



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:18 AM UTC

PDB ID : 9DZ7 / pdb\_00009dz7  
Title : Structure of ALAS bound to glycine from *S. cerevisiae*  
Authors : Tran, J.U.; Brown, B.L.  
Deposited on : 2024-10-15  
Resolution : 2.49 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

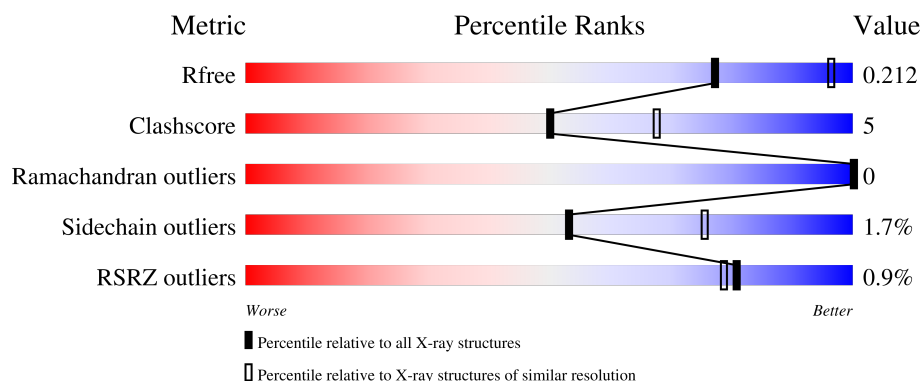
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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  $\geq 3$ , 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	491	<div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	B	491	<div> <div>82%</div> <div>11%</div> <div>• 7%</div> </div>
1	C	491	<div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	D	491	<div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div>
1	E	491	<div> <div>88%</div> <div>8%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	491	 85% 9% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	E	604	-	-	X	-

## 2 Entry composition [i](#)

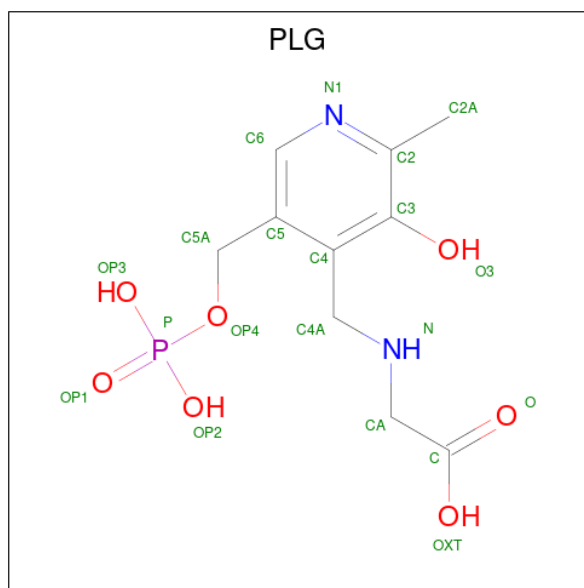
There are 4 unique types of molecules in this entry. The entry contains 22739 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5-aminolevulinate synthase, mitochondrial.

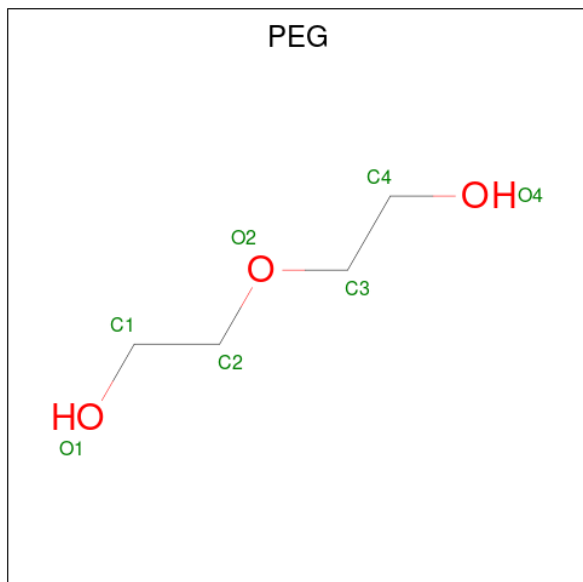
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	468	Total	C	N	O	S	0	0	0
			3639	2305	638	682	14			
1	A	476	Total	C	N	O	S	0	0	0
			3686	2331	647	694	14			
1	C	473	Total	C	N	O	S	0	0	0
			3667	2321	643	689	14			
1	E	472	Total	C	N	O	S	0	0	0
			3658	2316	642	686	14			
1	D	464	Total	C	N	O	S	0	0	0
			3613	2288	633	678	14			
1	B	459	Total	C	N	O	S	0	0	0
			3565	2259	625	667	14			

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL-METHANE] (CCD ID: PLG) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



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

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



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	88	Total O 88 88	0	0
4	A	125	Total O 125 125	0	0

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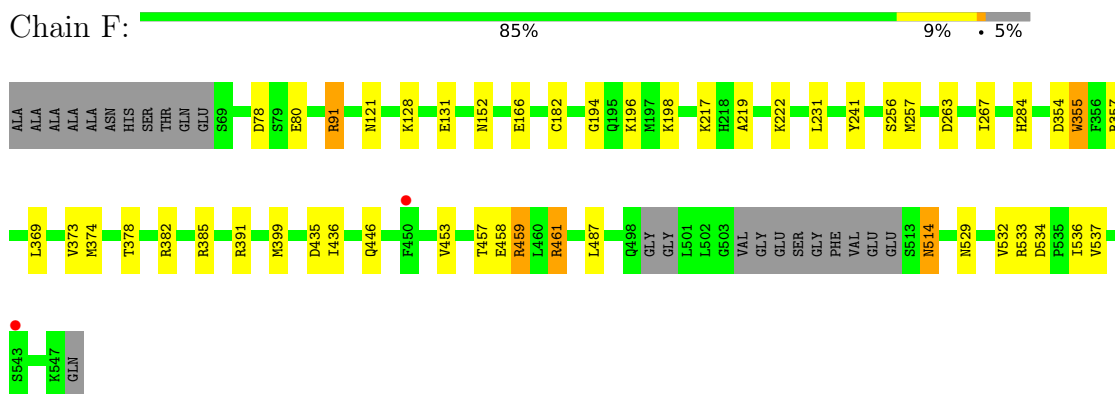
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	101	Total 101	O 101	0	0
4	E	119	Total 119	O 119	0	0
4	D	111	Total 111	O 111	0	0
4	B	86	Total 86	O 86	0	0

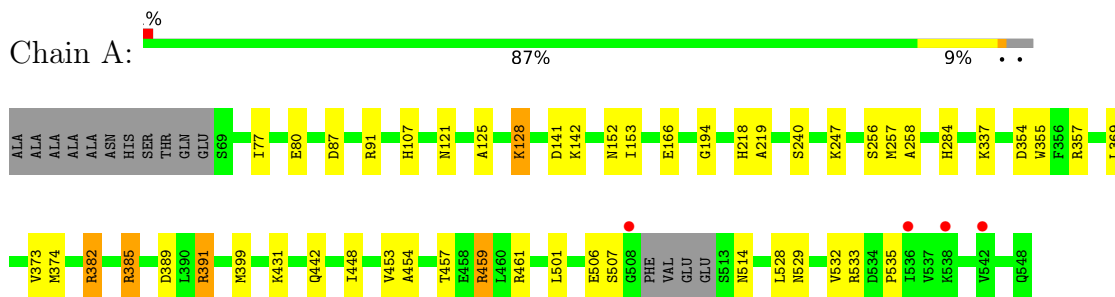
### 3 Residue-property plots

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.

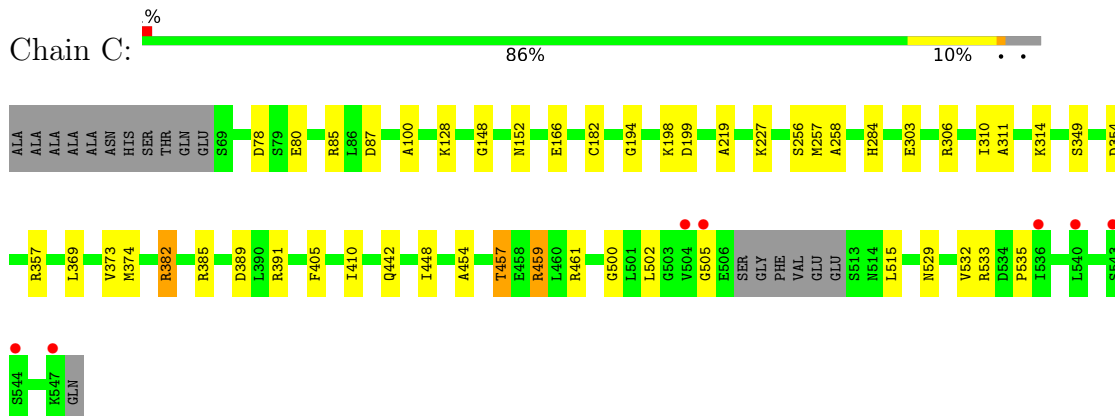
- Molecule 1: 5-aminolevulinate synthase, mitochondrial



- Molecule 1: 5-aminolevulinate synthase, mitochondrial

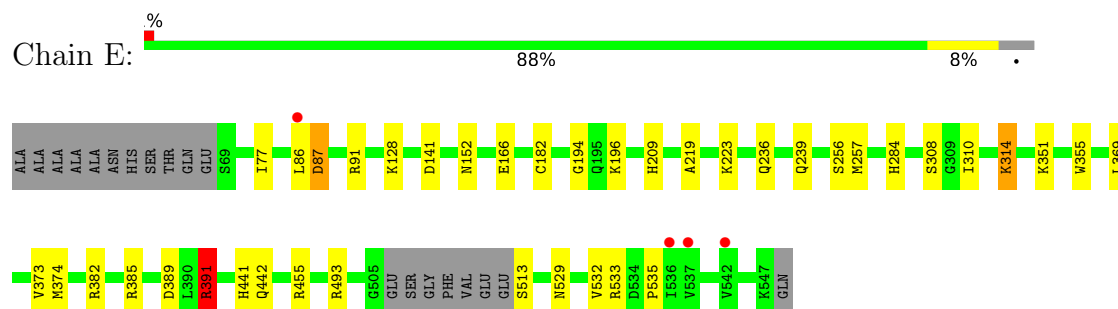


- Molecule 1: 5-aminolevulinate synthase, mitochondrial

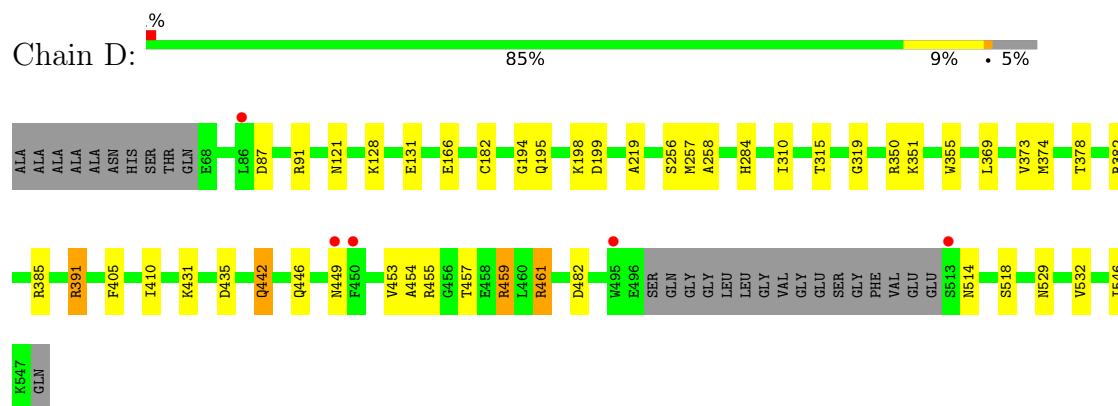




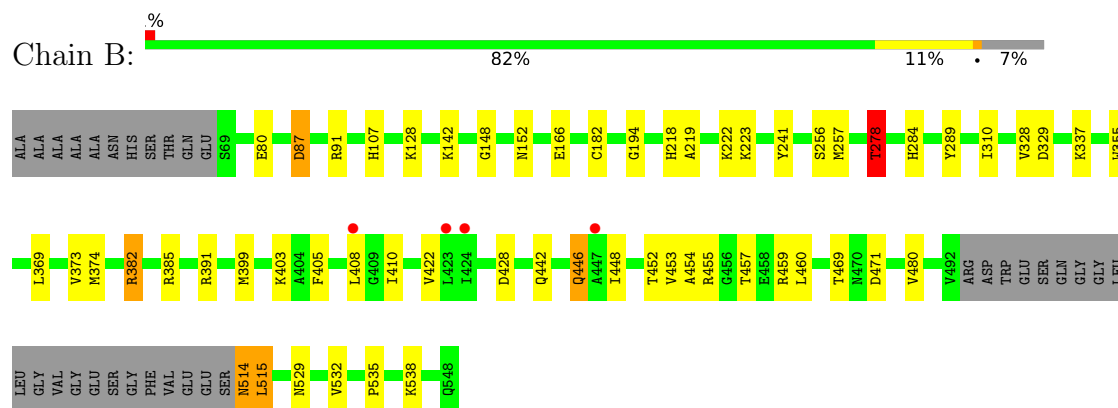
- Molecule 1: 5-aminolevulinate synthase, mitochondrial



- Molecule 1: 5-aminolevulinate synthase, mitochondrial



- Molecule 1: 5-aminolevulinate synthase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.67Å 112.52Å 117.39Å 115.76° 98.31° 91.49°	Depositor
Resolution (Å)	48.91 – 2.49 48.91 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.91-2.49) 97.2 (48.91-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.168 , 0.207 0.176 , 0.212	Depositor DCC
$R_{free}$ test set	5044 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PEG

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	0.58	0/3762	0.98	2/5095 (0.0%)
1	B	0.57	0/3639	0.99	5/4930 (0.1%)
1	C	0.59	0/3743	0.98	1/5070 (0.0%)
1	D	0.58	0/3689	0.97	3/4998 (0.1%)
1	E	0.60	0/3734	1.02	5/5058 (0.1%)
1	F	0.56	0/3714	0.96	1/5030 (0.0%)
All	All	0.58	0/22281	0.98	17/30181 (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	4
1	B	0	3
1	C	0	4
1	D	0	5
1	E	0	2
1	F	0	3
All	All	0	21

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	391	ARG	NE-CZ-NH2	11.76	129.79	119.20
1	E	391	ARG	NE-CZ-NH1	-11.53	109.97	121.50
1	E	391	ARG	CD-NE-CZ	7.67	135.13	124.40
1	B	278	THR	CB-CA-C	7.58	123.59	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	389	ASP	CA-CB-CG	6.68	119.28	112.60
1	F	355	TRP	CA-CB-CG	6.53	126.00	113.60
1	A	389	ASP	CA-CB-CG	6.48	119.08	112.60
1	E	389	ASP	CA-CB-CG	5.98	118.58	112.60
1	D	482	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	428	ASP	CA-CB-CG	5.74	118.33	112.60
1	E	239	GLN	CB-CG-CD	-5.73	102.86	112.60
1	D	391	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	B	403	LYS	CB-CG-CD	5.48	123.90	111.30
1	D	258	ALA	N-CA-CB	-5.29	103.56	110.59
1	B	278	THR	N-CA-CB	-5.27	101.83	110.68
1	A	391	ARG	NE-CZ-NH2	-5.07	114.63	119.20
1	B	446	GLN	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ARG	Sidechain
1	A	385	ARG	Sidechain
1	A	391	ARG	Sidechain
1	A	459	ARG	Sidechain
1	B	382	ARG	Sidechain
1	B	391	ARG	Sidechain
1	B	459	ARG	Sidechain
1	C	382	ARG	Sidechain
1	C	391	ARG	Sidechain
1	C	459	ARG	Sidechain
1	C	533	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	391	ARG	Sidechain
1	D	455	ARG	Sidechain
1	D	459	ARG	Sidechain
1	D	461	ARG	Sidechain
1	E	391	ARG	Sidechain
1	E	493	ARG	Sidechain
1	F	391	ARG	Sidechain
1	F	459	ARG	Sidechain
1	F	461	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	3686	0	3679	40	0
1	B	3565	0	3571	49	0
1	C	3667	0	3663	39	0
1	D	3613	0	3607	31	0
1	E	3658	0	3657	33	0
1	F	3639	0	3638	44	0
2	A	20	0	12	3	0
2	B	20	0	12	6	0
2	C	20	0	12	2	0
2	D	20	0	12	4	0
2	E	20	0	12	5	0
2	F	20	0	12	3	0
3	A	42	0	60	1	0
3	B	7	0	10	0	0
3	C	28	0	40	6	0
3	D	7	0	10	0	0
3	E	77	0	110	12	0
4	A	125	0	0	11	0
4	B	86	0	0	4	0
4	C	101	0	0	10	1
4	D	111	0	0	8	0
4	E	119	0	0	11	0
4	F	88	0	0	8	1
All	All	22739	0	22117	234	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 5.

All (234) 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:469:THR:HG23	1:B:471:ASP:OD1	1.61	1.01
4:A:793:HOH:O	1:B:152:ASN:HB2	1.64	0.96
2:B:601:PLG:O3	2:B:601:PLG:HA1	1.66	0.95
2:D:601:PLG:HA2	4:D:717:HOH:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:446:GLN:HB3	4:F:745:HOH:O	1.70	0.90
1:B:399:MET:HE2	1:B:514:ASN:OD1	1.74	0.87
1:C:357:ARG:NH2	1:D:91:ARG:O	2.08	0.86
1:F:152:ASN:HB2	4:F:765:HOH:O	1.74	0.86
2:B:601:PLG:O3	2:B:601:PLG:CA	2.25	0.84
1:F:399:MET:HE2	1:F:514:ASN:OD1	1.76	0.83
1:C:448:ILE:HD11	1:C:461:ARG:HB2	1.60	0.82
1:F:436:ILE:CD1	1:F:487:LEU:HD11	2.10	0.81
2:E:601:PLG:C4A	4:E:706:HOH:O	2.29	0.80
1:E:236:GLN:NE2	4:E:701:HOH:O	2.13	0.80
1:F:80:GLU:HG2	1:E:355:TRP:HE1	1.44	0.80
1:F:217:LYS:HD3	4:F:771:HOH:O	1.80	0.79
1:F:436:ILE:HD12	1:F:487:LEU:HD11	1.65	0.78
1:F:222:LYS:HB3	4:F:768:HOH:O	1.86	0.75
1:C:314:LYS:HE2	3:C:602:PEG:H41	1.68	0.74
1:A:141:ASP:HB3	4:A:728:HOH:O	1.88	0.74
1:F:357:ARG:NH2	1:E:91:ARG:O	2.20	0.74
1:A:357:ARG:NH2	1:B:91:ARG:O	2.22	0.73
1:C:128:LYS:HE2	3:C:605:PEG:H31	1.69	0.73
1:C:454:ALA:O	1:C:457:THR:HG22	1.89	0.73
2:D:601:PLG:CA	4:D:717:HOH:O	2.32	0.72
1:E:86:LEU:HD21	4:E:809:HOH:O	1.90	0.72
1:F:196:LYS:HG3	1:F:355:TRP:CH2	2.25	0.72
1:C:257:MET:HB2	4:C:776:HOH:O	1.91	0.71
1:C:303:GLU:OE1	1:C:306:ARG:NH1	2.25	0.70
1:A:166:GLU:OE2	1:A:385:ARG:NH2	2.24	0.70
1:F:78:ASP:OD1	1:E:351:LYS:HE3	1.92	0.69
1:C:448:ILE:CD1	1:C:461:ARG:HB2	2.21	0.69
1:B:278:THR:HG22	1:B:329:ASP:H	1.57	0.69
1:B:148:GLY:C	4:B:706:HOH:O	2.36	0.68
1:E:166:GLU:OE2	1:E:385:ARG:NH2	2.25	0.68
2:D:601:PLG:O3	2:D:601:PLG:N	2.26	0.67
1:F:453:VAL:HG22	1:F:457:THR:OG1	1.94	0.66
1:B:422:VAL:HG23	1:B:460:LEU:HB2	1.78	0.65
1:B:337:LYS:HZ2	2:B:601:PLG:H	1.42	0.65
1:A:453:VAL:HG12	1:A:457:THR:OG1	1.97	0.65
1:D:453:VAL:HG12	1:D:457:THR:OG1	1.97	0.65
2:E:601:PLG:H4A2	4:E:706:HOH:O	1.93	0.64
1:E:382:ARG:HD2	4:E:788:HOH:O	1.98	0.64
1:D:182:CYS:HB3	2:D:601:PLG:OP4	1.97	0.63
1:A:453:VAL:HG11	1:A:459:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG2	1:B:355:TRP:HE1	1.65	0.62
1:B:453:VAL:HG12	1:B:457:THR:OG1	1.99	0.62
1:C:198:LYS:HD3	4:C:736:HOH:O	2.00	0.61
1:B:310:ILE:HD11	1:B:535:PRO:HG3	1.82	0.61
1:A:128:LYS:HD2	1:A:128:LYS:C	2.26	0.61
1:D:369:LEU:HB2	1:D:374:MET:HE3	1.83	0.60
1:F:182:CYS:HB3	2:F:601:PLG:OP4	2.01	0.60
1:B:422:VAL:CG2	1:B:460:LEU:HB2	2.32	0.60
1:A:369:LEU:HB2	1:A:374:MET:HE3	1.83	0.60
1:D:166:GLU:OE2	1:D:382:ARG:NH1	2.33	0.60
1:B:446:GLN:O	4:B:701:HOH:O	2.17	0.60
2:B:601:PLG:HA1	2:B:601:PLG:HO3	1.65	0.60
1:A:77:ILE:HD12	1:B:355:TRP:CD2	2.37	0.59
1:B:256:SER:HB3	1:B:284:HIS:CD2	2.36	0.59
1:C:152:ASN:HB2	4:D:797:HOH:O	2.01	0.59
1:E:441:HIS:HD2	4:E:805:HOH:O	1.85	0.59
1:C:78:ASP:OD1	1:D:351:LYS:HD3	2.04	0.57
1:D:256:SER:HB3	1:D:284:HIS:CD2	2.39	0.56
1:B:529:ASN:O	1:B:532:VAL:HG22	2.04	0.56
1:F:458:GLU:OE2	4:F:701:HOH:O	2.18	0.56
1:F:529:ASN:O	1:F:532:VAL:HG22	2.05	0.56
1:A:247:LYS:HE2	4:A:702:HOH:O	2.05	0.56
1:B:222:LYS:HE3	1:B:241:TYR:OH	2.05	0.56
1:F:369:LEU:HB2	1:F:374:MET:HE3	1.88	0.56
1:A:256:SER:OG	1:A:257:MET:HE2	2.05	0.56
3:E:608:PEG:H11	4:E:800:HOH:O	2.05	0.56
1:F:91:ARG:NH2	4:F:705:HOH:O	2.39	0.56
1:F:166:GLU:OE2	1:F:382:ARG:NH1	2.39	0.55
1:E:314:LYS:HE3	3:E:605:PEG:H21	1.87	0.55
1:D:529:ASN:O	1:D:532:VAL:HG22	2.05	0.55
1:F:166:GLU:OE1	1:F:385:ARG:NH2	2.23	0.55
1:F:256:SER:HB3	1:F:284:HIS:CD2	2.40	0.55
1:E:369:LEU:HB2	1:E:374:MET:HE3	1.89	0.55
1:C:529:ASN:O	1:C:532:VAL:HG22	2.06	0.55
1:F:194:GLY:O	1:F:198:LYS:HE2	2.07	0.54
1:A:501:LEU:HD13	3:A:606:PEG:H31	1.89	0.54
1:D:453:VAL:HG11	1:D:459:ARG:NH1	2.22	0.54
1:C:369:LEU:HB2	1:C:374:MET:HE3	1.90	0.54
1:F:399:MET:CE	1:F:514:ASN:OD1	2.54	0.54
1:E:256:SER:OG	1:E:257:MET:HE2	2.07	0.54
1:D:194:GLY:O	1:D:198:LYS:HE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:604:PEG:O4	3:E:605:PEG:O4	2.26	0.53
1:E:87:ASP:OD1	1:E:455:ARG:NH2	2.41	0.53
1:F:196:LYS:HG3	1:F:355:TRP:HH2	1.74	0.53
1:B:399:MET:CE	1:B:514:ASN:OD1	2.53	0.53
1:D:256:SER:OG	1:D:257:MET:HE2	2.09	0.53
1:B:369:LEU:HB2	1:B:374:MET:HE3	1.91	0.53
1:C:85:ARG:NH2	1:D:546:ILE:O	2.42	0.53
1:A:337:LYS:NZ	2:A:601:PLG:H	2.07	0.53
1:B:87:ASP:OD2	1:B:455:ARG:NH1	2.41	0.52
1:F:453:VAL:HG21	1:F:459:ARG:CZ	2.39	0.52
1:E:455:ARG:NH1	4:E:705:HOH:O	2.40	0.52
1:A:529:ASN:O	1:A:532:VAL:HG22	2.10	0.52
1:C:166:GLU:OE1	1:C:385:ARG:NH2	2.24	0.52
1:F:166:GLU:OE2	1:F:537:VAL:HG21	2.10	0.52
1:D:198:LYS:HE2	1:D:198:LYS:HA	1.91	0.52
1:B:448:ILE:HG22	1:B:453:VAL:HG23	1.92	0.52
1:D:166:GLU:OE1	1:D:385:ARG:NH2	2.22	0.52
1:D:514:ASN:OD1	4:D:701:HOH:O	2.19	0.52
1:E:529:ASN:O	1:E:532:VAL:HG22	2.08	0.52
1:B:289:TYR:CD1	1:B:515:LEU:HD23	2.45	0.51
1:D:194:GLY:O	1:D:198:LYS:CE	2.58	0.51
1:C:199:ASP:HB2	4:C:755:HOH:O	2.10	0.51
1:B:91:ARG:NH2	1:B:452:THR:OG1	2.38	0.51
2:E:601:PLG:O3	2:E:601:PLG:N	2.44	0.50
1:B:337:LYS:NZ	2:B:601:PLG:H	2.07	0.50
1:A:128:LYS:HD2	1:A:128:LYS:O	2.11	0.50
2:A:601:PLG:CA	4:A:804:HOH:O	2.58	0.50
1:C:349:SER:HB2	4:C:731:HOH:O	2.11	0.50
1:F:453:VAL:HG21	1:F:459:ARG:NH1	2.26	0.50
1:A:256:SER:HB3	1:A:284:HIS:CD2	2.47	0.50
1:A:461:ARG:NH1	4:A:705:HOH:O	2.44	0.50
2:A:601:PLG:HA2	4:A:804:HOH:O	2.10	0.50
1:E:256:SER:HB3	1:E:284:HIS:CD2	2.46	0.50
1:B:278:THR:CG2	1:B:328:VAL:HA	2.41	0.50
1:B:453:VAL:HG12	1:B:454:ALA:N	2.27	0.50
1:C:257:MET:SD	1:C:448:ILE:HD13	2.52	0.50
1:F:263:ASP:O	1:F:267:ILE:HG12	2.12	0.49
1:F:537:VAL:HG23	1:F:537:VAL:O	2.12	0.49
1:C:148:GLY:C	4:C:734:HOH:O	2.54	0.49
1:E:314:LYS:NZ	3:E:604:PEG:H31	2.27	0.49
1:F:131:GLU:OE2	4:F:702:HOH:O	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:ASP:OD1	1:F:357:ARG:NH1	2.44	0.49
1:B:382:ARG:NH2	1:B:535:PRO:O	2.44	0.49
1:F:256:SER:OG	1:F:257:MET:HE2	2.11	0.49
1:B:310:ILE:CD1	1:B:535:PRO:HB3	2.43	0.49
1:B:166:GLU:OE1	1:B:385:ARG:NH2	2.23	0.49
1:A:77:ILE:HD12	1:B:355:TRP:CE2	2.48	0.48
1:C:405:PHE:CD1	1:C:410:ILE:HD12	2.48	0.48
1:B:405:PHE:CD1	1:B:410:ILE:HD12	2.48	0.48
1:A:153:ILE:HD11	1:B:448:ILE:CD1	2.42	0.48
1:A:258:ALA:HB3	4:A:787:HOH:O	2.13	0.48
1:A:354:ASP:OD1	1:A:357:ARG:NH1	2.43	0.48
1:D:405:PHE:CD1	1:D:410:ILE:HD12	2.47	0.48
1:C:500:GLY:HA2	1:C:505:GLY:HA3	1.95	0.48
1:E:194:GLY:HA3	1:E:219:ALA:HB1	1.95	0.48
1:B:469:THR:CG2	1:B:471:ASP:OD1	2.47	0.48
1:F:231:LEU:HD21	1:F:267:ILE:HD11	1.96	0.48
1:A:107:HIS:NE2	1:B:142:LYS:NZ	2.57	0.48
1:C:100:ALA:O	4:C:701:HOH:O	2.20	0.48
3:C:605:PEG:H21	4:C:701:HOH:O	2.12	0.48
1:C:256:SER:OG	1:C:257:MET:HE2	2.12	0.48
1:E:128:LYS:C	1:E:128:LYS:HD2	2.38	0.48
1:C:354:ASP:OD1	1:C:357:ARG:NH1	2.44	0.48
1:E:314:LYS:HZ3	3:E:604:PEG:H21	1.79	0.47
1:E:314:LYS:HB2	3:E:606:PEG:H11	1.95	0.47
1:D:128:LYS:HD2	1:D:128:LYS:C	2.39	0.47
1:B:182:CYS:HB3	2:B:601:PLG:OP4	2.14	0.47
1:C:258:ALA:HB3	4:C:732:HOH:O	2.15	0.47
3:E:608:PEG:H31	4:E:800:HOH:O	2.14	0.47
1:B:278:THR:CG2	1:B:329:ASP:H	2.24	0.47
1:A:153:ILE:HD11	1:B:448:ILE:HD12	1.96	0.47
1:A:142:LYS:NZ	1:B:107:HIS:NE2	2.51	0.47
1:D:199:ASP:HB2	4:D:770:HOH:O	2.13	0.47
1:C:256:SER:HB3	1:C:284:HIS:CD2	2.49	0.47
1:D:166:GLU:HG3	1:D:378:THR:HG23	1.96	0.47
1:D:453:VAL:HG11	1:D:459:ARG:CZ	2.45	0.47
1:B:194:GLY:HA3	1:B:219:ALA:HB1	1.96	0.47
1:A:194:GLY:HA3	1:A:219:ALA:HB1	1.96	0.46
1:D:453:VAL:HG12	1:D:454:ALA:N	2.30	0.46
1:F:80:GLU:OE2	1:E:196:LYS:HD2	2.16	0.46
1:E:182:CYS:HB3	2:E:601:PLG:OP4	2.15	0.46
1:C:382:ARG:NH2	1:C:535:PRO:O	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:OG	1:B:257:MET:HE2	2.15	0.46
1:F:128:LYS:HD2	1:F:128:LYS:C	2.39	0.46
1:A:453:VAL:HG13	4:A:806:HOH:O	2.14	0.46
1:D:442:GLN:NE2	4:D:711:HOH:O	2.49	0.46
1:A:453:VAL:HG12	1:A:454:ALA:N	2.31	0.46
1:A:453:VAL:HG11	1:A:459:ARG:CZ	2.46	0.46
1:C:80:GLU:HG2	1:D:355:TRP:HE1	1.80	0.46
4:A:739:HOH:O	1:B:91:ARG:HD2	2.17	0.45
1:B:128:LYS:HD2	1:B:128:LYS:C	2.41	0.45
1:C:310:ILE:HG23	1:C:532:VAL:HG12	1.99	0.45
1:F:194:GLY:HA3	1:F:219:ALA:HB1	1.98	0.45
2:F:601:PLG:CA	2:F:601:PLG:O3	2.65	0.45
1:C:194:GLY:HA3	1:C:219:ALA:HB1	1.98	0.45
1:D:194:GLY:HA3	1:D:219:ALA:HB1	1.97	0.45
1:F:533:ARG:O	1:F:534:ASP:C	2.59	0.45
1:C:128:LYS:C	1:C:128:LYS:HD2	2.42	0.45
1:C:457:THR:OG1	1:C:502:LEU:HD11	2.17	0.45
1:F:399:MET:HE2	1:F:514:ASN:CG	2.40	0.45
1:A:399:MET:HE2	4:A:810:HOH:O	2.17	0.44
1:B:538:LYS:HA	1:B:538:LYS:HE2	1.99	0.44
1:D:315:THR:OG1	1:D:319:GLY:HA2	2.17	0.44
1:B:453:VAL:HG12	1:B:454:ALA:H	1.83	0.44
1:C:457:THR:OG1	1:C:502:LEU:CD1	2.66	0.44
1:E:310:ILE:HD13	1:E:535:PRO:HB3	2.00	0.44
1:E:310:ILE:HG23	1:E:532:VAL:HG12	1.99	0.44
1:B:278:THR:HG21	1:B:328:VAL:HA	1.99	0.44
1:C:500:GLY:CA	1:C:505:GLY:HA3	2.47	0.44
1:F:241:TYR:CD2	1:A:507:SER:HB3	2.52	0.44
3:C:605:PEG:C3	4:C:701:HOH:O	2.66	0.44
1:D:121:ASN:OD1	1:D:461:ARG:NH2	2.50	0.44
1:A:382:ARG:NH2	1:A:535:PRO:O	2.46	0.43
1:C:182:CYS:HB3	2:C:601:PLG:OP4	2.17	0.43
1:B:399:MET:HE2	1:B:514:ASN:CG	2.43	0.43
3:C:604:PEG:H31	3:C:604:PEG:O1	2.17	0.43
1:D:431:LYS:HE3	1:D:449:ASN:ND2	2.33	0.43
1:F:80:GLU:HG2	1:E:355:TRP:NE1	2.21	0.43
1:A:125:ALA:O	1:A:128:LYS:HE2	2.19	0.43
1:E:209:HIS:NE2	2:E:601:PLG:HA1	2.33	0.43
1:A:152:ASN:HB2	4:B:774:HOH:O	2.18	0.43
1:A:355:TRP:HE1	1:B:80:GLU:HG2	1.84	0.42
1:A:528:LEU:HB2	1:A:533:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ARG:NH1	1:E:152:ASN:HB2	2.34	0.42
1:A:141:ASP:CB	4:A:728:HOH:O	2.58	0.42
1:A:121:ASN:HB2	4:B:706:HOH:O	2.18	0.42
1:A:218:HIS:CE1	1:B:218:HIS:CE1	3.07	0.42
1:C:457:THR:HG23	1:C:459:ARG:NH1	2.34	0.42
1:D:131:GLU:OE2	4:D:702:HOH:O	2.21	0.42
1:F:78:ASP:OD1	1:E:351:LYS:CE	2.66	0.42
3:E:608:PEG:C3	4:E:800:HOH:O	2.68	0.41
2:F:601:PLG:H2A1	4:F:704:HOH:O	2.20	0.41
1:C:311:ALA:HA	3:C:604:PEG:H42	2.02	0.41
1:A:448:ILE:HG22	1:A:453:VAL:HG23	2.03	0.41
1:B:410:ILE:HD13	1:B:480:VAL:HG12	2.03	0.41
1:F:166:GLU:HG3	1:F:378:THR:HG23	2.02	0.41
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.91	0.41
1:E:314:LYS:HZ3	3:E:604:PEG:H31	1.85	0.41
1:D:446:GLN:HB3	4:D:715:HOH:O	2.20	0.41
1:E:533:ARG:NH1	4:E:716:HOH:O	2.54	0.40
1:E:314:LYS:HE3	3:E:605:PEG:C2	2.51	0.40
1:A:240:SER:HB2	3:E:611:PEG:H11	2.03	0.40
1:C:457:THR:HG23	1:C:457:THR:O	2.22	0.40
1:F:121:ASN:OD1	1:F:461:ARG:NH2	2.52	0.40
2:C:601:PLG:N	4:C:704:HOH:O	2.37	0.40
1:D:195:GLN:HA	1:D:198:LYS:HE3	2.03	0.40
1:F:355:TRP:HB2	1:E:77:ILE:HG23	2.03	0.40
1:E:308:SER:HB3	3:E:606:PEG:H32	2.02	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)
4:F:776:HOH:O	4:C:793:HOH:O[1_454]	2.09	0.11

## 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	472/491 (96%)	456 (97%)	16 (3%)	0	100	100
1	B	455/491 (93%)	440 (97%)	15 (3%)	0	100	100
1	C	469/491 (96%)	451 (96%)	18 (4%)	0	100	100
1	D	460/491 (94%)	445 (97%)	15 (3%)	0	100	100
1	E	468/491 (95%)	451 (96%)	17 (4%)	0	100	100
1	F	462/491 (94%)	446 (96%)	16 (4%)	0	100	100
All	All	2786/2946 (95%)	2689 (96%)	97 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	401/411 (98%)	393 (98%)	8 (2%)	48	72
1	B	389/411 (95%)	381 (98%)	8 (2%)	47	71
1	C	399/411 (97%)	394 (99%)	5 (1%)	61	80
1	D	394/411 (96%)	388 (98%)	6 (2%)	57	78
1	E	398/411 (97%)	390 (98%)	8 (2%)	48	72
1	F	397/411 (97%)	392 (99%)	5 (1%)	61	80
All	All	2378/2466 (96%)	2338 (98%)	40 (2%)	53	75

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	91	ARG
1	F	373	VAL
1	F	435	ASP
1	F	514	ASN

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Mol	Chain	Res	Type
1	F	536	ILE
1	A	87	ASP
1	A	91	ARG
1	A	128	LYS
1	A	373	VAL
1	A	431	LYS
1	A	442	GLN
1	A	506	GLU
1	A	514	ASN
1	C	87	ASP
1	C	227	LYS
1	C	373	VAL
1	C	442	GLN
1	C	457	THR
1	E	87	ASP
1	E	141	ASP
1	E	223	LYS
1	E	314	LYS
1	E	373	VAL
1	E	391	ARG
1	E	442	GLN
1	E	513	SER
1	D	87	ASP
1	D	310	ILE
1	D	373	VAL
1	D	435	ASP
1	D	442	GLN
1	D	518	SER
1	B	87	ASP
1	B	223	LYS
1	B	278	THR
1	B	373	VAL
1	B	408	LEU
1	B	442	GLN
1	B	514	ASN
1	B	515	LEU

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

Mol	Chain	Res	Type
1	F	152	ASN
1	F	442	GLN

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Mol	Chain	Res	Type
1	A	82	GLN
1	A	449	ASN
1	A	485	ASN
1	C	94	ASN
1	C	109	GLN
1	C	446	GLN
1	C	485	ASN
1	E	82	GLN
1	E	109	GLN
1	E	441	HIS
1	E	442	GLN
1	E	449	ASN
1	D	442	GLN
1	D	449	ASN
1	D	514	ASN
1	B	432	GLN
1	B	441	HIS
1	B	442	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](#)

29 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	$\# Z  > 2$
3	PEG	C	605	-	6,6,6	0.63	0	5,5,5	0.69	0
3	PEG	B	602	-	6,6,6	0.50	0	5,5,5	0.25	0
2	PLG	A	601	-	20,20,20	0.89	0	26,28,28	1.32	3 (11%)
3	PEG	C	603	-	6,6,6	0.56	0	5,5,5	0.26	0
2	PLG	E	601	-	20,20,20	0.86	0	26,28,28	0.85	0
3	PEG	A	602	-	6,6,6	0.53	0	5,5,5	0.55	0
3	PEG	D	602	-	6,6,6	0.34	0	5,5,5	0.20	0
2	PLG	B	601	-	20,20,20	1.16	1 (5%)	26,28,28	1.14	2 (7%)
3	PEG	E	602	-	6,6,6	0.53	0	5,5,5	0.66	0
3	PEG	E	609	-	6,6,6	0.35	0	5,5,5	0.27	0
3	PEG	A	605	-	6,6,6	0.60	0	5,5,5	0.46	0
3	PEG	C	604	-	6,6,6	0.30	0	5,5,5	0.15	0
3	PEG	E	605	-	6,6,6	0.55	0	5,5,5	0.45	0
3	PEG	A	606	-	6,6,6	0.46	0	5,5,5	0.28	0
2	PLG	D	601	-	20,20,20	0.84	1 (5%)	26,28,28	1.04	3 (11%)
3	PEG	E	606	-	6,6,6	0.28	0	5,5,5	0.28	0
2	PLG	C	601	-	20,20,20	1.04	0	26,28,28	0.89	1 (3%)
3	PEG	E	611	-	6,6,6	0.29	0	5,5,5	0.19	0
3	PEG	E	610	-	6,6,6	0.74	0	5,5,5	0.59	0
3	PEG	A	603	-	6,6,6	0.26	0	5,5,5	0.25	0
3	PEG	A	607	-	6,6,6	0.51	0	5,5,5	0.38	0
3	PEG	E	603	-	6,6,6	0.46	0	5,5,5	0.24	0
3	PEG	E	604	-	6,6,6	0.60	0	5,5,5	0.55	0
3	PEG	C	602	-	6,6,6	0.50	0	5,5,5	0.28	0
3	PEG	A	604	-	6,6,6	0.43	0	5,5,5	0.40	0
3	PEG	E	608	-	6,6,6	0.34	0	5,5,5	0.11	0
3	PEG	E	612	-	6,6,6	0.28	0	5,5,5	0.12	0
2	PLG	F	601	-	20,20,20	1.17	1 (5%)	26,28,28	1.03	1 (3%)
3	PEG	E	607	-	6,6,6	0.37	0	5,5,5	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	C	605	-	-	4/4/4/4	-
3	PEG	B	602	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	A	601	-	-	8/12/12/12	0/1/1/1
3	PEG	C	603	-	-	3/4/4/4	-
2	PLG	E	601	-	-	4/12/12/12	0/1/1/1
3	PEG	A	602	-	-	3/4/4/4	-
3	PEG	D	602	-	-	3/4/4/4	-
2	PLG	B	601	-	-	8/12/12/12	0/1/1/1
3	PEG	E	602	-	-	2/4/4/4	-
3	PEG	E	609	-	-	3/4/4/4	-
3	PEG	A	605	-	-	2/4/4/4	-
3	PEG	C	604	-	-	2/4/4/4	-
3	PEG	E	605	-	-	3/4/4/4	-
3	PEG	A	606	-	-	1/4/4/4	-
2	PLG	D	601	-	-	6/12/12/12	0/1/1/1
3	PEG	E	606	-	-	1/4/4/4	-
2	PLG	C	601	-	-	3/12/12/12	0/1/1/1
3	PEG	E	611	-	-	2/4/4/4	-
3	PEG	E	610	-	-	1/4/4/4	-
3	PEG	A	603	-	-	3/4/4/4	-
3	PEG	A	607	-	-	2/4/4/4	-
3	PEG	E	603	-	-	1/4/4/4	-
3	PEG	E	604	-	-	3/4/4/4	-
3	PEG	C	602	-	-	1/4/4/4	-
3	PEG	A	604	-	-	3/4/4/4	-
3	PEG	E	608	-	-	3/4/4/4	-
3	PEG	E	612	-	-	2/4/4/4	-
2	PLG	F	601	-	-	7/12/12/12	0/1/1/1
3	PEG	E	607	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	PLG	C4A-C4	3.48	1.57	1.52
2	B	601	PLG	C4A-C4	3.35	1.56	1.52
2	D	601	PLG	O-C	2.47	1.30	1.22

All (10) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	PLG	O3-C3-C4	3.50	128.32	118.18
2	B	601	PLG	C4-C4A-N	2.79	116.65	111.50
2	A	601	PLG	O3-C3-C2	-2.52	112.36	117.58
2	A	601	PLG	C4A-C4-C3	2.45	123.24	119.98
2	F	601	PLG	C4-C4A-N	2.44	116.00	111.50
2	D	601	PLG	C4A-C4-C5	2.20	122.14	119.75
2	B	601	PLG	C4A-N-CA	2.17	115.25	112.72
2	D	601	PLG	C6-C5-C4	-2.08	116.48	118.06
2	D	601	PLG	OP3-P-OP2	2.07	115.57	107.80
2	C	601	PLG	C4A-C4-C5	2.07	122.00	119.75

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PLG	C5-C4-C4A-N
2	A	601	PLG	O-C-CA-N
2	E	601	PLG	C5-C4-C4A-N
2	E	601	PLG	C5A-OP4-P-OP3
2	D	601	PLG	C5-C4-C4A-N
2	D	601	PLG	O-C-CA-N
2	D	601	PLG	OXT-C-CA-N
2	B	601	PLG	C5-C4-C4A-N
2	F	601	PLG	C5-C4-C4A-N
2	C	601	PLG	C5-C4-C4A-N
3	A	603	PEG	O2-C3-C4-O4
2	A	601	PLG	OXT-C-CA-N
3	A	605	PEG	O2-C3-C4-O4
3	E	603	PEG	O1-C1-C2-O2
3	E	606	PEG	O1-C1-C2-O2
3	D	602	PEG	O2-C3-C4-O4
2	C	601	PLG	C4-C4A-N-CA
3	A	605	PEG	O1-C1-C2-O2
3	E	605	PEG	O2-C3-C4-O4
3	E	607	PEG	O1-C1-C2-O2
3	E	611	PEG	O1-C1-C2-O2
3	C	605	PEG	C1-C2-O2-C3
3	C	602	PEG	O2-C3-C4-O4
3	C	604	PEG	O2-C3-C4-O4
3	C	605	PEG	O1-C1-C2-O2
3	E	604	PEG	O1-C1-C2-O2
3	E	604	PEG	O2-C3-C4-O4
3	B	602	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	B	601	PLG	C3-C4-C4A-N
3	A	607	PEG	O1-C1-C2-O2
3	D	602	PEG	O1-C1-C2-O2
3	A	602	PEG	O1-C1-C2-O2
3	E	602	PEG	O2-C3-C4-O4
3	E	610	PEG	O2-C3-C4-O4
2	E	601	PLG	C4-C4A-N-CA
3	A	604	PEG	O2-C3-C4-O4
3	E	608	PEG	O1-C1-C2-O2
3	C	605	PEG	O2-C3-C4-O4
3	E	609	PEG	O2-C3-C4-O4
2	B	601	PLG	C5A-OP4-P-OP1
2	F	601	PLG	C3-C4-C4A-N
2	C	601	PLG	C3-C4-C4A-N
2	B	601	PLG	C5A-OP4-P-OP2
3	E	611	PEG	C1-C2-O2-C3
3	B	602	PEG	C4-C3-O2-C2
3	A	603	PEG	C1-C2-O2-C3
3	A	604	PEG	C1-C2-O2-C3
3	C	603	PEG	C4-C3-O2-C2
2	D	601	PLG	C4-C4A-N-CA
3	A	607	PEG	C4-C3-O2-C2
3	E	608	PEG	C4-C3-O2-C2
3	E	605	PEG	O1-C1-C2-O2
3	C	605	PEG	C4-C3-O2-C2
3	E	605	PEG	C1-C2-O2-C3
3	A	602	PEG	C4-C3-O2-C2
2	A	601	PLG	C3-C4-C4A-N
2	E	601	PLG	C3-C4-C4A-N
2	D	601	PLG	C3-C4-C4A-N
2	D	601	PLG	C4-C5-C5A-OP4
2	B	601	PLG	C4-C5-C5A-OP4
2	B	601	PLG	OXT-C-CA-N
3	C	603	PEG	O1-C1-C2-O2
3	A	606	PEG	C4-C3-O2-C2
2	F	601	PLG	C-CA-N-C4A
2	A	601	PLG	C-CA-N-C4A
2	F	601	PLG	C5A-OP4-P-OP1
2	A	601	PLG	C5A-OP4-P-OP1
2	F	601	PLG	C4-C4A-N-CA
3	C	603	PEG	C1-C2-O2-C3
3	C	604	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	E	608	PEG	C1-C2-O2-C3
3	E	602	PEG	C1-C2-O2-C3
2	B	601	PLG	O-C-CA-N
3	A	604	PEG	O1-C1-C2-O2
3	D	602	PEG	C1-C2-O2-C3
2	F	601	PLG	C6-C5-C5A-OP4
2	B	601	PLG	C6-C5-C5A-OP4
3	A	603	PEG	C4-C3-O2-C2
3	B	602	PEG	O1-C1-C2-O2
2	A	601	PLG	C4-C4A-N-CA
3	E	609	PEG	C4-C3-O2-C2
2	A	601	PLG	C5A-OP4-P-OP2
3	E	612	PEG	O2-C3-C4-O4
2	F	601	PLG	C4-C5-C5A-OP4
3	E	612	PEG	O1-C1-C2-O2
3	E	609	PEG	C1-C2-O2-C3
3	E	604	PEG	C1-C2-O2-C3
3	A	602	PEG	O2-C3-C4-O4

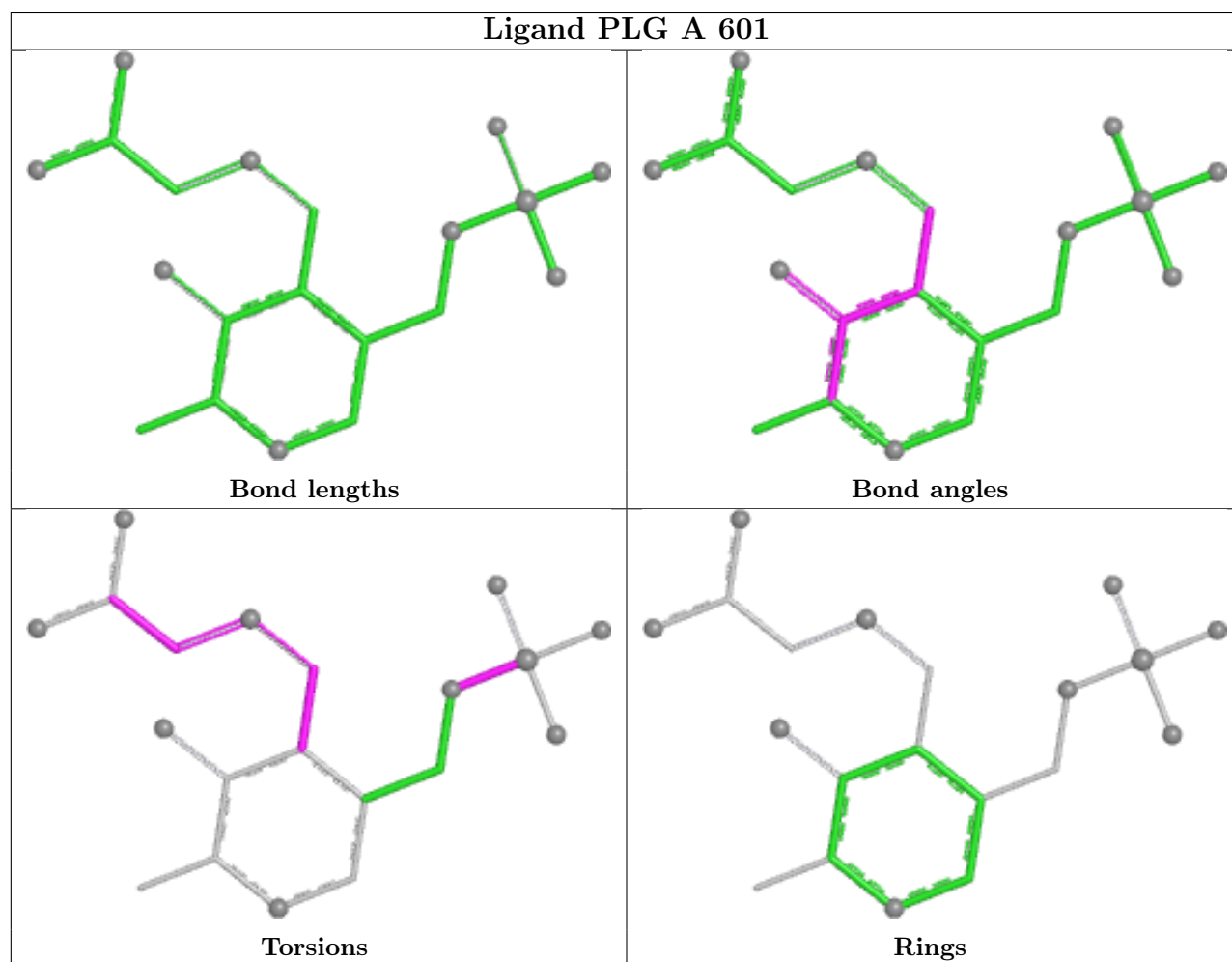
There are no ring outliers.

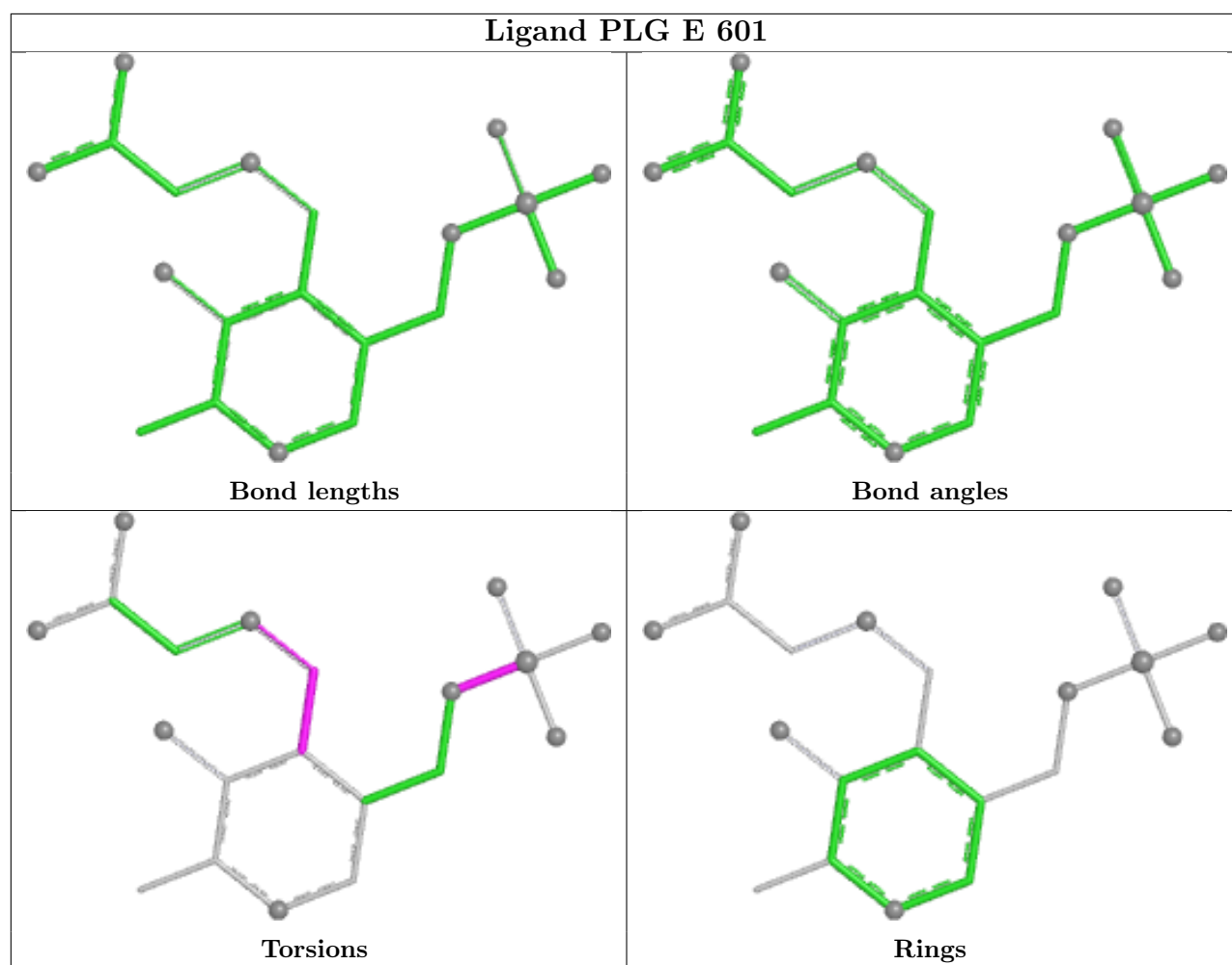
15 monomers are involved in 42 short contacts:

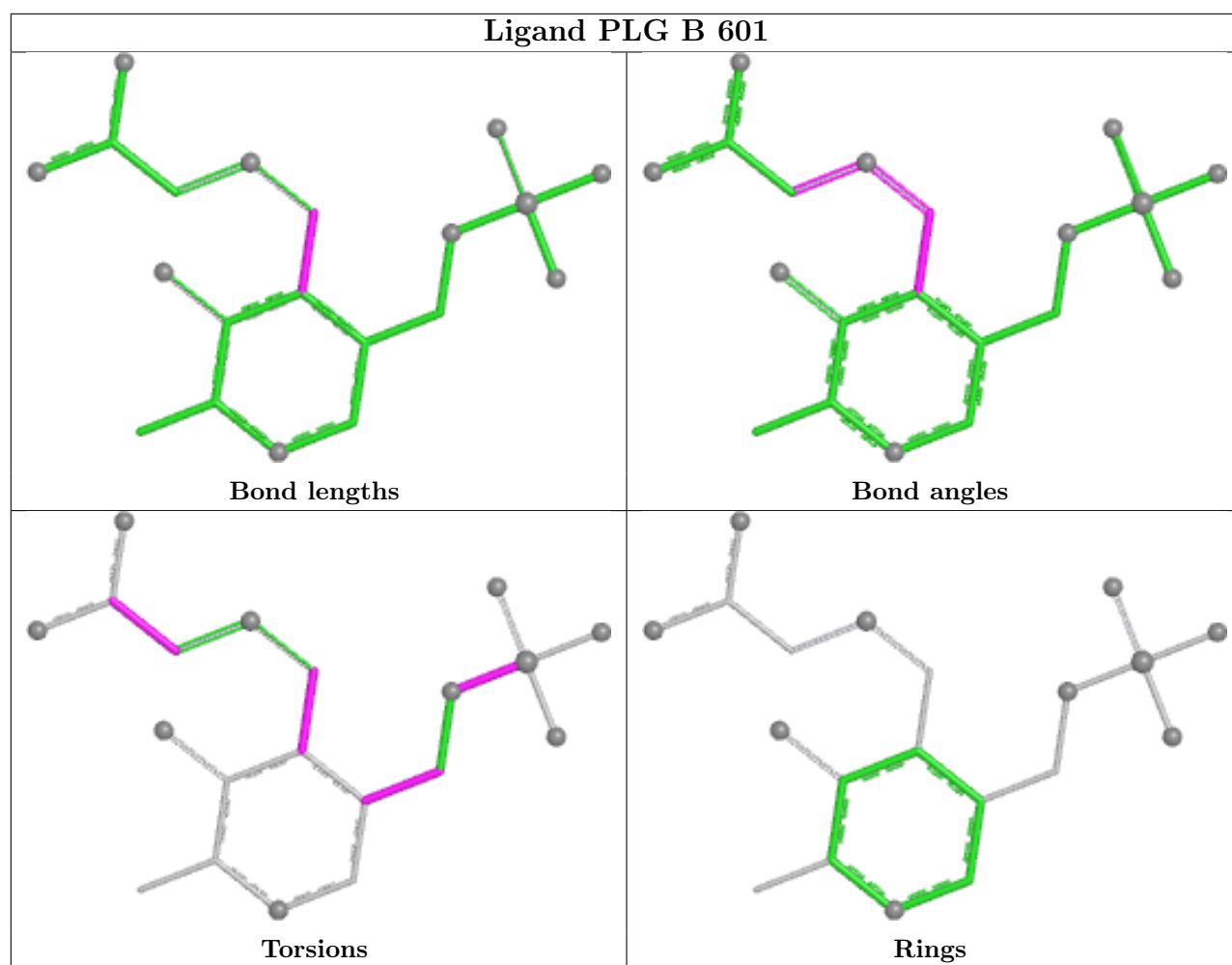
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	605	PEG	3	0
2	A	601	PLG	3	0
2	E	601	PLG	5	0
2	B	601	PLG	6	0
3	C	604	PEG	2	0
3	E	605	PEG	3	0
3	A	606	PEG	1	0
2	D	601	PLG	4	0
3	E	606	PEG	2	0
2	C	601	PLG	2	0
3	E	611	PEG	1	0
3	E	604	PEG	4	0
3	C	602	PEG	1	0
3	E	608	PEG	3	0
2	F	601	PLG	3	0

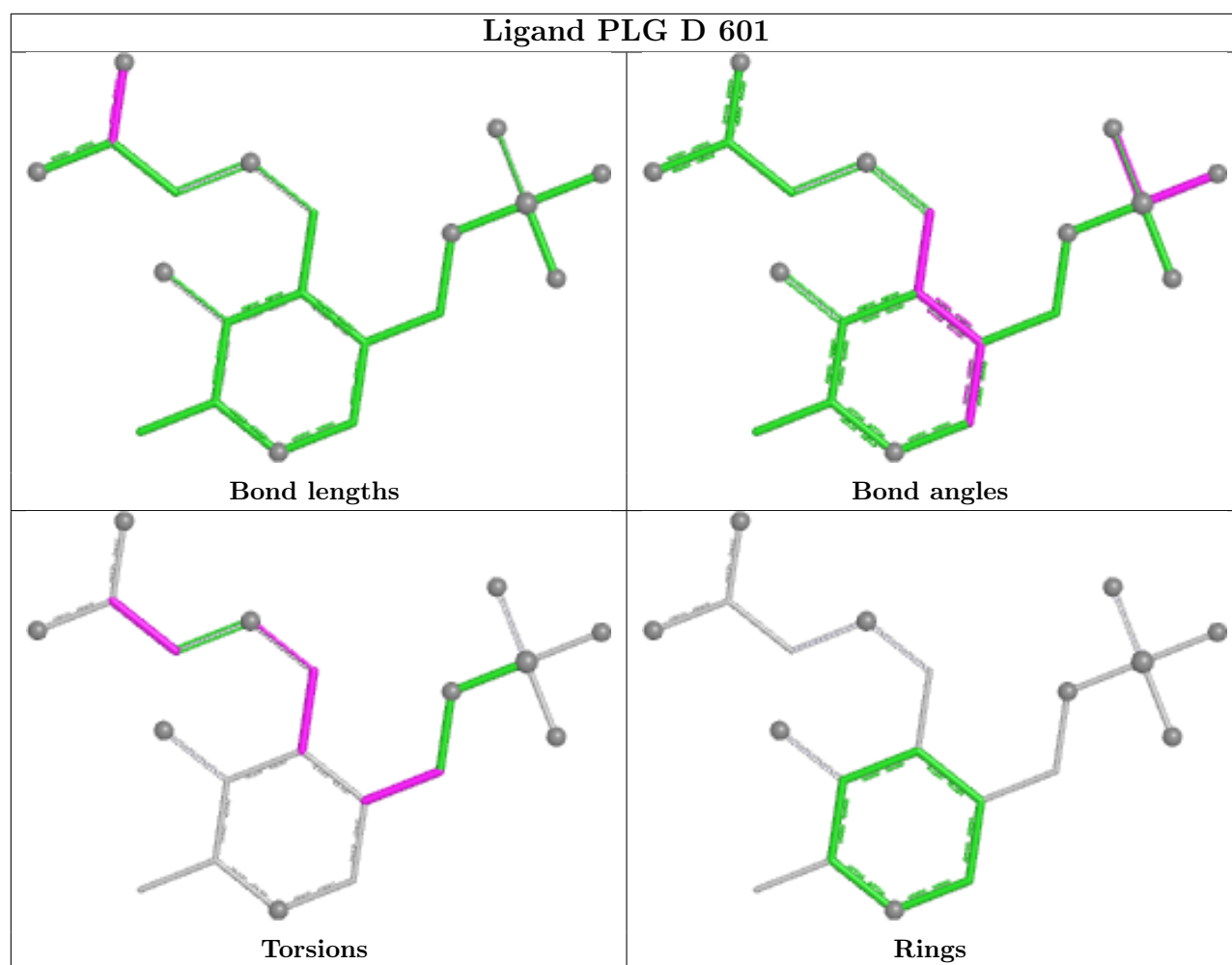
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

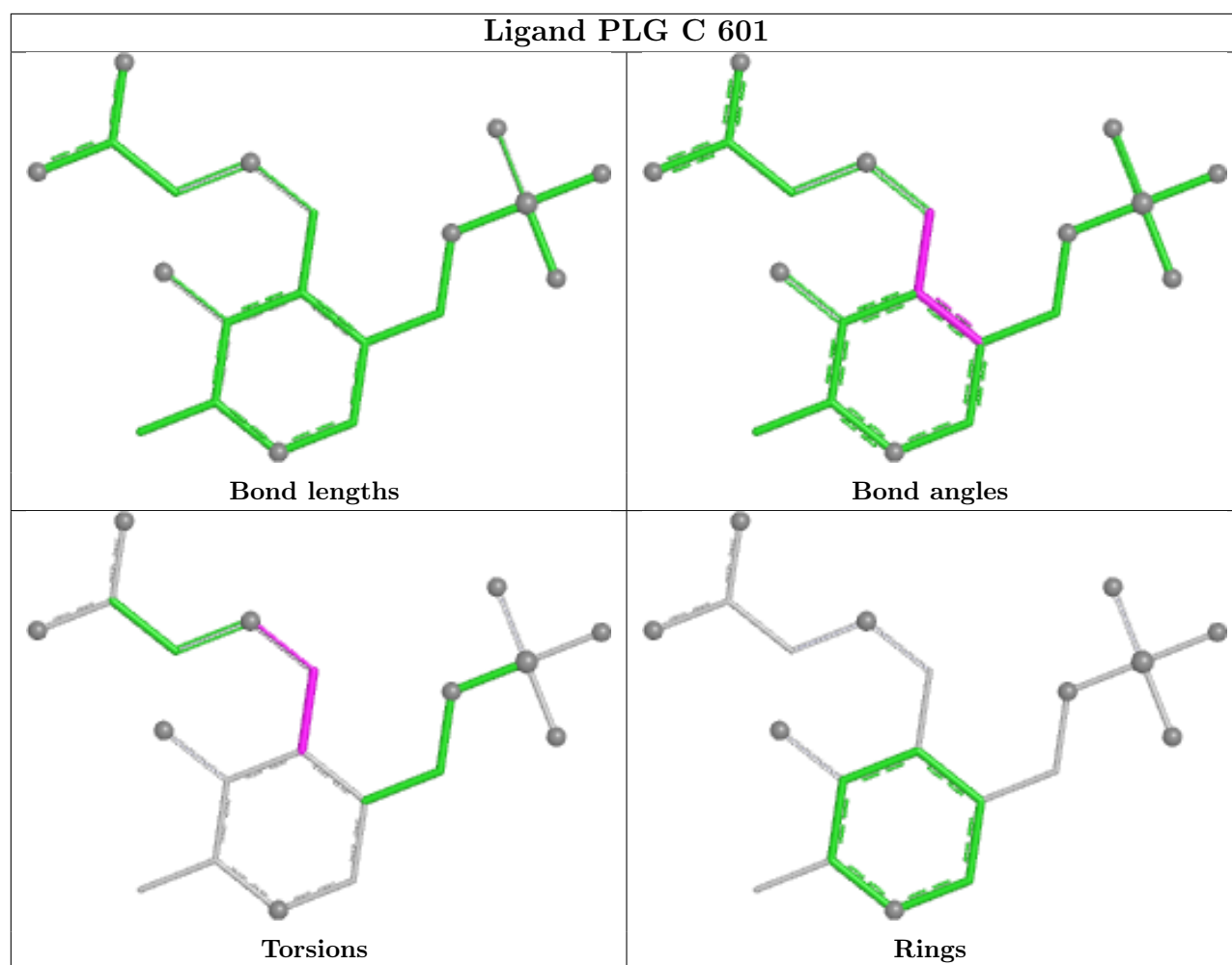
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



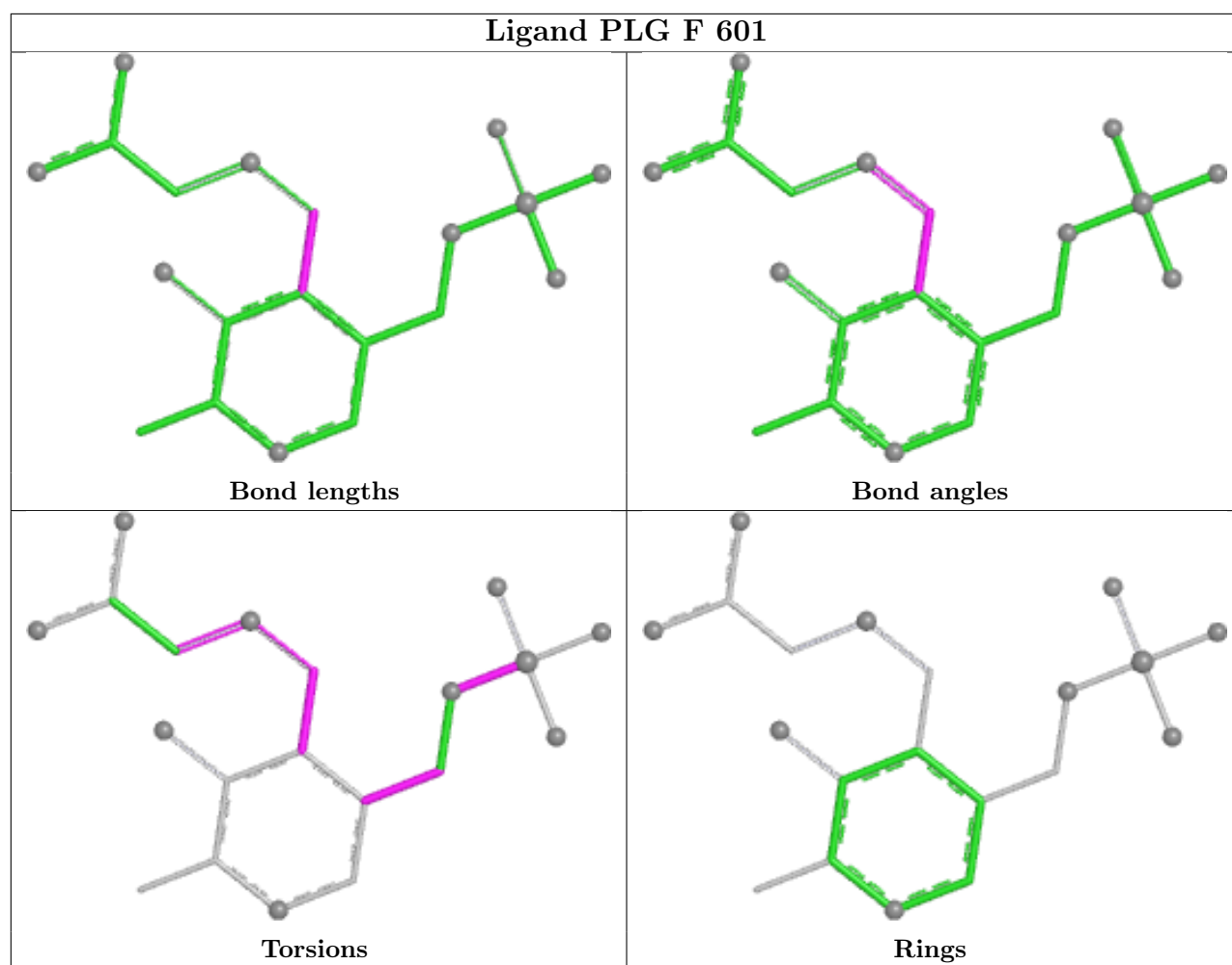












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	476/491 (96%)	-0.26	4 (0%) 82 80	27, 41, 76, 105	0
1	B	459/491 (93%)	-0.01	4 (0%) 81 79	31, 52, 91, 119	0
1	C	473/491 (96%)	-0.21	7 (1%) 72 69	28, 42, 75, 114	0
1	D	464/491 (94%)	-0.13	5 (1%) 78 76	28, 45, 88, 120	0
1	E	472/491 (96%)	-0.25	4 (0%) 82 80	26, 38, 96, 137	0
1	F	468/491 (95%)	0.10	2 (0%) 88 87	34, 55, 99, 121	0
All	All	2812/2946 (95%)	-0.13	26 (0%) 81 79	26, 44, 90, 137	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	GLY	3.5
1	B	423	LEU	3.3
1	E	536	ILE	3.1
1	F	450	PHE	2.8
1	A	536	ILE	2.7
1	E	542	VAL	2.7
1	E	537	VAL	2.6
1	C	505	GLY	2.6
1	E	86	LEU	2.6
1	D	449	ASN	2.5
1	C	543	SER	2.4
1	B	424	ILE	2.3
1	C	547	LYS	2.3
1	D	513	SER	2.3
1	C	540	LEU	2.2
1	B	408	LEU	2.2
1	C	536	ILE	2.2
1	B	447	ALA	2.1
1	C	544	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	495	TRP	2.1
1	C	504	VAL	2.1
1	D	86	LEU	2.1
1	A	538	LYS	2.1
1	F	543	SER	2.1
1	D	450	PHE	2.1
1	A	542	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	C	604	7/7	0.78	0.15	67,78,93,96	0
3	PEG	A	606	7/7	0.80	0.15	74,84,100,102	0
3	PEG	A	605	7/7	0.80	0.15	52,64,67,67	0
3	PEG	C	605	7/7	0.84	0.14	46,53,64,64	0
3	PEG	C	603	7/7	0.85	0.15	62,63,72,73	0
3	PEG	E	609	7/7	0.85	0.11	53,67,78,78	0
3	PEG	E	608	7/7	0.86	0.14	50,65,75,76	0
3	PEG	E	611	7/7	0.86	0.14	62,73,92,97	0
3	PEG	B	602	7/7	0.86	0.16	61,70,83,83	0
3	PEG	E	612	7/7	0.87	0.12	58,63,74,77	0
3	PEG	A	607	7/7	0.88	0.13	60,63,73,74	0
3	PEG	E	610	7/7	0.89	0.13	47,54,67,68	0
3	PEG	A	604	7/7	0.89	0.12	42,47,59,61	0
2	PLG	B	601	20/20	0.90	0.11	45,53,79,86	0
3	PEG	A	603	7/7	0.90	0.11	48,50,54,57	0
3	PEG	D	602	7/7	0.90	0.11	53,57,67,69	0

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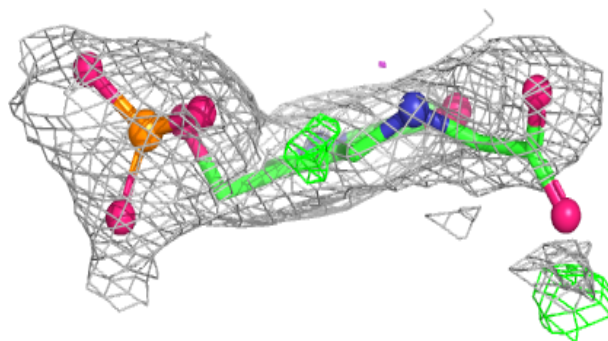
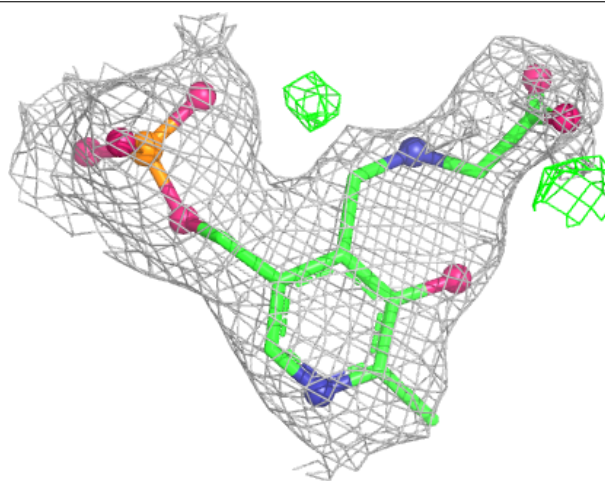
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	C	602	7/7	0.90	0.11	47,55,61,62	0
3	PEG	E	607	7/7	0.91	0.10	41,50,54,57	0
3	PEG	A	602	7/7	0.91	0.10	39,42,42,43	0
2	PLG	F	601	20/20	0.91	0.10	43,54,80,89	0
3	PEG	E	606	7/7	0.91	0.11	58,59,63,67	0
3	PEG	E	604	7/7	0.92	0.12	34,41,48,49	0
3	PEG	E	603	7/7	0.93	0.10	37,46,54,55	0
3	PEG	E	602	7/7	0.93	0.08	35,42,45,46	0
3	PEG	E	605	7/7	0.93	0.12	40,49,67,72	0
2	PLG	A	601	20/20	0.94	0.09	37,43,67,74	0
2	PLG	D	601	20/20	0.95	0.09	39,45,69,73	0
2	PLG	C	601	20/20	0.96	0.08	35,47,56,63	0
2	PLG	E	601	20/20	0.97	0.07	34,46,65,67	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.

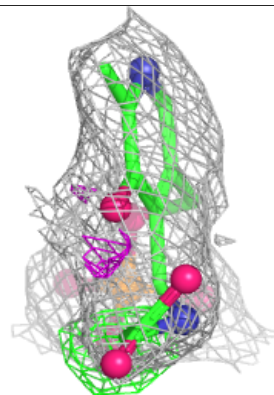
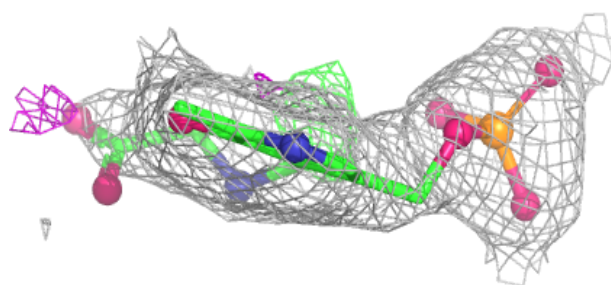
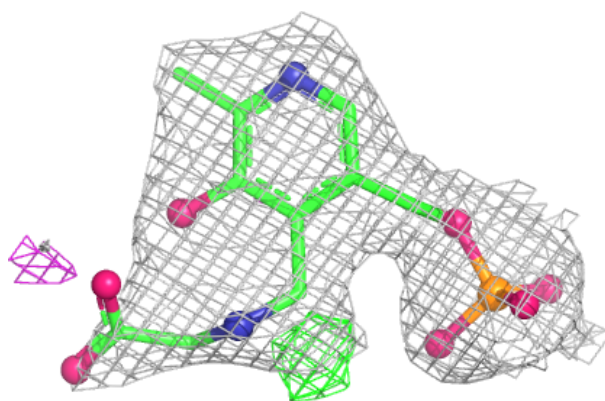
**Electron density around PLG B 601:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



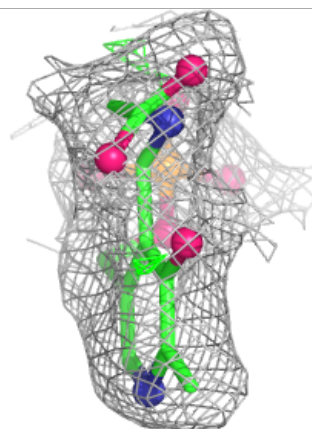
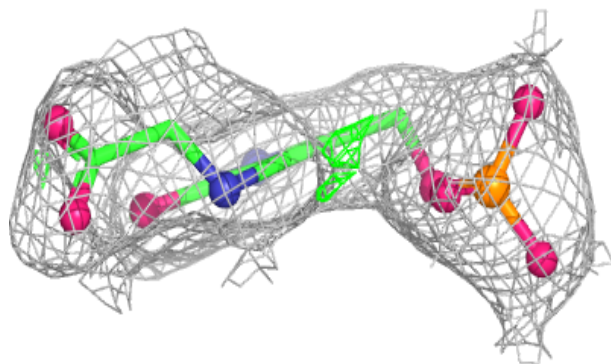
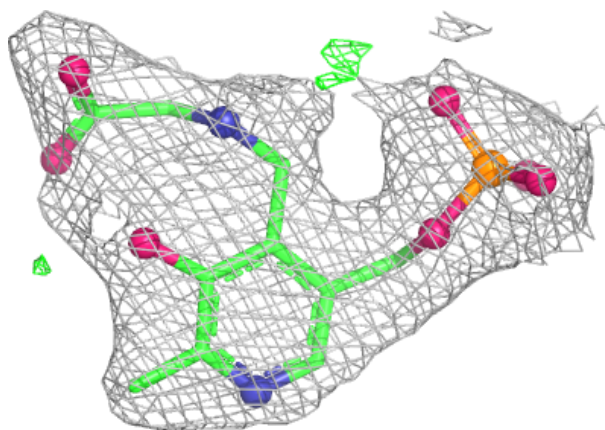
**Electron density around PLG F 601:**

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



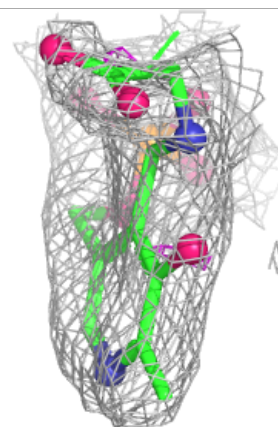
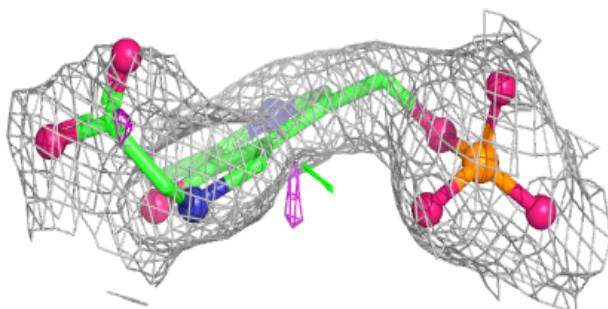
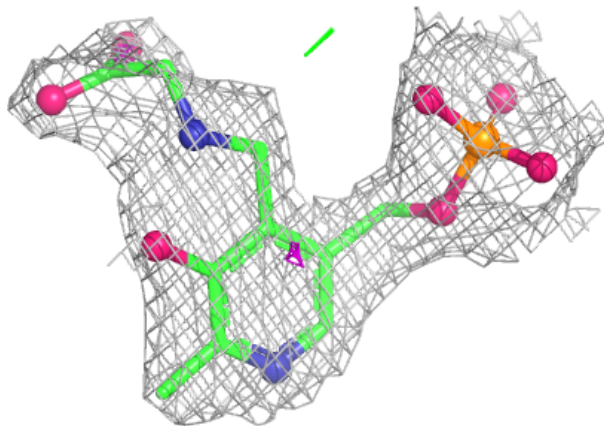
**Electron density around PLG A 601:**

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



**Electron density around PLG D 601:**

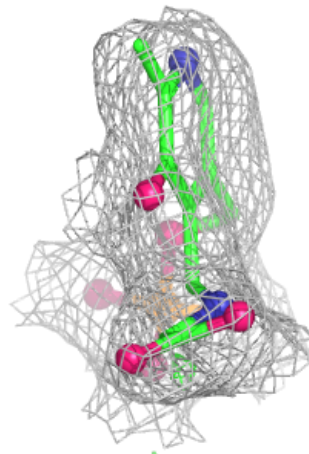
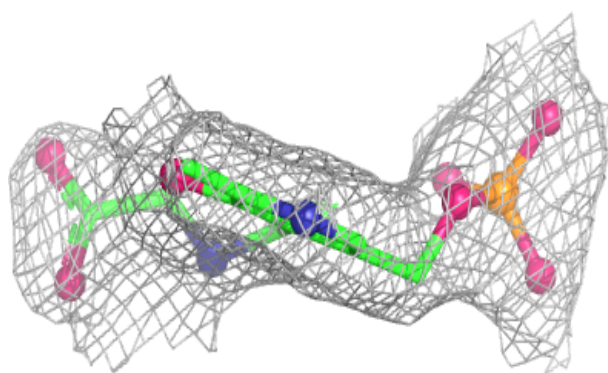
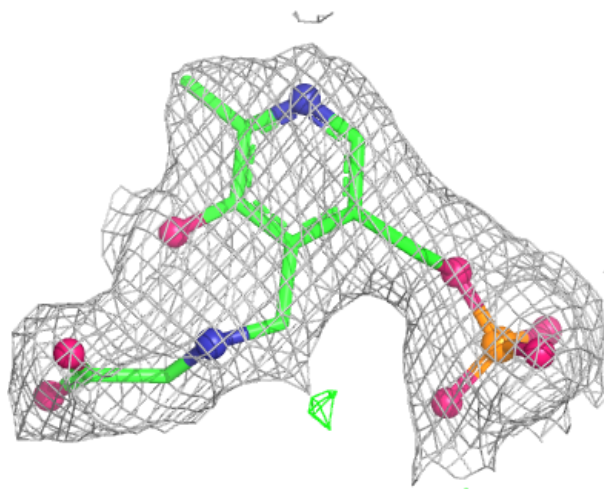
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PLG C 601:**

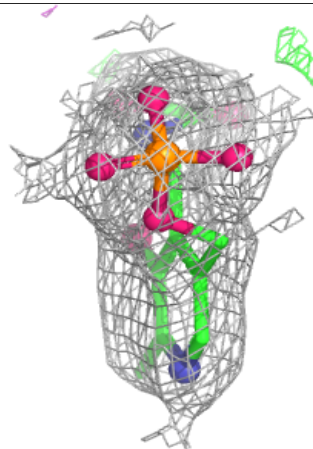
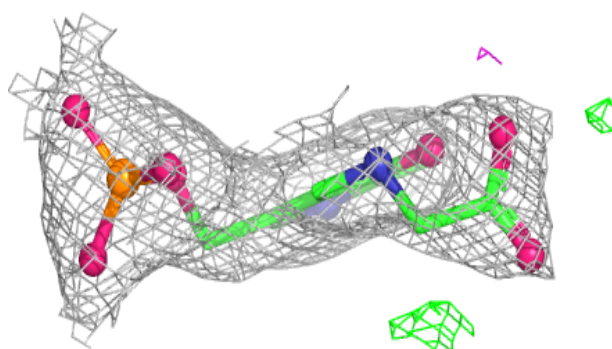
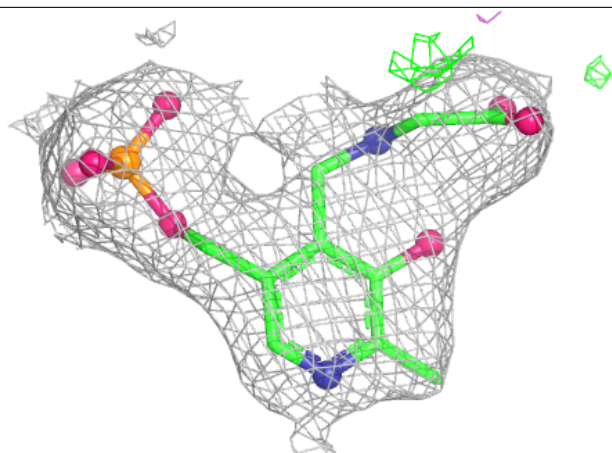
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PLG E 601:**

$2mF_o-DF_c$  (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.