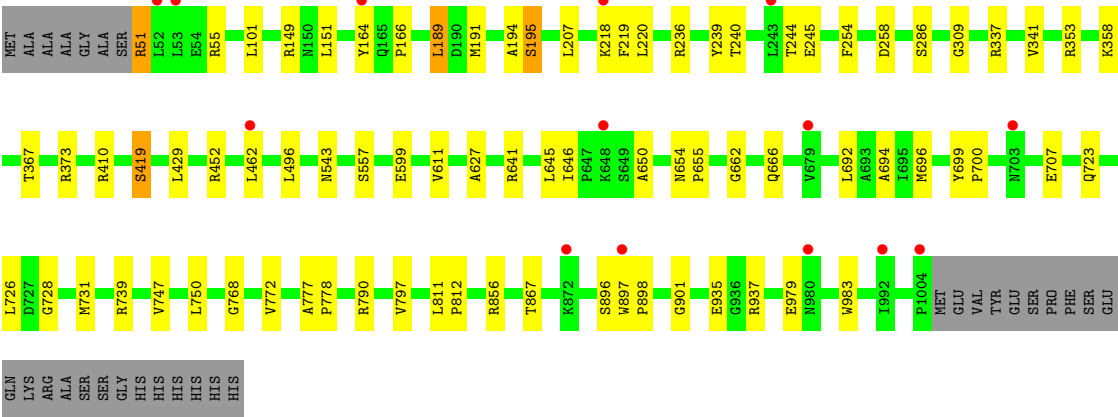
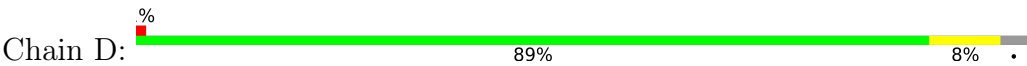


- Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial





• Molecule 1: Glycine dehydrogenase (decarboxylating), mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.66Å 123.44Å 197.67Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	49.33 – 2.00 49.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.33-2.00) 99.0 (49.33-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.215 , 0.240 0.222 , 0.245	Depositor DCC
R_{free} test set	13576 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	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	0.97	EDS
Total number of atoms	30932	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.09 % 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 5.1082e-05. 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: PLG, EDO, BCT, PEG, GOL

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	0.91	4/7599 (0.1%)	0.98	10/10291 (0.1%)
1	B	0.86	0/7609	0.95	8/10306 (0.1%)
1	C	0.92	3/7599 (0.0%)	0.98	6/10291 (0.1%)
1	D	0.87	0/7609	0.95	4/10306 (0.0%)
All	All	0.89	7/30416 (0.0%)	0.97	28/41194 (0.1%)

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	8
1	B	0	8
1	C	0	5
1	D	0	6
All	All	0	27

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	754	LYS	N-CA	-6.19	1.40	1.46
1	A	981	LYS	C-O	-5.60	1.17	1.24
1	C	393	ALA	C-O	-5.38	1.17	1.24
1	A	68	ILE	C-O	-5.35	1.18	1.24
1	C	832	THR	C-O	-5.32	1.17	1.24
1	A	191	MET	C-O	-5.25	1.17	1.23
1	C	744	GLY	C-O	-5.08	1.18	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	LEU	N-CA-C	7.72	119.77	111.36
1	A	197	LEU	N-CA-C	7.09	119.09	111.36
1	D	309	GLY	N-CA-C	6.98	125.35	115.30
1	B	309	GLY	N-CA-C	6.98	125.35	115.30
1	C	959	HIS	CA-CB-CG	6.82	120.62	113.80
1	A	304	PRO	N-CA-C	6.50	118.62	110.70
1	C	309	GLY	N-CA-C	6.38	123.85	115.36
1	A	309	GLY	N-CA-C	6.30	124.02	115.32
1	A	959	HIS	CA-CB-CG	6.18	119.98	113.80
1	A	194	ALA	CA-C-N	6.11	133.20	121.54
1	A	194	ALA	C-N-CA	6.11	133.20	121.54
1	D	194	ALA	CA-C-N	6.05	133.10	121.54
1	D	194	ALA	C-N-CA	6.05	133.10	121.54
1	B	194	ALA	CA-C-N	6.05	133.09	121.54
1	B	194	ALA	C-N-CA	6.05	133.09	121.54
1	A	705	VAL	N-CA-C	6.02	118.12	108.85
1	C	194	ALA	CA-C-N	5.76	132.55	121.54
1	C	194	ALA	C-N-CA	5.76	132.55	121.54
1	C	980	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	304	PRO	CA-C-N	5.54	125.64	119.32
1	A	304	PRO	C-N-CA	5.54	125.64	119.32
1	B	195	SER	N-CA-C	5.45	122.41	110.80
1	D	195	SER	N-CA-C	5.36	122.22	110.80
1	A	708	GLU	N-CA-C	5.24	117.74	111.71
1	B	980	ASN	CA-CB-CG	5.18	117.78	112.60
1	B	688	HIS	CA-C-N	5.08	128.44	120.82
1	B	688	HIS	C-N-CA	5.08	128.44	120.82
1	B	197	LEU	N-CA-C	5.04	117.89	111.69

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	337	ARG	Sidechain
1	A	373	ARG	Sidechain
1	A	452	ARG	Sidechain
1	A	630	ARG	Sidechain
1	A	849	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	342	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	347	ARG	Sidechain
1	B	424	ARG	Sidechain
1	B	452	ARG	Sidechain
1	B	55	ARG	Sidechain
1	B	849	ARG	Sidechain
1	B	962	ARG	Sidechain
1	C	103	ARG	Sidechain
1	C	337	ARG	Sidechain
1	C	452	ARG	Sidechain
1	C	849	ARG	Sidechain
1	C	853	ARG	Sidechain
1	D	236	ARG	Sidechain
1	D	337	ARG	Sidechain
1	D	410	ARG	Sidechain
1	D	452	ARG	Sidechain
1	D	51	ARG	Sidechain
1	D	55	ARG	Sidechain

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	7433	0	7371	43	0
1	B	7442	0	7373	49	0
1	C	7433	0	7371	40	1
1	D	7442	0	7373	60	0
2	A	20	0	11	0	0
2	B	20	0	11	1	0
2	C	20	0	11	0	0
2	D	20	0	11	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	C	12	0	16	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	7	0	10	1	0
6	C	14	0	20	3	0
6	D	7	0	10	2	0
7	A	318	0	0	2	0
7	B	192	0	0	1	0
7	C	314	0	0	0	0
7	D	200	0	0	2	0
All	All	30932	0	29636	185	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (185) 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:856:ARG:HH11	1:B:856:ARG:HG3	1.13	1.06
1:B:580:HIS:ND1	1:B:581:PRO:HD2	1.94	0.82
1:A:191:MET:SD	1:A:341:VAL:HG21	2.20	0.81
1:C:495:GLU:OE2	1:D:51:ARG:HD2	1.81	0.81
1:D:191:MET:SD	1:D:341:VAL:HG21	2.23	0.78
1:D:654:ASN:HB2	1:D:655:PRO:CD	2.14	0.77
1:D:419:SER:HB2	1:D:429:LEU:HD11	1.68	0.76
1:B:555:LEU:HD21	1:B:891:HIS:HE1	1.54	0.70
1:B:856:ARG:HG3	1:B:856:ARG:NH1	1.91	0.70
1:D:654:ASN:HB2	1:D:655:PRO:HD3	1.75	0.69
1:A:610:GLN:HE22	1:A:790:ARG:HG3	1.58	0.68
1:B:419:SER:HB2	1:B:429:LEU:HD11	1.76	0.68
1:C:495:GLU:OE2	1:D:51:ARG:CD	2.42	0.68
1:A:495:GLU:OE2	1:B:51:ARG:HD2	1.95	0.65
1:D:650:ALA:HB1	1:D:654:ASN:ND2	2.12	0.65
1:B:580:HIS:CG	1:B:581:PRO:HD2	2.32	0.64
1:C:207:LEU:HD23	1:C:207:LEU:C	2.22	0.64
1:A:608:TYR:CE2	1:A:748:SER:HB2	2.34	0.62
1:D:207:LEU:HD13	1:D:219:PHE:CG	2.35	0.62
1:D:646:ILE:CD1	1:D:696:MET:CE	2.78	0.61
1:C:88:ASP:O	1:C:92:GLU:HG3	2.01	0.60
1:B:654:ASN:OD1	1:B:696:MET:HE2	2.01	0.60
1:D:646:ILE:HD11	1:D:696:MET:CE	2.33	0.59
1:D:983:TRP:H	6:D:1103:PEG:H31	1.68	0.58
1:B:555:LEU:HD21	1:B:891:HIS:CE1	2.38	0.58
1:B:149:ARG:NH2	7:B:3102:HOH:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ALA:HB1	1:A:797:VAL:HG21	1.86	0.58
1:D:627:ALA:HB1	1:D:797:VAL:HG21	1.86	0.57
1:A:148:LEU:HD23	1:A:148:LEU:C	2.30	0.57
1:D:654:ASN:CB	1:D:655:PRO:CD	2.81	0.57
1:D:218:LYS:HE2	1:D:220:LEU:HD21	1.87	0.57
1:D:207:LEU:HD12	1:D:207:LEU:O	2.05	0.57
1:D:646:ILE:HD11	1:D:696:MET:HE2	1.86	0.57
1:A:193:ASN:HB2	1:A:347:ARG:O	2.04	0.56
1:D:419:SER:HB2	1:D:429:LEU:CD1	2.35	0.56
1:D:646:ILE:CD1	1:D:696:MET:HE3	2.35	0.56
1:D:207:LEU:HD12	1:D:207:LEU:C	2.31	0.56
1:A:608:TYR:HE2	1:A:748:SER:HB2	1.72	0.55
1:B:419:SER:HB2	1:B:429:LEU:CD1	2.37	0.55
1:D:240:THR:HG22	1:D:240:THR:O	2.05	0.55
1:C:627:ALA:HB1	1:C:797:VAL:HG21	1.88	0.55
1:A:430:GLN:HG3	1:A:439:LYS:HG2	1.89	0.55
1:A:499:GLU:HA	1:B:52:LEU:HD23	1.89	0.54
1:A:191:MET:SD	1:A:341:VAL:CG2	2.93	0.54
1:D:462:LEU:HD12	1:D:462:LEU:O	2.06	0.54
1:B:649:SER:O	1:B:702:THR:OG1	2.20	0.53
1:D:207:LEU:HD13	1:D:219:PHE:CD1	2.43	0.53
1:D:654:ASN:O	1:D:696:MET:HE1	2.08	0.53
1:B:627:ALA:HB1	1:B:797:VAL:HG21	1.90	0.53
1:A:636:LYS:HE2	1:A:638:GLU:HG3	1.89	0.53
1:B:240:THR:O	1:B:240:THR:HG22	2.07	0.53
1:D:641:ARG:HD3	1:D:692:LEU:O	2.08	0.53
1:C:193:ASN:HB2	1:C:347:ARG:O	2.09	0.52
1:C:726:LEU:C	1:C:726:LEU:HD23	2.35	0.52
1:B:305:PRO:HA	1:B:308:PHE:CZ	2.45	0.52
1:D:419:SER:CB	1:D:429:LEU:HD11	2.39	0.51
1:A:523:GLN:HB3	1:A:1005:MET:HG3	1.93	0.51
1:B:207:LEU:HD13	1:B:233:VAL:HG13	1.93	0.51
1:B:580:HIS:CE1	1:B:581:PRO:HD2	2.46	0.50
1:D:218:LYS:HE3	1:D:245:GLU:OE1	2.12	0.50
1:C:305:PRO:HA	1:C:308:PHE:CZ	2.47	0.50
6:C:1106:PEG:O1	6:D:1103:PEG:H22	2.13	0.49
1:B:207:LEU:CD1	1:B:233:VAL:HG13	2.42	0.49
1:C:495:GLU:CD	1:D:51:ARG:HD2	2.38	0.49
1:A:239:TYR:O	1:A:662:GLY:HA3	2.13	0.49
1:A:726:LEU:C	1:A:726:LEU:HD23	2.38	0.49
1:C:254:PHE:HB3	1:C:286:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HE2	1:B:979:GLU:HB2	1.95	0.48
1:C:789:LYS:HE2	1:C:796:PRO:HG2	1.94	0.48
1:A:708:GLU:HA	1:A:708:GLU:OE2	2.14	0.48
1:B:705:VAL:CG1	1:B:854:GLY:HA2	2.43	0.48
1:A:610:GLN:NE2	1:A:790:ARG:HG3	2.27	0.47
1:B:897:TRP:CG	1:B:898:PRO:HA	2.49	0.47
1:C:164:TYR:O	1:C:166:PRO:HD3	2.14	0.47
1:D:599:GLU:OE2	1:D:790:ARG:NH2	2.48	0.47
1:C:992:ILE:HD12	1:C:992:ILE:N	2.29	0.47
1:D:254:PHE:HB3	1:D:286:SER:OG	2.15	0.47
1:D:897:TRP:CG	1:D:898:PRO:HA	2.50	0.47
1:A:664:LYS:NZ	7:A:1211:HOH:O	2.48	0.47
1:D:191:MET:SD	1:D:341:VAL:CG2	2.99	0.47
1:C:239:TYR:O	1:C:662:GLY:HA3	2.15	0.47
1:A:897:TRP:CG	1:A:898:PRO:HA	2.51	0.46
1:A:649:SER:O	1:A:702:THR:OG1	2.23	0.46
1:A:694:ALA:HA	1:A:723:GLN:O	2.16	0.46
1:A:77:GLU:HB3	1:A:913:LYS:HE3	1.98	0.46
1:A:151:LEU:C	1:A:151:LEU:HD23	2.40	0.46
1:A:254:PHE:HB3	1:A:286:SER:OG	2.15	0.46
1:B:151:LEU:HD23	1:B:151:LEU:C	2.40	0.46
1:D:646:ILE:HD13	1:D:696:MET:HE3	1.98	0.45
1:B:219:PHE:O	1:B:244:THR:HA	2.16	0.45
1:C:694:ALA:HA	1:C:723:GLN:O	2.17	0.45
1:D:627:ALA:CB	1:D:797:VAL:HG21	2.46	0.45
1:D:694:ALA:HA	1:D:723:GLN:O	2.17	0.45
1:A:627:ALA:CB	1:A:797:VAL:HG21	2.46	0.45
1:C:151:LEU:C	1:C:151:LEU:HD23	2.41	0.45
1:C:636:LYS:HE2	1:C:638:GLU:HG3	1.98	0.45
1:B:353:ARG:HA	1:B:358:LYS:O	2.16	0.45
1:A:811:LEU:N	1:A:812:PRO:CD	2.80	0.45
1:C:207:LEU:HD23	1:C:207:LEU:O	2.17	0.45
1:B:750:LEU:O	1:B:768:GLY:HA2	2.17	0.45
1:D:750:LEU:O	1:D:768:GLY:HA2	2.17	0.45
1:D:218:LYS:HB3	1:D:258:ASP:O	2.17	0.45
1:B:728:GLY:O	1:B:731:MET:HG2	2.16	0.44
1:D:151:LEU:C	1:D:151:LEU:HD23	2.42	0.44
1:D:239:TYR:O	1:D:662:GLY:HA3	2.17	0.44
1:A:57:LEU:HD12	1:B:410:ARG:HG3	1.99	0.44
1:C:897:TRP:CG	1:C:898:PRO:HA	2.52	0.44
1:C:207:LEU:C	1:C:207:LEU:CD2	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:ALA:CB	1:C:797:VAL:HG21	2.48	0.44
1:D:219:PHE:O	1:D:244:THR:HA	2.17	0.44
1:D:726:LEU:C	1:D:726:LEU:HD23	2.43	0.44
1:D:189:LEU:HD12	1:D:189:LEU:HA	1.75	0.44
1:A:164:TYR:O	1:A:166:PRO:HD3	2.18	0.44
1:B:164:TYR:O	1:B:166:PRO:HD3	2.17	0.43
1:A:728:GLY:O	1:A:731:MET:HG2	2.19	0.43
1:A:219:PHE:O	1:A:244:THR:HA	2.18	0.43
1:B:726:LEU:C	1:B:726:LEU:HD23	2.43	0.43
1:D:935:GLU:OE1	1:D:937:ARG:NH2	2.52	0.43
1:B:705:VAL:HG11	1:B:854:GLY:HA2	1.99	0.43
1:C:353:ARG:HA	1:C:358:LYS:O	2.18	0.43
1:D:353:ARG:HA	1:D:358:LYS:O	2.19	0.43
1:C:897:TRP:HZ3	1:C:904:MET:HE1	1.84	0.43
1:B:239:TYR:O	1:B:662:GLY:HA3	2.18	0.43
1:B:347:ARG:HG2	1:B:363:LEU:HD22	2.01	0.43
1:B:694:ALA:HA	1:B:723:GLN:O	2.18	0.43
1:C:219:PHE:O	1:C:244:THR:HA	2.18	0.43
6:C:1106:PEG:H41	7:D:1330:HOH:O	2.18	0.43
1:D:240:THR:O	1:D:240:THR:CG2	2.66	0.43
1:D:164:TYR:O	1:D:166:PRO:HD3	2.18	0.43
1:A:353:ARG:HD2	7:A:1469:HOH:O	2.17	0.43
1:C:196:LEU:HD23	1:C:196:LEU:HA	1.85	0.43
1:D:777:ALA:N	1:D:778:PRO:CD	2.81	0.43
1:D:811:LEU:N	1:D:812:PRO:CD	2.82	0.43
1:B:217:ARG:HH11	1:B:217:ARG:HG2	1.83	0.42
1:C:750:LEU:O	1:C:768:GLY:HA2	2.19	0.42
1:B:777:ALA:N	1:B:778:PRO:CD	2.81	0.42
1:C:419:SER:HB2	1:C:429:LEU:HD11	2.02	0.42
1:C:777:ALA:N	1:C:778:PRO:CD	2.82	0.42
1:A:777:ALA:N	1:A:778:PRO:CD	2.82	0.42
1:B:982:PHE:CD2	6:B:3002:PEG:H21	2.55	0.42
1:A:207:LEU:HD12	1:A:219:PHE:CD1	2.54	0.42
1:A:935:GLU:OE1	1:A:937:ARG:NH1	2.51	0.42
6:C:1106:PEG:H42	1:D:543:ASN:HD22	1.85	0.42
1:C:217:ARG:HG2	1:C:217:ARG:HH11	1.84	0.42
1:A:207:LEU:HD13	1:A:233:VAL:HG13	2.02	0.42
1:C:565:SER:OG	1:D:149:ARG:HD2	2.19	0.42
1:C:811:LEU:N	1:C:812:PRO:CD	2.82	0.42
1:B:729:ALA:HB3	2:B:3003:PLG:C2A	2.49	0.42
1:B:924:ILE:O	1:B:928:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG12	1:A:336:VAL:HG12	2.01	0.42
1:A:750:LEU:O	1:A:768:GLY:HA2	2.19	0.42
1:B:207:LEU:HD12	1:B:219:PHE:CD1	2.54	0.42
1:B:627:ALA:CB	1:B:797:VAL:HG21	2.49	0.41
1:C:544:LYS:HE2	1:D:979:GLU:HB3	2.02	0.41
1:B:424:ARG:HH11	1:B:424:ARG:HG3	1.85	0.41
1:D:867:THR:OG1	1:D:901:GLY:O	2.35	0.41
1:A:419:SER:OG	1:A:429:LEU:HD11	2.20	0.41
1:B:647:PRO:HD2	1:B:696:MET:O	2.20	0.41
1:C:77:GLU:HB3	1:C:913:LYS:HE3	2.02	0.41
1:D:728:GLY:O	1:D:731:MET:HG2	2.20	0.41
1:A:867:THR:OG1	1:A:901:GLY:O	2.35	0.41
1:D:101:LEU:HD21	1:D:739:ARG:HG3	2.02	0.41
1:D:149:ARG:NH2	7:D:1202:HOH:O	2.35	0.41
1:C:645:LEU:HD23	1:C:666:GLN:HB3	2.02	0.41
1:A:699:TYR:HA	1:A:700:PRO:C	2.45	0.41
1:B:811:LEU:N	1:B:812:PRO:CD	2.83	0.41
1:C:897:TRP:CZ3	1:C:904:MET:HE1	2.56	0.41
1:B:240:THR:O	1:B:240:THR:CG2	2.69	0.41
1:B:699:TYR:HA	1:B:700:PRO:C	2.45	0.41
1:C:352:THR:HG21	1:C:362:ARG:CD	2.51	0.41
1:D:496:LEU:HD23	1:D:496:LEU:HA	1.91	0.41
1:D:699:TYR:HA	1:D:700:PRO:C	2.46	0.41
1:D:645:LEU:HD23	1:D:666:GLN:HB3	2.03	0.41
1:B:758:ILE:HG23	1:B:759:PRO:HD2	2.03	0.40
1:C:197:LEU:HD13	1:C:620:GLN:HG3	2.03	0.40
1:D:747:VAL:HG23	1:D:772:VAL:HG12	2.03	0.40
1:B:77:GLU:HB3	1:B:913:LYS:HE3	2.03	0.40
1:A:647:PRO:HD2	1:A:696:MET:O	2.22	0.40
1:C:740:PRO:HA	1:C:743:PHE:CZ	2.56	0.40
1:C:755:THR:HB	1:C:756:PHE:CD2	2.57	0.40
1:D:367:THR:O	1:D:373:ARG:HG3	2.22	0.40
1:D:599:GLU:HG3	1:D:611:VAL:HB	2.02	0.40
1:A:207:LEU:CD1	1:A:233:VAL:HG13	2.52	0.40
1:B:791:ASN:OD1	1:B:793:ASP:HB3	2.22	0.40
1:C:747:VAL:HG23	1:C:772:VAL:HG12	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:GLU:OE2	1:C:853:ARG:NH1[1_455]	1.99	0.21

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	949/984 (96%)	922 (97%)	26 (3%)	1 (0%)	48	46
1	B	952/984 (97%)	922 (97%)	29 (3%)	1 (0%)	48	46
1	C	949/984 (96%)	923 (97%)	25 (3%)	1 (0%)	48	46
1	D	952/984 (97%)	920 (97%)	31 (3%)	1 (0%)	48	46
All	All	3802/3936 (97%)	3687 (97%)	111 (3%)	4 (0%)	48	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	C	195	SER
1	D	195	SER
1	B	195	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	805/829 (97%)	802 (100%)	3 (0%)	84	89
1	B	806/829 (97%)	800 (99%)	6 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	805/829 (97%)	801 (100%)	4 (0%)	81	87
1	D	806/829 (97%)	800 (99%)	6 (1%)	76	82
All	All	3222/3316 (97%)	3203 (99%)	19 (1%)	78	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	SER
1	A	670	VAL
1	A	708	GLU
1	B	557	SER
1	B	579	ILE
1	B	707	GLU
1	B	791	ASN
1	B	856	ARG
1	B	896	SER
1	C	52	LEU
1	C	496	LEU
1	C	557	SER
1	C	791	ASN
1	D	189	LEU
1	D	419	SER
1	D	557	SER
1	D	707	GLU
1	D	856	ARG
1	D	896	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	399	HIS
1	A	563	ASN
1	A	620	GLN
1	A	928	GLN
1	B	399	HIS
1	B	459	ASN
1	B	587	GLN
1	B	589	GLN
1	B	959	HIS

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Mol	Chain	Res	Type
1	C	441	GLN
1	C	592	GLN
1	C	928	GLN
1	D	459	ASN
1	D	526	ASN
1	D	587	GLN
1	D	589	GLN
1	D	928	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLG	B	3003	-	20,20,20	2.76	3 (15%)	26,28,28	2.21	8 (30%)
5	BCT	A	1105	-	3,3,3	1.62	1 (33%)	2,3,3	0.38	0
2	PLG	D	1101	-	20,20,20	2.51	6 (30%)	26,28,28	2.40	9 (34%)
4	GOL	A	1104	-	5,5,5	0.55	0	5,5,5	1.18	0
6	PEG	C	1106	-	6,6,6	0.71	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	C	1104	-	6,6,6	0.64	0	5,5,5	0.62	0
3	EDO	A	1102	-	3,3,3	0.70	0	2,2,2	0.27	0
4	GOL	C	1105	-	5,5,5	0.58	0	5,5,5	0.20	0
6	PEG	D	1103	-	6,6,6	0.54	0	5,5,5	0.68	0
3	EDO	D	1102	-	3,3,3	0.43	0	2,2,2	1.11	0
4	GOL	A	1103	-	5,5,5	0.45	0	5,5,5	0.59	0
4	GOL	C	1103	-	5,5,5	0.64	0	5,5,5	0.74	0
6	PEG	B	3002	-	6,6,6	0.60	0	5,5,5	0.67	0
2	PLG	A	1101	-	20,20,20	2.06	3 (15%)	26,28,28	2.42	13 (50%)
3	EDO	C	1102	-	3,3,3	0.45	0	2,2,2	0.30	0
3	EDO	B	3001	-	3,3,3	0.40	0	2,2,2	0.45	0
4	GOL	B	3004	-	5,5,5	0.26	0	5,5,5	0.31	0
2	PLG	C	1101	-	20,20,20	2.15	9 (45%)	26,28,28	2.03	9 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	B	3003	-	-	3/12/12/12	0/1/1/1
2	PLG	D	1101	-	-	3/12/12/12	0/1/1/1
4	GOL	A	1104	-	-	3/4/4/4	-
6	PEG	C	1106	-	-	2/4/4/4	-
6	PEG	C	1104	-	-	3/4/4/4	-
3	EDO	A	1102	-	-	1/1/1/1	-
4	GOL	C	1105	-	-	2/4/4/4	-
6	PEG	D	1103	-	-	3/4/4/4	-
3	EDO	D	1102	-	-	1/1/1/1	-
4	GOL	A	1103	-	-	2/4/4/4	-
4	GOL	C	1103	-	-	4/4/4/4	-
6	PEG	B	3002	-	-	3/4/4/4	-
2	PLG	A	1101	-	-	3/12/12/12	0/1/1/1
3	EDO	C	1102	-	-	0/1/1/1	-
3	EDO	B	3001	-	-	1/1/1/1	-
4	GOL	B	3004	-	-	3/4/4/4	-
2	PLG	C	1101	-	-	2/12/12/12	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3003	PLG	C3-C2	7.66	1.48	1.41
2	B	3003	PLG	C5-C4	6.83	1.50	1.40
2	A	1101	PLG	C3-C2	6.36	1.47	1.41
2	D	1101	PLG	C3-C2	6.03	1.47	1.41
2	B	3003	PLG	C3-C4	6.03	1.48	1.40
2	D	1101	PLG	C5-C4	5.76	1.48	1.40
2	D	1101	PLG	C3-C4	4.78	1.47	1.40
2	A	1101	PLG	C5-C4	4.33	1.46	1.40
2	A	1101	PLG	C3-C4	3.89	1.45	1.40
2	C	1101	PLG	C3-C2	3.85	1.45	1.41
2	C	1101	PLG	C5-C4	3.37	1.45	1.40
2	C	1101	PLG	P-OP3	-3.19	1.43	1.54
2	C	1101	PLG	P-OP1	-3.13	1.40	1.50
2	C	1101	PLG	P-OP2	-2.91	1.44	1.54
2	C	1101	PLG	C3-C4	2.85	1.44	1.40
2	C	1101	PLG	OXT-C	-2.74	1.21	1.30
2	D	1101	PLG	P-OP3	-2.70	1.44	1.54
2	D	1101	PLG	P-OP2	-2.54	1.45	1.54
2	C	1101	PLG	O3-C3	-2.50	1.31	1.36
2	D	1101	PLG	OXT-C	-2.23	1.23	1.30
5	A	1105	BCT	O1-C	2.19	1.33	1.25
2	C	1101	PLG	C2-N1	-2.09	1.30	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	PLG	C4A-N-CA	7.76	121.76	112.72
2	B	3003	PLG	C4A-N-CA	6.75	120.58	112.72
2	A	1101	PLG	OP3-P-OP4	-4.57	94.75	106.67
2	A	1101	PLG	OP4-P-OP1	4.47	118.52	106.44
2	D	1101	PLG	C4A-C4-C5	4.47	124.61	119.75
2	A	1101	PLG	C4A-C4-C3	4.08	125.40	119.98
2	C	1101	PLG	C4A-N-CA	3.97	117.34	112.72
2	A	1101	PLG	C4A-N-CA	3.93	117.30	112.72
2	B	3003	PLG	OP3-P-OP4	-3.84	96.65	106.67
2	C	1101	PLG	C2A-C2-C3	-3.82	116.33	120.80
2	D	1101	PLG	OP4-P-OP1	-3.56	96.82	106.44
2	C	1101	PLG	OP2-P-OP4	-3.54	97.43	106.67
2	C	1101	PLG	C2A-C2-N1	3.39	124.03	117.64
2	B	3003	PLG	C3-C4-C5	-3.32	115.72	118.73
2	A	1101	PLG	OP2-P-OP4	-3.00	98.84	106.67
2	B	3003	PLG	OP3-P-OP2	2.94	118.81	107.80
2	A	1101	PLG	O3-C3-C4	2.93	126.67	118.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	PLG	OP3-P-OP1	2.84	121.91	110.83
2	C	1101	PLG	OP2-P-OP1	2.77	121.61	110.83
2	D	1101	PLG	C6-N1-C2	2.75	124.18	119.20
2	B	3003	PLG	C6-C5-C4	2.67	120.08	118.06
2	A	1101	PLG	C6-C5-C4	2.66	120.07	118.06
2	A	1101	PLG	C3-C4-C5	-2.61	116.36	118.73
2	A	1101	PLG	OP4-C5A-C5	2.60	114.24	109.36
2	D	1101	PLG	OP4-C5A-C5	2.57	114.17	109.36
2	C	1101	PLG	OP4-C5A-C5	2.56	114.16	109.36
2	D	1101	PLG	OP3-P-OP1	2.53	120.70	110.83
2	C	1101	PLG	C3-C4-C5	-2.51	116.45	118.73
2	A	1101	PLG	C4-C4A-N	2.49	116.11	111.50
2	B	3003	PLG	C4A-C4-C3	2.49	123.28	119.98
2	D	1101	PLG	C4-C4A-N	-2.47	106.95	111.50
2	C	1101	PLG	C6-N1-C2	2.41	123.56	119.20
2	C	1101	PLG	C4A-C4-C3	2.39	123.16	119.98
2	B	3003	PLG	C4-C4A-N	2.34	115.82	111.50
2	A	1101	PLG	C2A-C2-C3	-2.33	118.07	120.80
2	B	3003	PLG	C6-N1-C2	2.25	123.28	119.20
2	D	1101	PLG	C2A-C2-N1	2.16	121.70	117.64
2	D	1101	PLG	C2A-C2-C3	-2.11	118.32	120.80
2	A	1101	PLG	C6-N1-C2	2.08	122.97	119.20

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	PLG	C3-C4-C4A-N
2	A	1101	PLG	C5-C4-C4A-N
2	B	3003	PLG	C5-C4-C4A-N
2	C	1101	PLG	C3-C4-C4A-N
2	C	1101	PLG	C5-C4-C4A-N
4	A	1103	GOL	C1-C2-C3-O3
4	A	1104	GOL	O1-C1-C2-C3
4	B	3004	GOL	O1-C1-C2-O2
4	B	3004	GOL	O1-C1-C2-C3
4	C	1103	GOL	C1-C2-C3-O3
4	C	1105	GOL	C1-C2-C3-O3
6	C	1106	PEG	O1-C1-C2-O2
6	D	1103	PEG	O1-C1-C2-O2
6	B	3002	PEG	O1-C1-C2-O2
4	A	1103	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	1104	GOL	O1-C1-C2-O2
4	C	1103	GOL	O2-C2-C3-O3
4	C	1105	GOL	O2-C2-C3-O3
6	C	1104	PEG	O2-C3-C4-O4
6	C	1106	PEG	O2-C3-C4-O4
2	D	1101	PLG	C5-C4-C4A-N
3	D	1102	EDO	O1-C1-C2-O2
6	C	1104	PEG	O1-C1-C2-O2
4	B	3004	GOL	O2-C2-C3-O3
6	C	1104	PEG	C4-C3-O2-C2
4	C	1103	GOL	O1-C1-C2-C3
6	D	1103	PEG	C1-C2-O2-C3
2	B	3003	PLG	C3-C4-C4A-N
2	B	3003	PLG	C4-C4A-N-CA
6	B	3002	PEG	C4-C3-O2-C2
3	B	3001	EDO	O1-C1-C2-O2
2	A	1101	PLG	C4-C4A-N-CA
4	A	1104	GOL	O2-C2-C3-O3
3	A	1102	EDO	O1-C1-C2-O2
2	D	1101	PLG	C4-C4A-N-CA
6	D	1103	PEG	C4-C3-O2-C2
2	D	1101	PLG	C3-C4-C4A-N
6	B	3002	PEG	C1-C2-O2-C3
4	C	1103	GOL	O1-C1-C2-O2

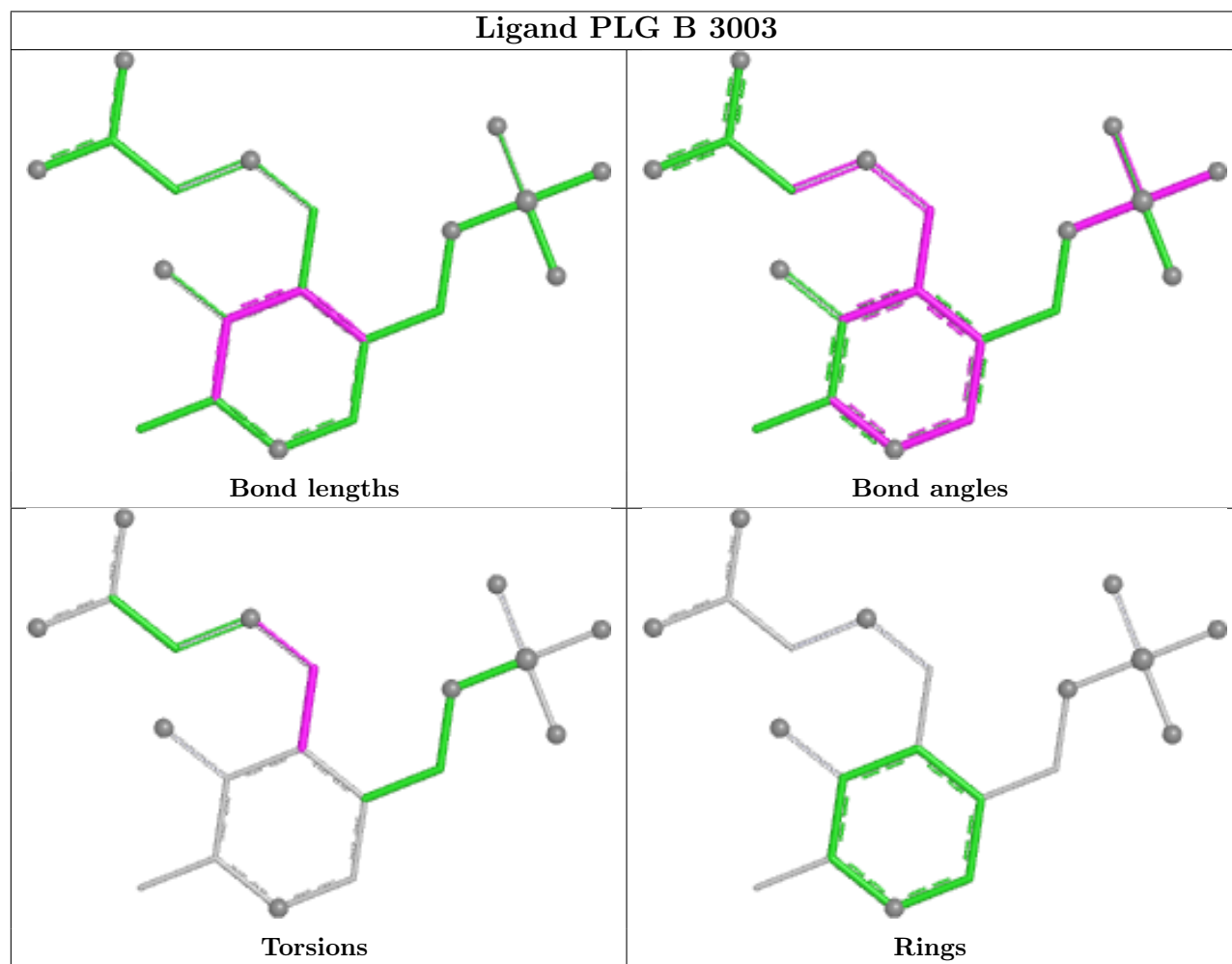
There are no ring outliers.

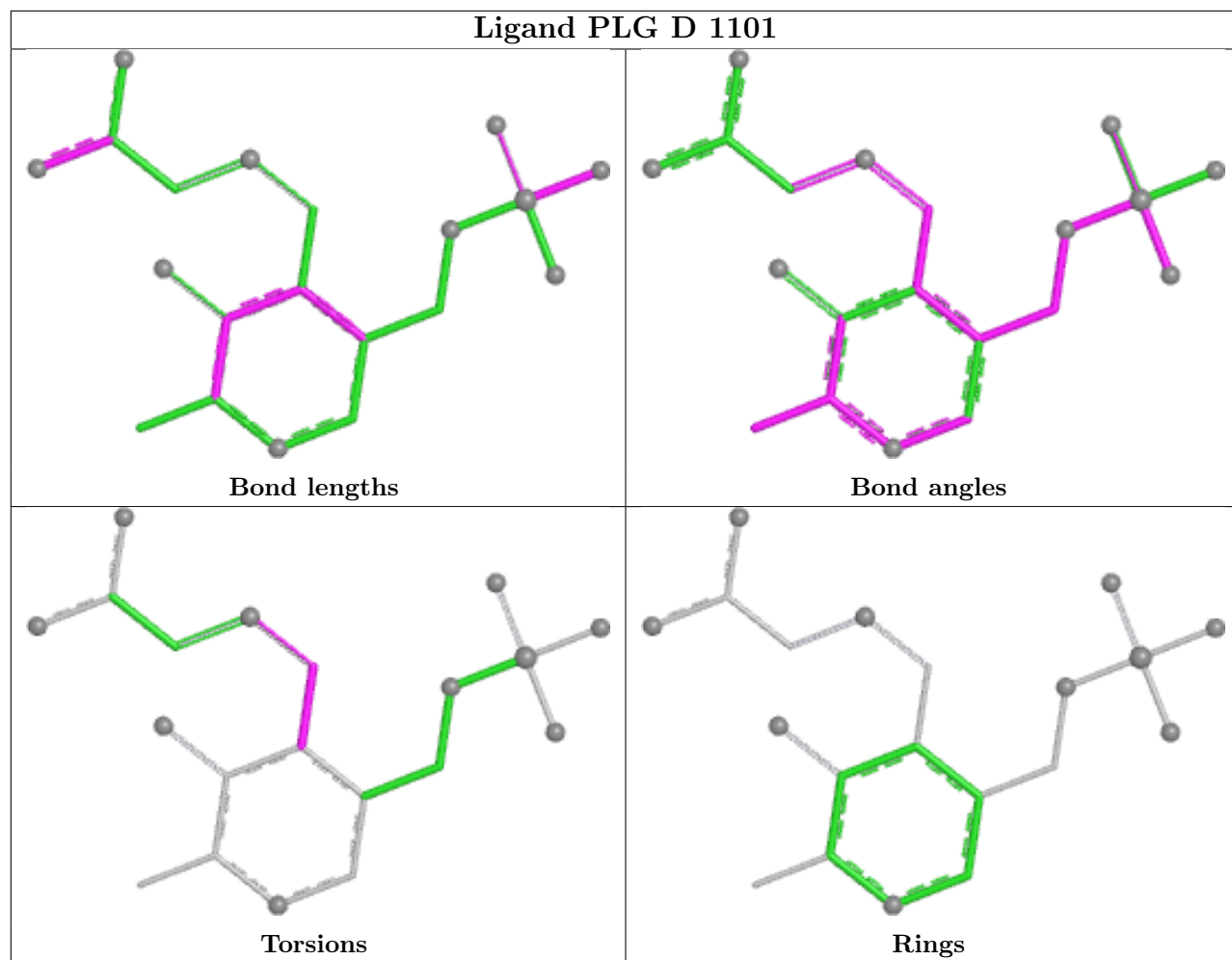
4 monomers are involved in 6 short contacts:

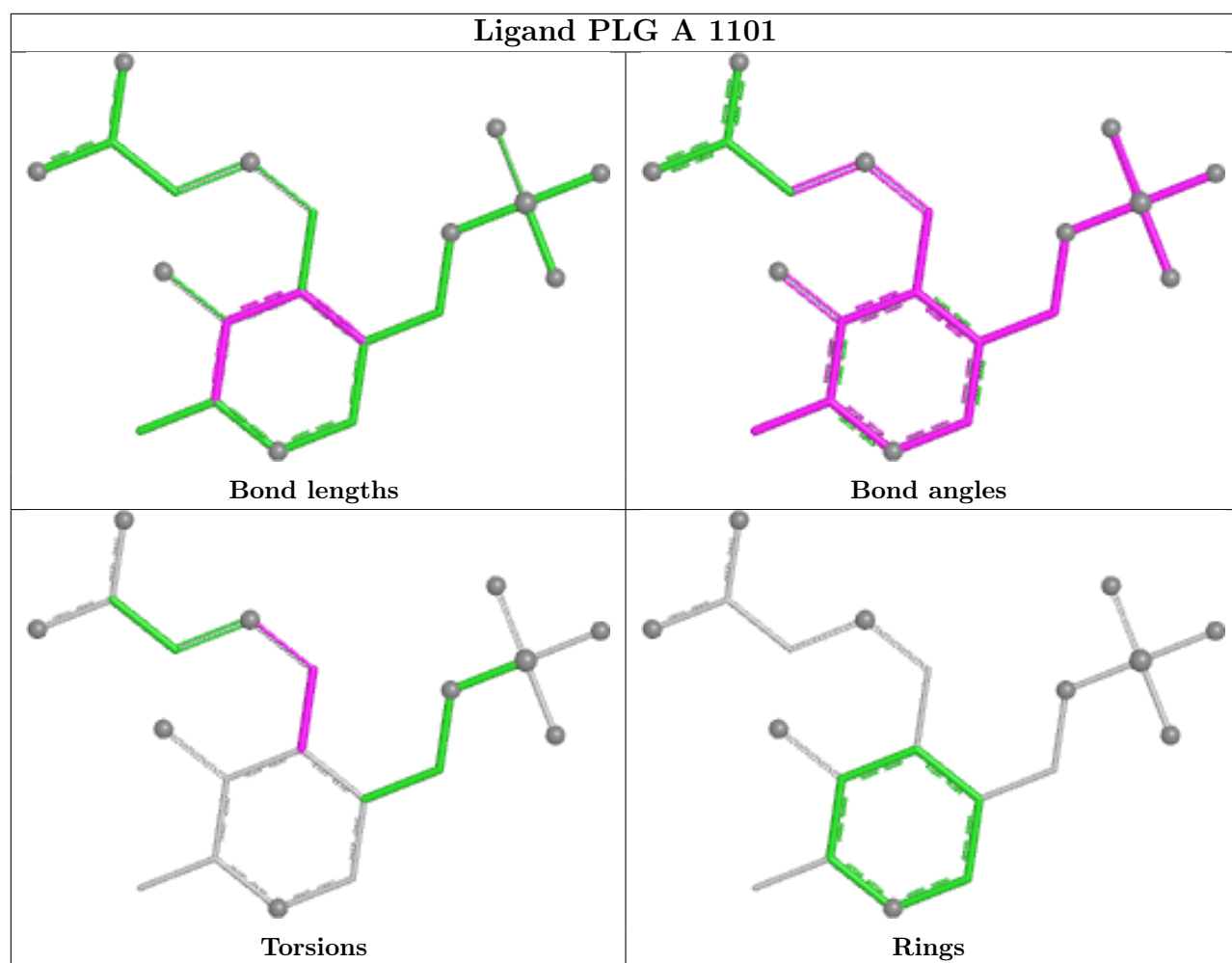
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3003	PLG	1	0
6	C	1106	PEG	3	0
6	D	1103	PEG	2	0
6	B	3002	PEG	1	0

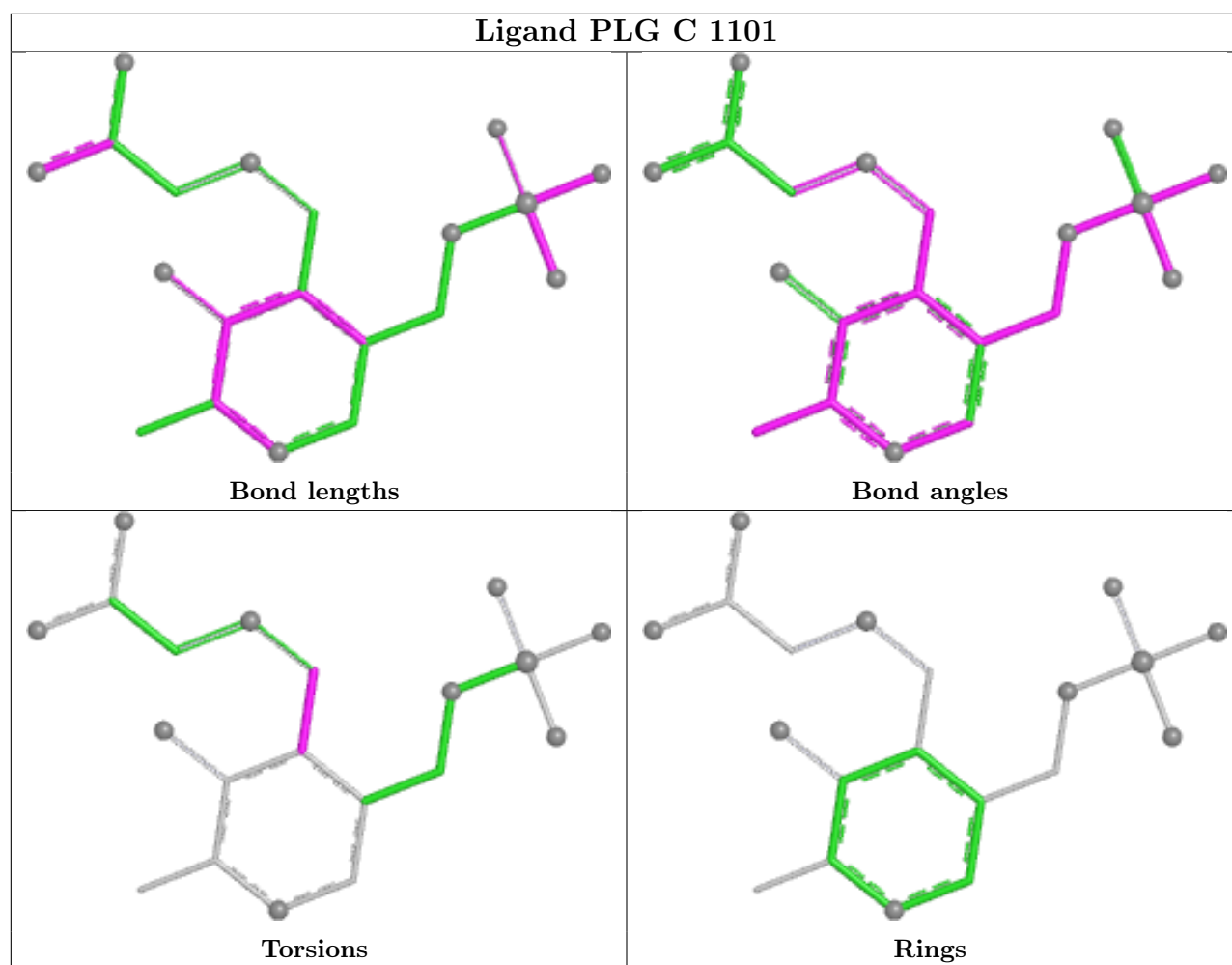
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	953/984 (96%)	-0.04	8 (0%) 82 82	28, 41, 62, 99	0
1	B	954/984 (96%)	0.33	16 (1%) 69 68	32, 54, 80, 99	0
1	C	953/984 (96%)	-0.04	8 (0%) 82 82	26, 40, 61, 92	0
1	D	954/984 (96%)	0.24	14 (1%) 72 71	31, 52, 80, 99	0
All	All	3814/3936 (96%)	0.12	46 (1%) 76 76	26, 46, 76, 99	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	959	HIS	4.6
1	A	788	LEU	3.6
1	A	1005	MET	3.6
1	A	791	ASN	3.6
1	A	959	HIS	3.5
1	D	164	TYR	3.3
1	D	897	TRP	3.2
1	C	788	LEU	3.2
1	D	992	ILE	3.2
1	D	462	LEU	3.1
1	B	243	LEU	2.9
1	D	980	ASN	2.9
1	D	648	LYS	2.8
1	D	52	LEU	2.7
1	D	1004	PRO	2.6
1	D	243	LEU	2.5
1	B	629	ILE	2.5
1	B	1004	PRO	2.5
1	C	791	ASN	2.5
1	B	164	TYR	2.5
1	C	49	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	2.4
1	B	634	ASN	2.4
1	A	790	ARG	2.4
1	A	446	VAL	2.3
1	B	980	ASN	2.3
1	A	496	LEU	2.3
1	B	259	VAL	2.2
1	B	83	GLY	2.2
1	B	650	ALA	2.2
1	B	722	GLY	2.2
1	B	979	GLU	2.2
1	B	992	ILE	2.2
1	D	703	ASN	2.2
1	D	679	VAL	2.2
1	B	793	ASP	2.2
1	B	353	ARG	2.2
1	C	790	ARG	2.2
1	D	53	LEU	2.2
1	B	91	ILE	2.1
1	C	1005	MET	2.1
1	D	872	LYS	2.1
1	A	634	ASN	2.1
1	C	164	TYR	2.0
1	C	496	LEU	2.0
1	D	218	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

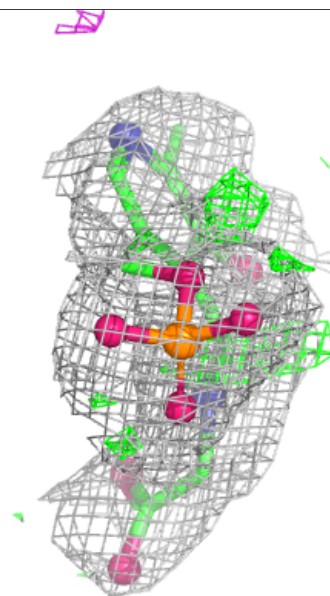
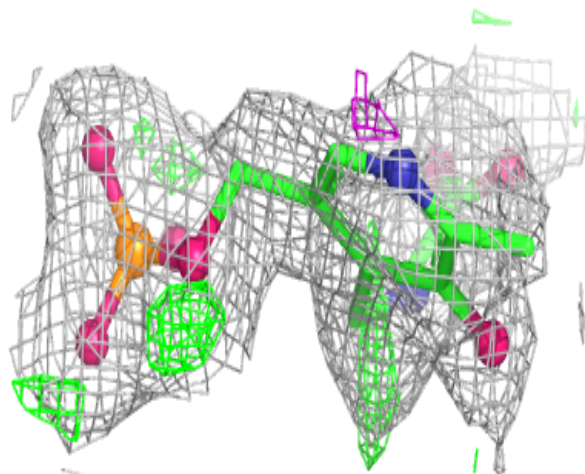
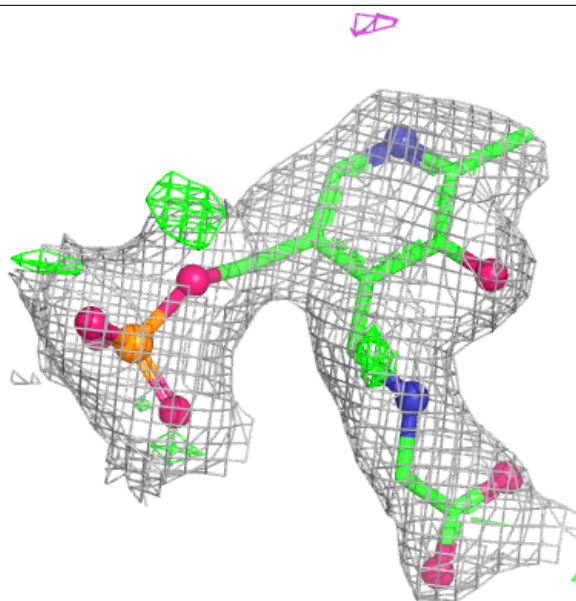
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	1102	4/4	0.63	0.25	59,59,61,62	0
6	PEG	C	1106	7/7	0.69	0.26	63,65,68,69	0
6	PEG	B	3002	7/7	0.73	0.21	54,57,67,70	0
5	BCT	A	1105	4/4	0.82	0.13	53,56,62,64	0
6	PEG	D	1103	7/7	0.82	0.18	52,64,65,71	0
6	PEG	C	1104	7/7	0.83	0.16	46,58,68,70	0
3	EDO	D	1102	4/4	0.83	0.19	40,41,45,47	0
4	GOL	C	1103	6/6	0.83	0.16	45,58,58,62	0
4	GOL	A	1103	6/6	0.86	0.14	55,62,65,67	0
4	GOL	B	3004	6/6	0.89	0.13	48,50,53,59	0
4	GOL	C	1105	6/6	0.90	0.14	39,44,45,50	0
3	EDO	B	3001	4/4	0.90	0.12	63,63,63,64	0
2	PLG	D	1101	20/20	0.91	0.12	42,60,71,73	0
3	EDO	C	1102	4/4	0.91	0.12	57,60,60,61	0
4	GOL	A	1104	6/6	0.93	0.13	49,53,56,63	0
2	PLG	B	3003	20/20	0.94	0.10	44,58,65,66	0
2	PLG	C	1101	20/20	0.95	0.09	25,32,49,52	0
2	PLG	A	1101	20/20	0.97	0.08	26,33,49,54	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.

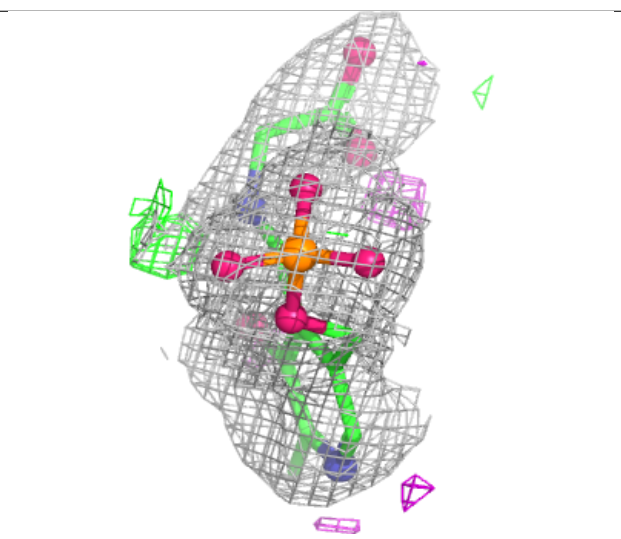
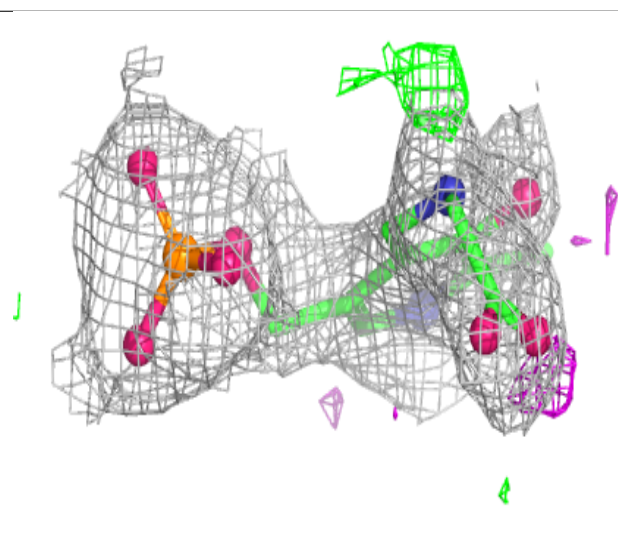
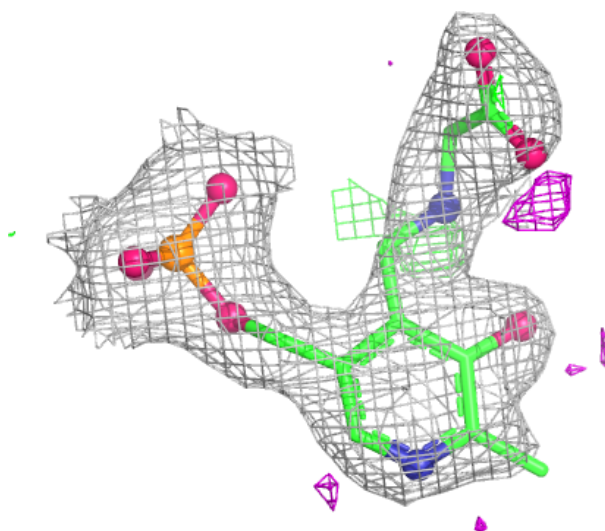
Electron density around PLG D 1101:

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



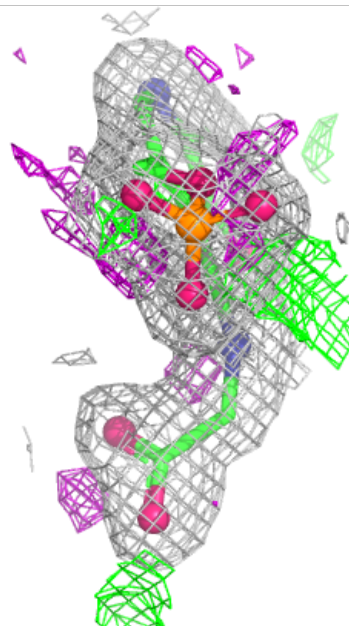
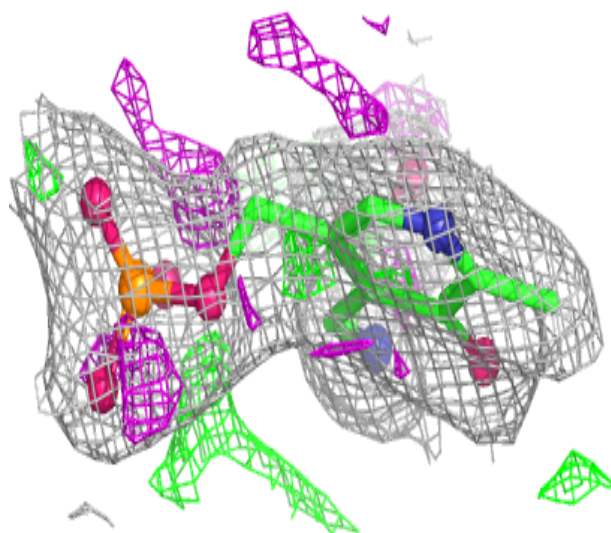
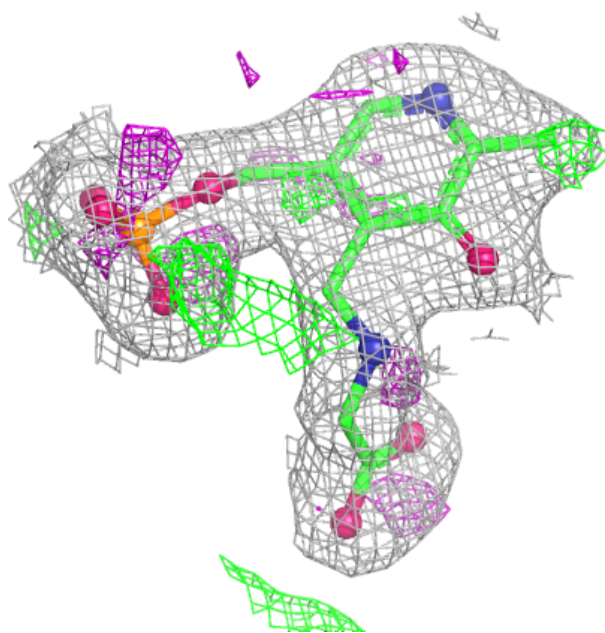
Electron density around PLG B 3003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



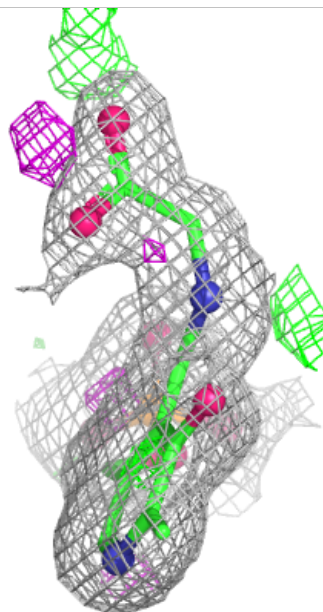
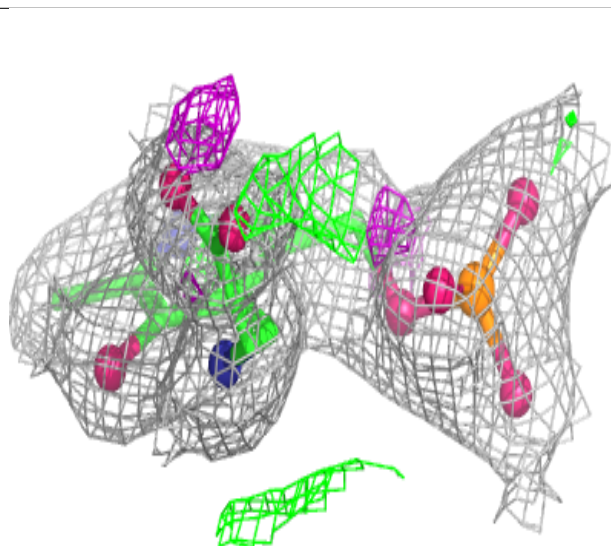
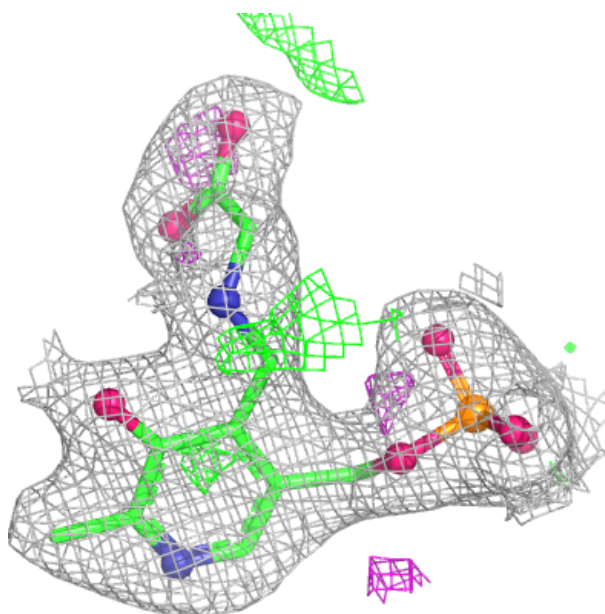
Electron density around PLG C 1101:

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



Electron density around PLG A 1101:

$2mF_o-DF_c$ (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.