



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:51 PM UTC

PDB ID : 8JG7 / pdb_00008jg7
Title : Serine decarboxylase
Authors : Wang, H.; Gong, W.
Deposited on : 2023-05-19
Resolution : 2.85 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

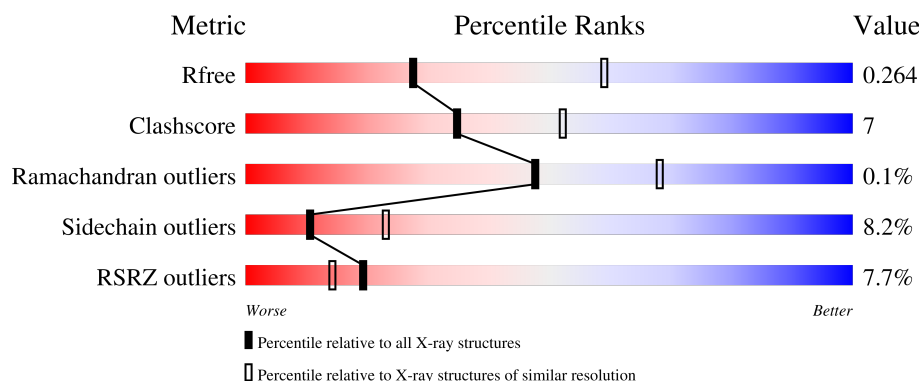
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	418	7% 73% 21% • •
1	C	418	8% 72% 22% • •
1	D	418	6% 72% 22% • •
1	E	418	9% 74% 20% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13088 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 Serine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3247	2064	563	596	24			
1	C	407	Total	C	N	O	S	0	0	0
			3246	2064	563	595	24			
1	D	408	Total	C	N	O	S	0	0	0
			3251	2067	564	596	24			
1	E	409	Total	C	N	O	S	0	0	0
			3256	2070	565	597	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	483	ALA	-	expression tag	UNP Q9MA74
A	484	ALA	-	expression tag	UNP Q9MA74
C	483	ALA	-	expression tag	UNP Q9MA74
C	484	ALA	-	expression tag	UNP Q9MA74
D	483	ALA	-	expression tag	UNP Q9MA74
D	484	ALA	-	expression tag	UNP Q9MA74
E	483	ALA	-	expression tag	UNP Q9MA74
E	484	ALA	-	expression tag	UNP Q9MA74

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

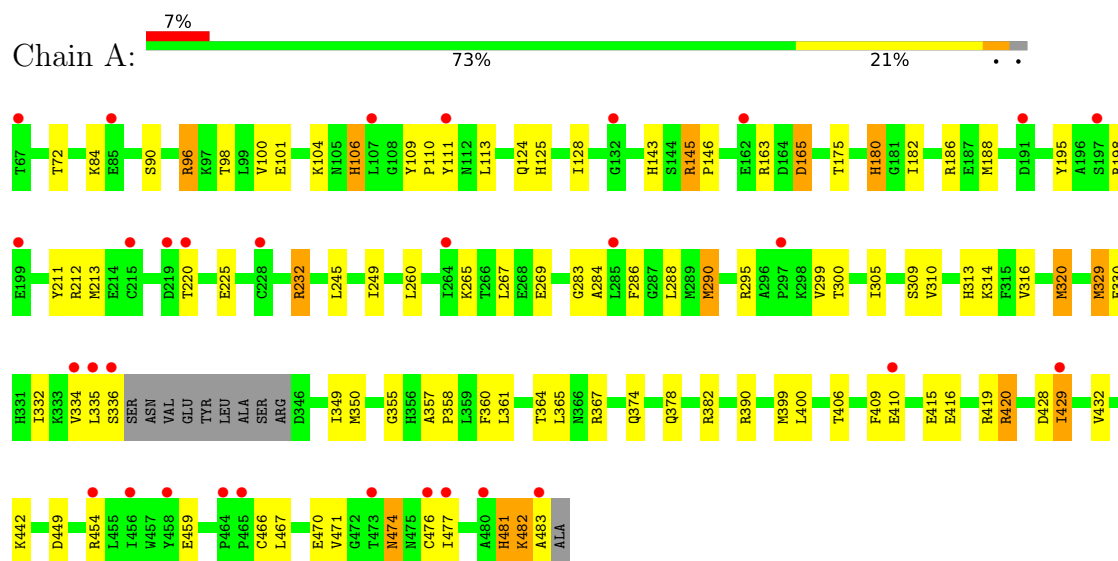


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

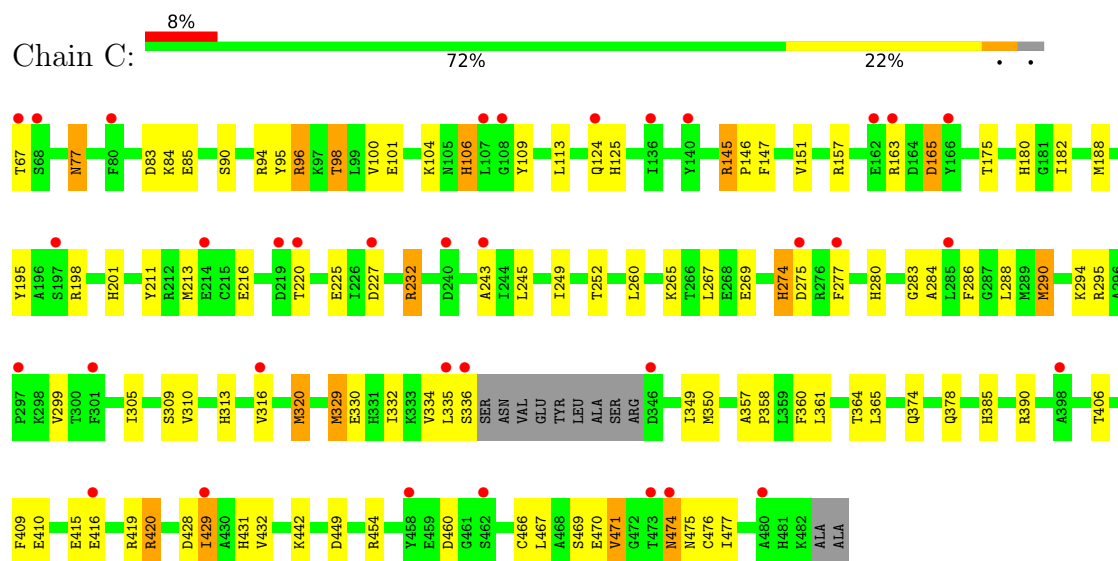
3 Residue-property plots [i](#)

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.

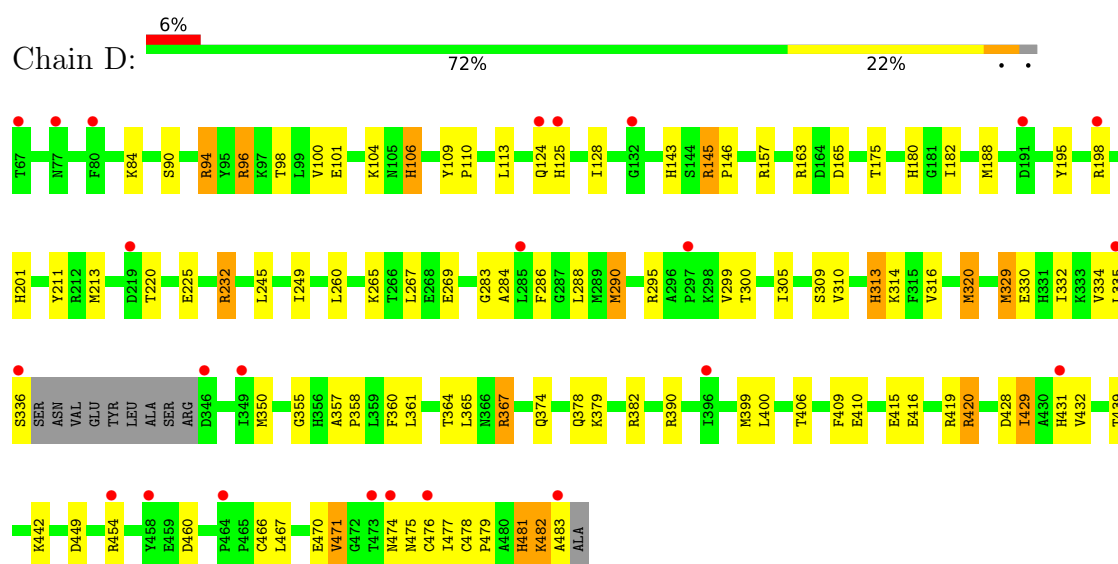
• Molecule 1: Serine decarboxylase



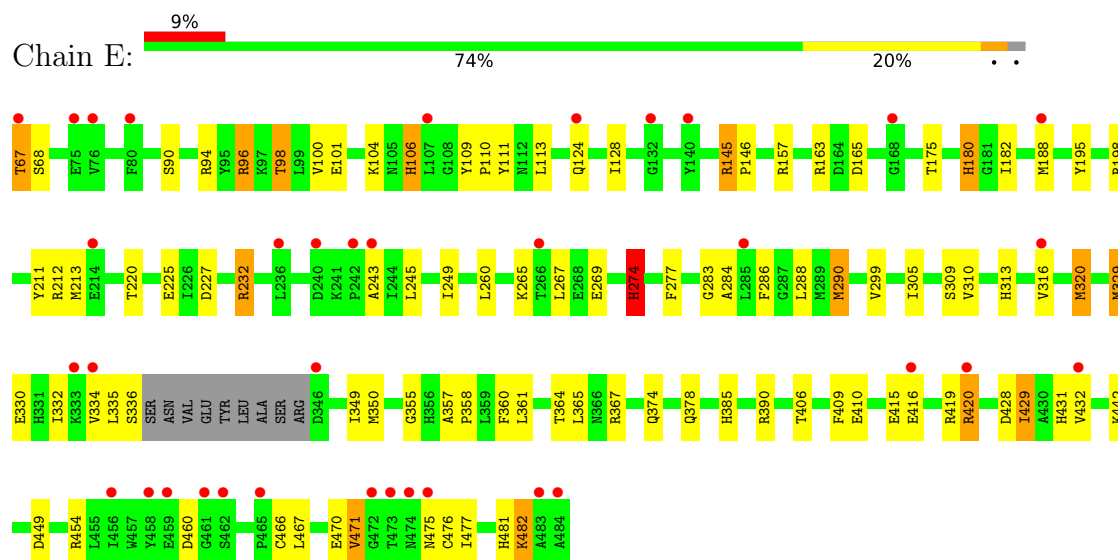
• Molecule 1: Serine decarboxylase



• Molecule 1: Serine decarboxylase



• Molecule 1: Serine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.36Å 149.45Å 139.13Å 90.00° 109.18° 90.00°	Depositor
Resolution (Å)	49.39 – 2.85 49.39 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.39-2.85) 99.6 (49.39-2.85)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.214 , 0.262 0.221 , 0.264	Depositor DCC
R_{free} test set	2576 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13088	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% 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: ZN, PLP, 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	0.63	5/3323 (0.2%)	1.05	3/4492 (0.1%)
1	C	0.64	7/3322 (0.2%)	1.06	5/4489 (0.1%)
1	D	0.66	7/3327 (0.2%)	1.08	2/4496 (0.0%)
1	E	0.63	5/3332 (0.2%)	1.07	3/4503 (0.1%)
All	All	0.64	24/13304 (0.2%)	1.06	13/17980 (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	11
1	C	0	9
1	D	0	10
1	E	0	9
All	All	0	39

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	431	HIS	CE1-NE2	6.99	1.39	1.32
1	A	143	HIS	CE1-NE2	6.91	1.39	1.32
1	D	180	HIS	CE1-NE2	6.61	1.39	1.32
1	D	106	HIS	CE1-NE2	6.35	1.38	1.32
1	C	274	HIS	CE1-NE2	6.28	1.38	1.32
1	C	201	HIS	CE1-NE2	5.98	1.38	1.32
1	D	313	HIS	CE1-NE2	5.92	1.38	1.32
1	A	481	HIS	CE1-NE2	5.79	1.38	1.32
1	E	431	HIS	CE1-NE2	5.74	1.38	1.32
1	C	280	HIS	CE1-NE2	5.74	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	HIS	CE1-NE2	5.72	1.38	1.32
1	E	180	HIS	CE1-NE2	5.68	1.38	1.32
1	E	385	HIS	CE1-NE2	5.65	1.38	1.32
1	A	180	HIS	CE1-NE2	5.57	1.38	1.32
1	D	125	HIS	CE1-NE2	5.44	1.38	1.32
1	A	125	HIS	CE1-NE2	5.38	1.38	1.32
1	C	385	HIS	CE1-NE2	5.37	1.38	1.32
1	D	201	HIS	CE1-NE2	5.32	1.37	1.32
1	C	125	HIS	CE1-NE2	5.32	1.37	1.32
1	E	106	HIS	CE1-NE2	5.30	1.37	1.32
1	E	274	HIS	CE1-NE2	5.15	1.37	1.32
1	D	481	HIS	CE1-NE2	5.04	1.37	1.32
1	A	106	HIS	CE1-NE2	5.03	1.37	1.32
1	D	431	HIS	CE1-NE2	5.02	1.37	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	GLU	CB-CA-C	-6.58	97.85	109.62
1	A	165	ASP	CA-CB-CG	6.22	118.82	112.60
1	E	225	GLU	CB-CA-C	-6.16	98.59	109.62
1	A	225	GLU	CB-CA-C	-5.90	99.06	109.62
1	D	232	ARG	CB-CA-C	-5.65	101.94	110.92
1	C	227	ASP	CA-CB-CG	5.45	118.05	112.60
1	E	232	ARG	CB-CA-C	-5.38	102.36	110.92
1	A	232	ARG	CB-CA-C	-5.36	102.41	110.92
1	C	232	ARG	CB-CA-C	-5.35	102.41	110.92
1	C	225	GLU	CB-CA-C	-5.35	100.05	109.62
1	C	165	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	274	HIS	N-CA-C	-5.11	103.59	110.24
1	E	227	ASP	CA-CB-CG	5.09	117.69	112.60

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain
1	A	163	ARG	Sidechain
1	A	198	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	295	ARG	Sidechain
1	A	367	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	382	ARG	Sidechain
1	A	390	ARG	Sidechain
1	A	419	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	96	ARG	Sidechain
1	C	145	ARG	Sidechain
1	C	157	ARG	Sidechain
1	C	163	ARG	Sidechain
1	C	198	ARG	Sidechain
1	C	295	ARG	Sidechain
1	C	390	ARG	Sidechain
1	C	419	ARG	Sidechain
1	C	420	ARG	Sidechain
1	C	96	ARG	Sidechain
1	D	145	ARG	Sidechain
1	D	157	ARG	Sidechain
1	D	163	ARG	Sidechain
1	D	198	ARG	Sidechain
1	D	295	ARG	Sidechain
1	D	367	ARG	Sidechain
1	D	390	ARG	Sidechain
1	D	419	ARG	Sidechain
1	D	420	ARG	Sidechain
1	D	96	ARG	Sidechain
1	E	145	ARG	Sidechain
1	E	157	ARG	Sidechain
1	E	163	ARG	Sidechain
1	E	198	ARG	Sidechain
1	E	367	ARG	Sidechain
1	E	390	ARG	Sidechain
1	E	419	ARG	Sidechain
1	E	420	ARG	Sidechain
1	E	96	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	3247	0	3186	51	0
1	C	3246	0	3192	50	0
1	D	3251	0	3197	53	0
1	E	3256	0	3202	47	0
2	A	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	2	0
2	E	15	0	7	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	6	0	7	1	0
4	C	6	0	7	1	0
4	D	6	0	7	1	0
4	E	6	0	7	2	0
All	All	13088	0	12833	194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (194) 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:D:94:ARG:HH21	1:D:94:ARG:HG3	1.39	0.87
1:C:175:THR:HG23	2:C:501:PLP:O2P	1.91	0.70
1:D:420:ARG:NH2	1:D:449:ASP:OD2	2.24	0.70
1:E:182:ILE:HG22	1:E:213:MET:HE1	1.74	0.69
1:A:420:ARG:NH2	1:A:449:ASP:OD2	2.25	0.69
1:D:182:ILE:HG22	1:D:213:MET:HE1	1.76	0.68
1:A:182:ILE:HG22	1:A:213:MET:HE1	1.75	0.67
1:C:182:ILE:HG22	1:C:213:MET:HE1	1.74	0.67
1:C:420:ARG:NH2	1:C:449:ASP:OD2	2.27	0.67
1:D:94:ARG:HH21	1:D:94:ARG:CG	2.06	0.67
1:C:374:GLN:HG3	1:C:378:GLN:HE21	1.61	0.66
1:C:252:THR:HG23	4:C:503:GOL:H31	1.77	0.66
1:E:420:ARG:NH2	1:E:449:ASP:OD2	2.28	0.66
1:C:350:MET:HE3	1:D:350:MET:HE3	1.77	0.66
1:E:175:THR:HG23	2:E:501:PLP:O1P	1.98	0.64
1:A:374:GLN:HG3	1:A:378:GLN:HE21	1.64	0.62
1:A:350:MET:HE3	1:E:350:MET:HE3	1.81	0.62
1:D:175:THR:HG23	2:D:501:PLP:O1P	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:GLN:HG3	1:D:378:GLN:HE21	1.66	0.61
1:A:429:ILE:HD12	1:A:470:GLU:HG2	1.83	0.60
1:A:175:THR:HG23	2:A:501:PLP:O2P	2.02	0.59
1:E:111:TYR:OH	4:E:503:GOL:O1	2.16	0.59
1:C:85:GLU:CD	1:D:367:ARG:HH11	2.10	0.59
1:D:429:ILE:HD12	1:D:470:GLU:HG2	1.85	0.58
1:E:232:ARG:HH22	1:E:269:GLU:HG3	1.69	0.58
1:C:232:ARG:HH22	1:C:269:GLU:HG3	1.68	0.57
1:C:466:CYS:O	1:C:476:CYS:SG	2.64	0.55
1:D:195:TYR:HB2	1:D:245:LEU:CD2	2.37	0.55
1:E:374:GLN:HG3	1:E:378:GLN:HE21	1.70	0.55
1:D:286:PHE:CD2	1:D:290:MET:HG3	2.41	0.55
1:A:195:TYR:HB2	1:A:245:LEU:CD2	2.37	0.55
1:A:286:PHE:CD2	1:A:290:MET:HG3	2.43	0.54
1:E:195:TYR:HB2	1:E:245:LEU:CD2	2.39	0.53
1:C:286:PHE:CD2	1:C:290:MET:HG3	2.44	0.53
1:D:466:CYS:O	1:D:476:CYS:SG	2.67	0.53
1:E:466:CYS:O	1:E:476:CYS:SG	2.67	0.53
1:A:466:CYS:O	1:A:476:CYS:SG	2.67	0.52
1:E:320:MET:HE1	1:E:360:PHE:CG	2.44	0.52
1:C:195:TYR:HB2	1:C:245:LEU:CD2	2.39	0.52
1:C:320:MET:HE1	1:C:360:PHE:CG	2.45	0.52
1:D:320:MET:HE1	1:D:360:PHE:CG	2.44	0.52
1:C:182:ILE:CG2	1:C:213:MET:HE1	2.40	0.52
1:C:104:LYS:O	1:C:442:LYS:HE2	2.10	0.52
1:D:410:GLU:OE2	1:D:454:ARG:NH1	2.33	0.52
1:E:104:LYS:O	1:E:442:LYS:HE2	2.10	0.51
1:E:165:ASP:O	1:E:329:MET:HB2	2.10	0.51
1:A:165:ASP:O	1:A:329:MET:HB2	2.11	0.51
1:A:320:MET:HE1	1:A:360:PHE:CG	2.46	0.51
1:E:182:ILE:CG2	1:E:213:MET:HE1	2.40	0.51
1:A:477:ILE:CG2	1:A:477:ILE:O	2.59	0.50
1:D:429:ILE:CD1	1:D:470:GLU:HG2	2.41	0.50
1:A:410:GLU:OE2	1:A:454:ARG:NH1	2.33	0.50
1:E:286:PHE:CD2	1:E:290:MET:HG3	2.45	0.50
1:A:260:LEU:HD11	1:A:305:ILE:HD11	1.92	0.50
1:A:481:HIS:O	1:A:482:LYS:C	2.53	0.50
1:D:481:HIS:O	1:D:482:LYS:C	2.54	0.50
1:E:260:LEU:HD11	1:E:305:ILE:HD11	1.92	0.50
1:C:249:ILE:HB	1:C:283:GLY:HA2	1.94	0.49
1:D:260:LEU:HD11	1:D:305:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:ILE:CG2	1:D:477:ILE:O	2.61	0.49
1:C:165:ASP:O	1:C:329:MET:HB2	2.12	0.49
1:A:232:ARG:HH22	1:A:269:GLU:HG3	1.78	0.49
1:A:429:ILE:CD1	1:A:470:GLU:HG2	2.42	0.49
1:C:410:GLU:OE2	1:C:454:ARG:NH1	2.34	0.48
1:A:182:ILE:CG2	1:A:213:MET:HE1	2.40	0.48
1:C:77:ASN:C	1:C:77:ASN:HD22	2.21	0.48
1:D:165:ASP:O	1:D:329:MET:HB2	2.14	0.48
1:D:211:TYR:HD2	1:D:213:MET:CE	2.27	0.48
1:D:182:ILE:CG2	1:D:213:MET:HE1	2.43	0.48
1:E:335:LEU:O	1:E:336:SER:C	2.57	0.48
1:C:245:LEU:CD1	1:C:267:LEU:HD11	2.44	0.48
1:C:350:MET:CE	1:D:350:MET:HE3	2.42	0.48
1:E:249:ILE:HB	1:E:283:GLY:HA2	1.95	0.47
1:E:477:ILE:O	1:E:477:ILE:CG2	2.61	0.47
1:A:249:ILE:HB	1:A:283:GLY:HA2	1.96	0.47
1:C:335:LEU:O	1:C:336:SER:C	2.58	0.47
1:E:245:LEU:CD1	1:E:267:LEU:HD11	2.44	0.47
1:D:104:LYS:O	1:D:442:LYS:HE2	2.14	0.47
1:D:249:ILE:HB	1:D:283:GLY:HA2	1.94	0.47
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.96	0.47
1:D:481:HIS:C	1:D:483:ALA:N	2.73	0.47
1:A:409:PHE:HE1	1:A:432:VAL:HG23	1.79	0.47
1:C:260:LEU:HD11	1:C:305:ILE:HD11	1.96	0.47
1:D:335:LEU:O	1:D:336:SER:C	2.57	0.47
1:A:335:LEU:O	1:A:336:SER:C	2.58	0.47
1:A:481:HIS:C	1:A:483:ALA:N	2.73	0.47
1:E:357:ALA:HB3	1:E:358:PRO:HD3	1.97	0.47
1:D:357:ALA:HB3	1:D:358:PRO:HD3	1.96	0.46
1:D:232:ARG:HH22	1:D:269:GLU:HG3	1.80	0.46
1:D:478:CYS:HB2	1:D:479:PRO:HD2	1.96	0.46
1:E:313:HIS:H	1:E:313:HIS:CD2	2.34	0.46
1:C:357:ALA:HB3	1:C:358:PRO:HD3	1.96	0.46
1:A:104:LYS:O	1:A:442:LYS:HE2	2.15	0.46
1:C:477:ILE:O	1:C:477:ILE:CG2	2.63	0.46
1:E:410:GLU:OE2	1:E:454:ARG:NH1	2.34	0.46
1:C:211:TYR:HD2	1:C:213:MET:CE	2.29	0.45
1:C:313:HIS:CD2	1:C:313:HIS:H	2.33	0.45
1:D:409:PHE:HE1	1:D:432:VAL:HG23	1.81	0.45
1:E:481:HIS:O	1:E:482:LYS:C	2.59	0.45
1:A:186:ARG:HD2	1:E:212:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:MET:HG2	1:A:400:LEU:N	2.31	0.45
1:C:409:PHE:HE1	1:C:432:VAL:HG23	1.81	0.45
1:A:361:LEU:O	1:A:365:LEU:HG	2.16	0.45
1:D:245:LEU:CD1	1:D:267:LEU:HD11	2.47	0.45
1:E:471:VAL:HG13	1:E:475:ASN:HB2	1.98	0.45
2:D:501:PLP:O3P	4:D:503:GOL:H32	2.17	0.44
1:E:211:TYR:HD2	1:E:213:MET:CE	2.29	0.44
1:A:245:LEU:CD1	1:A:267:LEU:HD11	2.48	0.44
1:D:361:LEU:O	1:D:365:LEU:HG	2.17	0.44
1:E:361:LEU:O	1:E:365:LEU:HG	2.17	0.44
1:E:145:ARG:N	1:E:146:PRO:CD	2.81	0.44
1:C:83:ASP:OD1	1:E:94:ARG:NH1	2.49	0.44
1:D:316:VAL:HG13	1:D:364:THR:HG21	2.00	0.44
1:A:211:TYR:HD2	1:A:213:MET:CE	2.31	0.44
1:C:361:LEU:O	1:C:365:LEU:HG	2.17	0.44
1:C:316:VAL:HG13	1:C:364:THR:HG21	1.99	0.44
1:D:283:GLY:O	1:D:284:ALA:C	2.61	0.44
1:E:106:HIS:CE1	1:E:109:TYR:HB2	2.53	0.44
1:C:195:TYR:HB2	1:C:245:LEU:HD22	1.99	0.44
1:D:286:PHE:HD2	1:D:290:MET:HG3	1.81	0.44
1:D:357:ALA:N	1:D:358:PRO:CD	2.81	0.44
1:D:474:ASN:OD1	1:D:474:ASN:N	2.51	0.44
1:C:145:ARG:N	1:C:146:PRO:CD	2.81	0.44
1:D:313:HIS:H	1:D:313:HIS:CD2	2.36	0.44
1:E:357:ALA:N	1:E:358:PRO:CD	2.81	0.44
1:E:180:HIS:HA	1:E:349:ILE:HD11	1.99	0.44
1:C:357:ALA:N	1:C:358:PRO:CD	2.81	0.43
1:C:374:GLN:CG	1:C:378:GLN:HE21	2.30	0.43
1:A:350:MET:CE	1:E:350:MET:HE3	2.46	0.43
1:C:95:TYR:OH	1:D:143:HIS:O	2.35	0.43
1:C:474:ASN:OD1	1:C:474:ASN:N	2.50	0.43
1:D:145:ARG:N	1:D:146:PRO:CD	2.81	0.43
1:C:274:HIS:O	1:C:275:ASP:CB	2.66	0.43
1:A:128:ILE:HG22	1:A:355:GLY:HA3	2.00	0.43
1:C:283:GLY:O	1:C:284:ALA:C	2.61	0.43
1:C:334:VAL:O	1:C:334:VAL:CG1	2.67	0.43
1:C:471:VAL:HG13	1:C:475:ASN:HB2	2.00	0.43
1:E:409:PHE:HE1	1:E:432:VAL:HG23	1.84	0.43
1:A:374:GLN:HG3	1:A:378:GLN:NE2	2.33	0.42
1:C:180:HIS:HA	1:C:349:ILE:HD11	2.00	0.42
1:D:94:ARG:CG	1:D:94:ARG:NH2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:HIS:CE1	1:D:109:TYR:HB2	2.53	0.42
1:A:283:GLY:O	1:A:284:ALA:C	2.62	0.42
1:C:94:ARG:O	1:C:98:THR:HG23	2.19	0.42
1:D:471:VAL:HG13	1:D:475:ASN:HB2	2.01	0.42
1:A:145:ARG:N	1:A:146:PRO:CD	2.81	0.42
1:E:286:PHE:HD2	1:E:290:MET:HG3	1.82	0.42
1:A:96:ARG:O	1:A:100:VAL:HG23	2.20	0.42
1:C:96:ARG:O	1:C:100:VAL:HG23	2.19	0.42
1:E:128:ILE:HG22	1:E:355:GLY:HA3	2.02	0.42
1:D:195:TYR:HB2	1:D:245:LEU:HD22	2.02	0.42
1:E:94:ARG:O	1:E:98:THR:HG23	2.20	0.42
1:A:195:TYR:HB2	1:A:245:LEU:HD22	2.02	0.42
1:D:110:PRO:O	1:D:314:LYS:HA	2.20	0.42
1:A:474:ASN:OD1	1:A:474:ASN:N	2.50	0.42
1:D:334:VAL:O	1:D:334:VAL:CG1	2.68	0.42
1:D:96:ARG:O	1:D:100:VAL:HG23	2.19	0.42
1:E:195:TYR:HB2	1:E:245:LEU:HD22	2.01	0.42
1:E:283:GLY:O	1:E:284:ALA:C	2.62	0.42
1:A:355:GLY:C	1:A:358:PRO:HD2	2.45	0.41
1:D:305:ILE:HD13	1:D:305:ILE:HA	1.81	0.41
1:D:399:MET:CB	1:D:471:VAL:HG22	2.50	0.41
1:E:96:ARG:O	1:E:100:VAL:HG23	2.20	0.41
1:E:316:VAL:HG13	1:E:364:THR:HG21	2.02	0.41
1:A:286:PHE:HD2	1:A:290:MET:HG3	1.84	0.41
1:C:286:PHE:HD2	1:C:290:MET:HG3	1.84	0.41
1:D:128:ILE:HG22	1:D:355:GLY:HA3	2.02	0.41
1:A:313:HIS:H	1:A:313:HIS:CD2	2.38	0.41
1:A:334:VAL:O	1:A:334:VAL:CG1	2.68	0.41
1:E:67:THR:HG22	1:E:68:SER:H	1.86	0.41
1:E:274:HIS:CD2	1:E:274:HIS:H	2.37	0.41
1:A:357:ALA:N	1:A:358:PRO:CD	2.82	0.41
1:C:106:HIS:CE1	1:C:109:TYR:HB2	2.55	0.41
1:D:355:GLY:C	1:D:358:PRO:HD2	2.46	0.41
1:C:147:PHE:O	1:C:151:VAL:HG23	2.21	0.41
1:D:399:MET:HG2	1:D:400:LEU:N	2.36	0.41
1:E:110:PRO:HG3	4:E:503:GOL:H32	2.03	0.41
1:E:429:ILE:HD12	1:E:470:GLU:HB3	2.02	0.41
1:A:110:PRO:O	1:A:314:LYS:HA	2.21	0.41
1:A:286:PHE:CE2	1:A:290:MET:HG3	2.56	0.41
1:C:195:TYR:CD1	1:C:216:GLU:HB3	2.56	0.41
1:C:429:ILE:HD12	1:C:470:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:LYS:HG3	1:D:382:ARG:HH21	1.85	0.41
1:E:243:ALA:O	1:E:277:PHE:HA	2.21	0.41
1:C:77:ASN:C	1:C:77:ASN:ND2	2.78	0.41
1:A:72:THR:O	1:A:84:LYS:NZ	2.54	0.40
1:A:106:HIS:CE1	1:A:109:TYR:HB2	2.56	0.40
1:A:316:VAL:HG13	1:A:364:THR:HG21	2.02	0.40
1:A:111:TYR:OH	4:A:503:GOL:H12	2.21	0.40
1:A:180:HIS:HA	1:A:349:ILE:HD11	2.03	0.40
1:E:334:VAL:O	1:E:334:VAL:CG1	2.68	0.40
1:A:410:GLU:CD	1:A:454:ARG:HH12	2.25	0.40
1:A:477:ILE:O	1:A:477:ILE:HG22	2.21	0.40
1:C:243:ALA:O	1:C:277:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/418 (97%)	380 (94%)	23 (6%)	1 (0%)	43	62
1	C	403/418 (96%)	379 (94%)	24 (6%)	0	100	100
1	D	404/418 (97%)	382 (95%)	21 (5%)	1 (0%)	43	62
1	E	405/418 (97%)	381 (94%)	24 (6%)	0	100	100
All	All	1616/1672 (97%)	1522 (94%)	92 (6%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	LYS
1	D	482	LYS

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	352/361 (98%)	325 (92%)	27 (8%)	12	25
1	C	353/361 (98%)	322 (91%)	31 (9%)	9	20
1	D	353/361 (98%)	324 (92%)	29 (8%)	10	23
1	E	353/361 (98%)	325 (92%)	28 (8%)	11	24
All	All	1411/1444 (98%)	1296 (92%)	115 (8%)	10	23

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	98	THR
1	A	101	GLU
1	A	113	LEU
1	A	124	GLN
1	A	188	MET
1	A	220	THR
1	A	265	LYS
1	A	288	LEU
1	A	290	MET
1	A	299	VAL
1	A	300	THR
1	A	309	SER
1	A	310	VAL
1	A	320	MET
1	A	329	MET
1	A	330	GLU
1	A	332	ILE
1	A	406	THR
1	A	415	GLU
1	A	416	GLU
1	A	428	ASP
1	A	429	ILE
1	A	459	GLU

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Mol	Chain	Res	Type
1	A	467	LEU
1	A	471	VAL
1	A	474	ASN
1	C	67	THR
1	C	77	ASN
1	C	84	LYS
1	C	90	SER
1	C	98	THR
1	C	101	GLU
1	C	113	LEU
1	C	124	GLN
1	C	188	MET
1	C	220	THR
1	C	265	LYS
1	C	288	LEU
1	C	290	MET
1	C	294	LYS
1	C	299	VAL
1	C	309	SER
1	C	310	VAL
1	C	320	MET
1	C	329	MET
1	C	330	GLU
1	C	332	ILE
1	C	406	THR
1	C	415	GLU
1	C	416	GLU
1	C	428	ASP
1	C	429	ILE
1	C	460	ASP
1	C	467	LEU
1	C	469	SER
1	C	471	VAL
1	C	474	ASN
1	D	84	LYS
1	D	90	SER
1	D	94	ARG
1	D	98	THR
1	D	101	GLU
1	D	113	LEU
1	D	124	GLN
1	D	188	MET

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Mol	Chain	Res	Type
1	D	220	THR
1	D	265	LYS
1	D	288	LEU
1	D	290	MET
1	D	299	VAL
1	D	300	THR
1	D	309	SER
1	D	310	VAL
1	D	320	MET
1	D	329	MET
1	D	330	GLU
1	D	332	ILE
1	D	406	THR
1	D	415	GLU
1	D	416	GLU
1	D	428	ASP
1	D	429	ILE
1	D	439	THR
1	D	460	ASP
1	D	467	LEU
1	D	471	VAL
1	E	67	THR
1	E	90	SER
1	E	98	THR
1	E	101	GLU
1	E	113	LEU
1	E	124	GLN
1	E	188	MET
1	E	220	THR
1	E	265	LYS
1	E	274	HIS
1	E	288	LEU
1	E	290	MET
1	E	299	VAL
1	E	309	SER
1	E	310	VAL
1	E	320	MET
1	E	329	MET
1	E	330	GLU
1	E	332	ILE
1	E	406	THR
1	E	415	GLU

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Mol	Chain	Res	Type
1	E	416	GLU
1	E	428	ASP
1	E	429	ILE
1	E	460	ASP
1	E	467	LEU
1	E	471	VAL
1	E	482	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	105	ASN
1	A	106	HIS
1	A	124	GLN
1	A	139	ASN
1	A	246	ASN
1	A	313	HIS
1	A	378	GLN
1	A	431	HIS
1	C	105	ASN
1	C	106	HIS
1	C	122	GLN
1	C	124	GLN
1	C	139	ASN
1	C	246	ASN
1	C	313	HIS
1	C	356	HIS
1	C	378	GLN
1	C	383	ASN
1	C	431	HIS
1	D	106	HIS
1	D	124	GLN
1	D	139	ASN
1	D	246	ASN
1	D	313	HIS
1	D	356	HIS
1	D	378	GLN
1	D	431	HIS
1	E	106	HIS
1	E	124	GLN
1	E	139	ASN

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Mol	Chain	Res	Type
1	E	246	ASN
1	E	313	HIS
1	E	378	GLN
1	E	431	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
4	GOL	E	503	2	5,5,5	0.34	0	5,5,5	0.56	0
4	GOL	D	503	2	5,5,5	0.24	0	5,5,5	0.63	0
4	GOL	C	503	2	5,5,5	0.17	0	5,5,5	0.44	0
2	PLP	D	501	4	15,15,16	1.01	1 (6%)	21,22,23	1.48	3 (14%)
4	GOL	A	503	2	5,5,5	0.23	0	5,5,5	0.63	0
2	PLP	C	501	4	15,15,16	0.81	0	21,22,23	1.17	3 (14%)
2	PLP	E	501	4	15,15,16	1.00	0	21,22,23	1.13	2 (9%)
2	PLP	A	501	4	15,15,16	0.72	0	21,22,23	1.06	2 (9%)

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
4	GOL	E	503	2	-	2/4/4/4	-
4	GOL	D	503	2	-	2/4/4/4	-
4	GOL	C	503	2	-	3/4/4/4	-
2	PLP	D	501	4	-	0/6/6/8	0/1/1/1
4	GOL	A	503	2	-	4/4/4/4	-
2	PLP	C	501	4	-	3/6/6/8	0/1/1/1
2	PLP	E	501	4	-	4/6/6/8	0/1/1/1
2	PLP	A	501	4	-	2/6/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	PLP	C5-C4	2.16	1.43	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	PLP	C4A-C4-C5	5.02	126.11	120.94
2	C	501	PLP	O4P-C5A-C5	3.58	116.06	109.36
2	A	501	PLP	C4A-C4-C5	2.79	123.81	120.94
2	E	501	PLP	O4P-C5A-C5	2.68	114.37	109.36
2	E	501	PLP	C4A-C4-C5	2.47	123.48	120.94
2	D	501	PLP	C4A-C4-C3	-2.39	116.54	120.52
2	C	501	PLP	O3-C3-C4	2.22	123.90	118.10
2	C	501	PLP	C4A-C4-C5	2.06	123.06	120.94
2	A	501	PLP	O3P-P-O4P	-2.06	101.31	106.67
2	D	501	PLP	O3-C3-C2	2.05	121.83	117.58

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	PLP	C5A-O4P-P-O2P
2	E	501	PLP	C5A-O4P-P-O1P
4	A	503	GOL	O1-C1-C2-C3
4	A	503	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	503	GOL	C1-C2-C3-O3
4	D	503	GOL	C1-C2-C3-O3
4	E	503	GOL	O1-C1-C2-C3
4	E	503	GOL	O1-C1-C2-O2
4	A	503	GOL	O2-C2-C3-O3
4	D	503	GOL	O2-C2-C3-O3
2	C	501	PLP	C5A-O4P-P-O3P
4	C	503	GOL	C1-C2-C3-O3
2	A	501	PLP	C4-C5-C5A-O4P
2	E	501	PLP	C4-C5-C5A-O4P
2	C	501	PLP	C5A-O4P-P-O1P
2	A	501	PLP	C6-C5-C5A-O4P
2	E	501	PLP	C6-C5-C5A-O4P
4	C	503	GOL	O2-C2-C3-O3
2	E	501	PLP	C5A-O4P-P-O2P
4	C	503	GOL	O1-C1-C2-O2

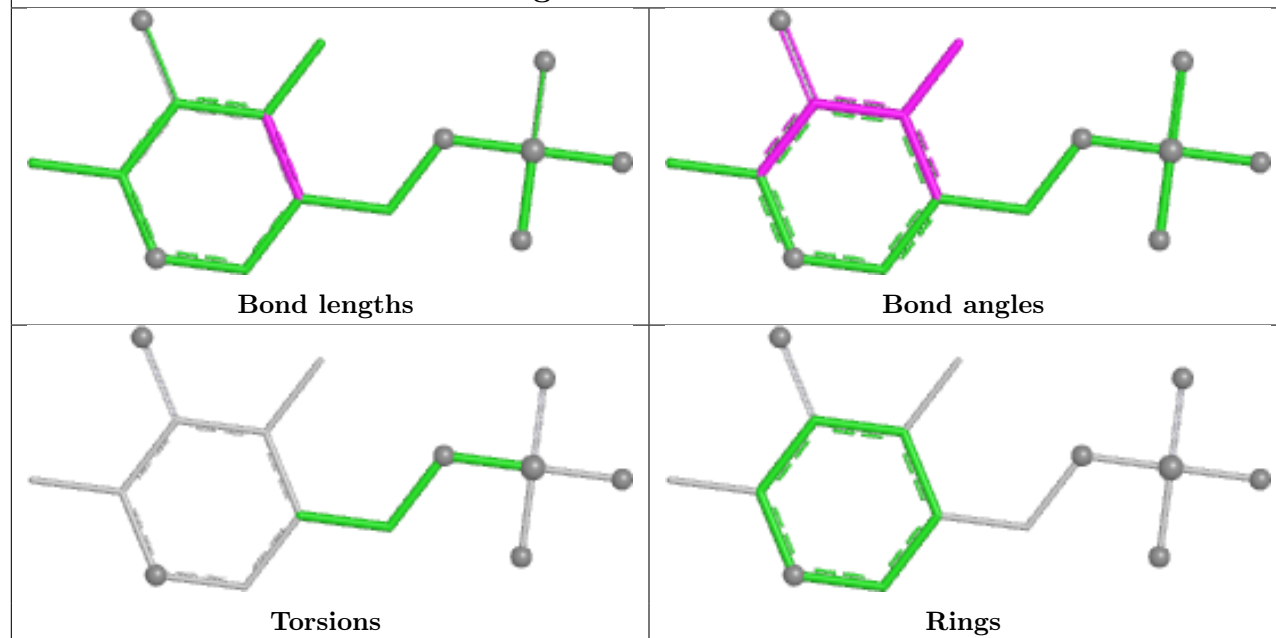
There are no ring outliers.

8 monomers are involved in 9 short contacts:

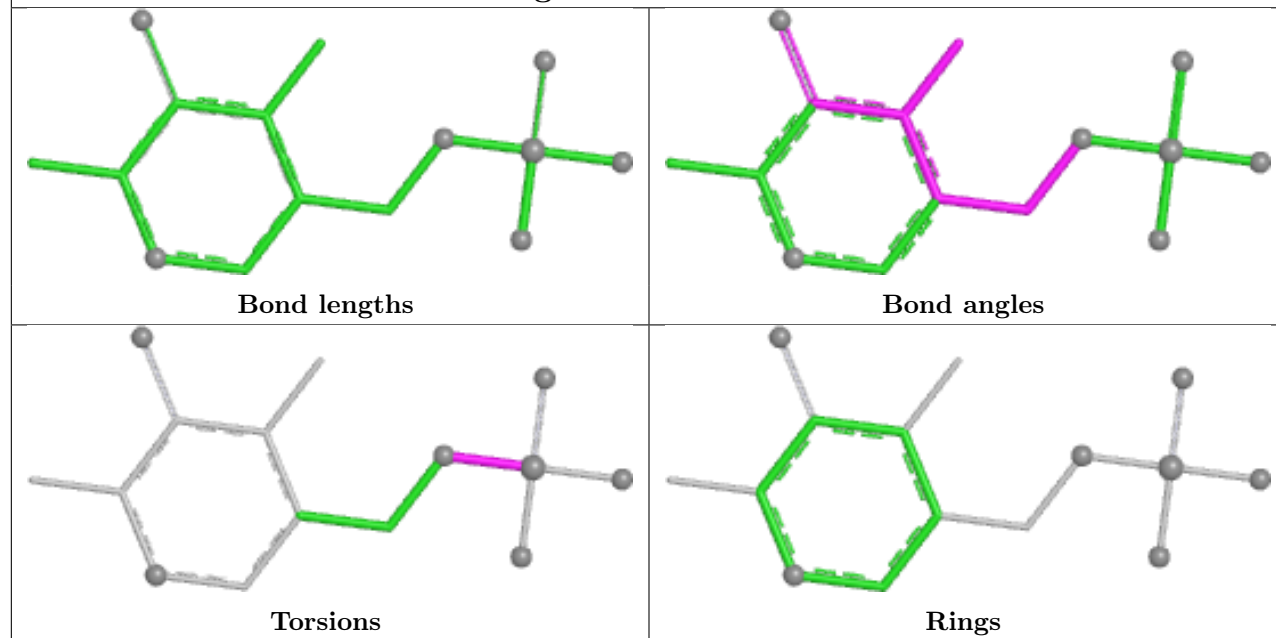
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	503	GOL	2	0
4	D	503	GOL	1	0
4	C	503	GOL	1	0
2	D	501	PLP	2	0
4	A	503	GOL	1	0
2	C	501	PLP	1	0
2	E	501	PLP	1	0
2	A	501	PLP	1	0

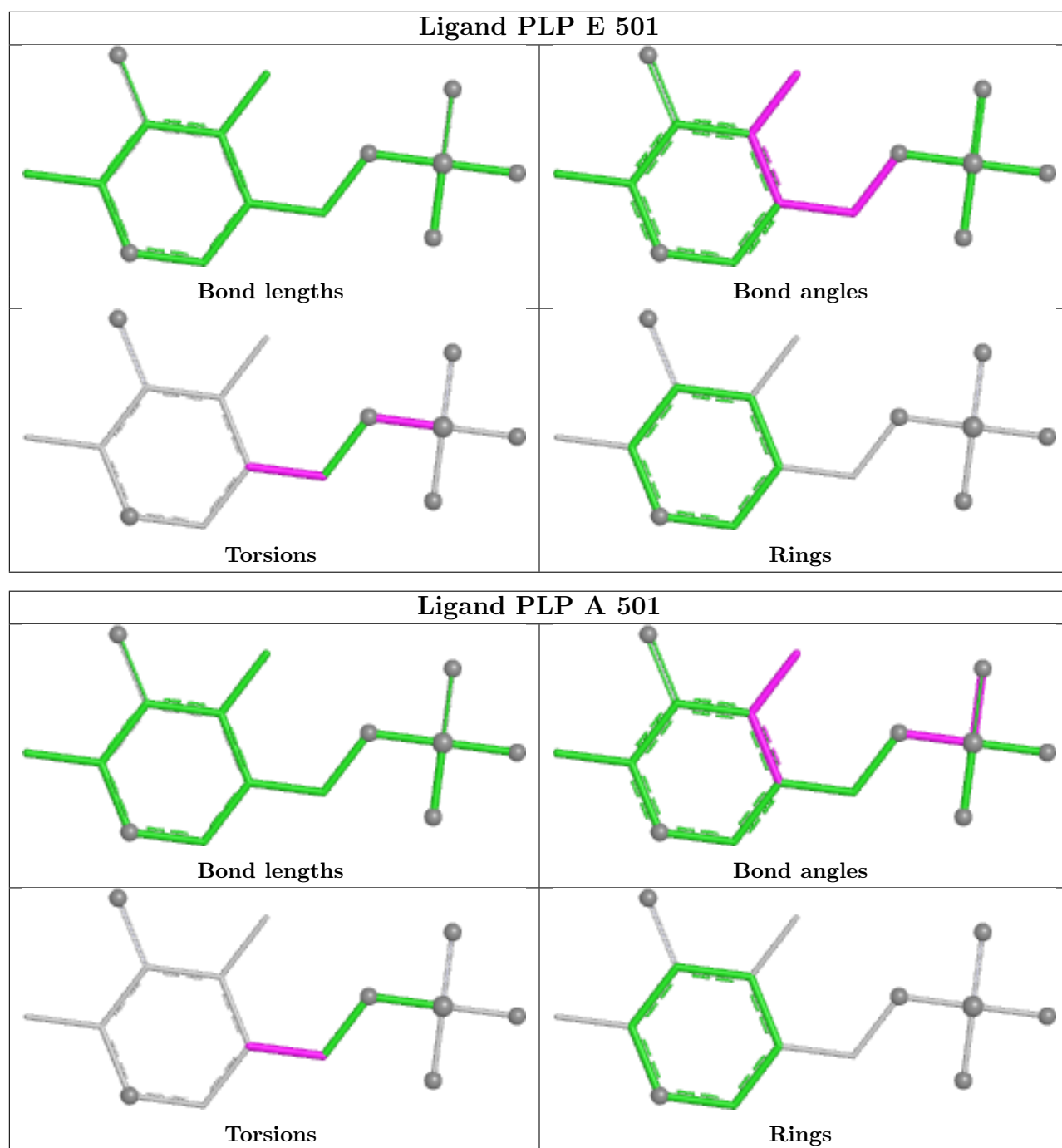
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand PLP D 501



Ligand PLP C 501





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	408/418 (97%)	0.73	31 (7%)	20	14	31, 57, 89, 120	0
1	C	407/418 (97%)	0.78	35 (8%)	16	12	27, 58, 91, 117	0
1	D	408/418 (97%)	0.40	24 (5%)	28	21	25, 47, 84, 107	0
1	E	409/418 (97%)	0.69	36 (8%)	15	12	31, 54, 85, 104	0
All	All	1632/1672 (97%)	0.65	126 (7%)	19	14	25, 55, 88, 120	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	484	ALA	6.6
1	E	462	SER	6.3
1	C	473	THR	5.7
1	C	416	GLU	5.6
1	A	473	THR	5.1
1	E	285	LEU	4.9
1	D	483	ALA	4.8
1	E	456	ILE	4.7
1	E	243	ALA	4.7
1	E	474	ASN	4.1
1	A	285	LEU	4.1
1	C	346	ASP	4.1
1	A	220	THR	4.1
1	A	132	GLY	4.1
1	C	163	ARG	3.9
1	A	483	ALA	3.8
1	D	125	HIS	3.8
1	E	346	ASP	3.7
1	C	219	ASP	3.7
1	E	475	ASN	3.7
1	C	243	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	297	PRO	3.6
1	C	166	TYR	3.6
1	E	458	TYR	3.6
1	A	458	TYR	3.5
1	E	140	TYR	3.5
1	D	454	ARG	3.5
1	A	336	SER	3.5
1	C	107	LEU	3.4
1	A	464	PRO	3.4
1	E	80	PHE	3.3
1	E	107	LEU	3.3
1	E	483	ALA	3.3
1	E	124	GLN	3.2
1	A	219	ASP	3.1
1	C	277	PHE	3.1
1	C	67	THR	3.1
1	C	336	SER	3.0
1	E	473	THR	3.0
1	D	336	SER	3.0
1	C	136	ILE	3.0
1	C	124	GLN	3.0
1	C	285	LEU	3.0
1	A	199	GLU	3.0
1	D	77	ASN	3.0
1	A	228	CYS	3.0
1	C	474	ASN	2.9
1	A	480	ALA	2.9
1	A	334	VAL	2.9
1	D	458	TYR	2.9
1	A	465	PRO	2.9
1	A	107	LEU	2.9
1	E	334	VAL	2.9
1	D	198	ARG	2.9
1	D	473	THR	2.9
1	A	264	ILE	2.8
1	E	214	GLU	2.8
1	D	285	LEU	2.8
1	C	240	ASP	2.8
1	C	220	THR	2.7
1	E	188	MET	2.7
1	A	85	GLU	2.6
1	C	316	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	67	THR	2.6
1	D	431	HIS	2.5
1	A	197	SER	2.5
1	D	80	PHE	2.5
1	A	297	PRO	2.5
1	A	429	ILE	2.5
1	D	132	GLY	2.5
1	E	242	PRO	2.4
1	E	461	GLY	2.4
1	E	432	VAL	2.4
1	A	111	TYR	2.4
1	E	76	VAL	2.4
1	C	197	SER	2.4
1	C	462	SER	2.4
1	E	472	GLY	2.4
1	E	459	GLU	2.4
1	C	458	TYR	2.4
1	A	477	ILE	2.4
1	D	349	ILE	2.4
1	C	297	PRO	2.3
1	C	301	PHE	2.3
1	E	416	GLU	2.3
1	E	132	GLY	2.3
1	C	214	GLU	2.3
1	A	476	CYS	2.3
1	C	398	ALA	2.3
1	D	124	GLN	2.3
1	D	219	ASP	2.3
1	A	335	LEU	2.2
1	C	68	SER	2.2
1	C	429	ILE	2.2
1	C	275	ASP	2.2
1	D	464	PRO	2.2
1	D	346	ASP	2.2
1	C	108	GLY	2.2
1	E	333	LYS	2.2
1	D	396	ILE	2.2
1	E	420	ARG	2.2
1	C	227	ASP	2.2
1	C	80	PHE	2.2
1	E	316	VAL	2.1
1	A	67	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	168	GLY	2.1
1	C	335	LEU	2.1
1	D	335	LEU	2.1
1	E	465	PRO	2.1
1	E	236	LEU	2.1
1	E	266	THR	2.1
1	A	456	ILE	2.1
1	A	215	CYS	2.1
1	D	476	CYS	2.1
1	A	191	ASP	2.1
1	A	410	GLU	2.1
1	D	474	ASN	2.0
1	A	454	ARG	2.0
1	C	480	ALA	2.0
1	D	191	ASP	2.0
1	C	162	GLU	2.0
1	D	67	THR	2.0
1	A	162	GLU	2.0
1	E	75	GLU	2.0
1	E	240	ASP	2.0
1	C	140	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

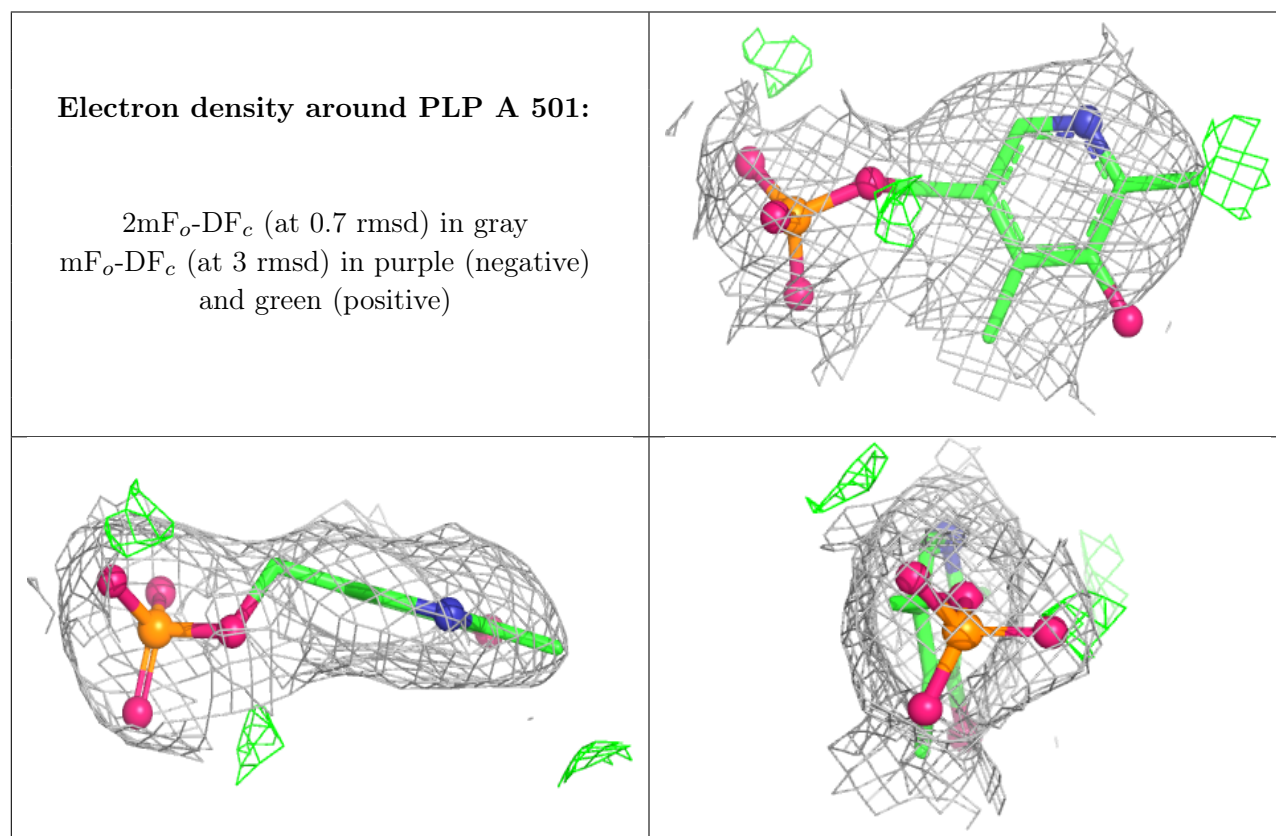
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	503	6/6	0.90	0.12	42,56,62,66	0
4	GOL	E	503	6/6	0.90	0.13	48,56,58,67	0

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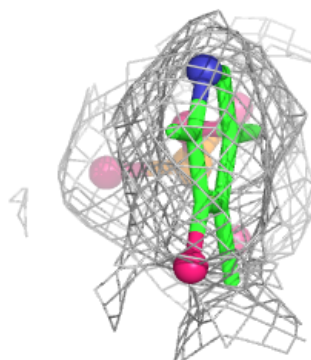
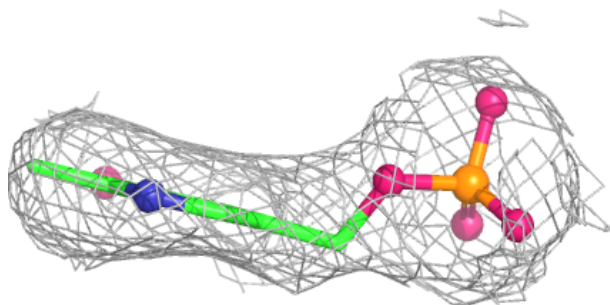
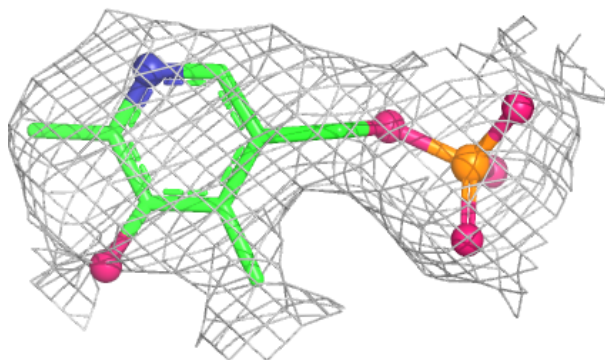
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	D	503	6/6	0.92	0.08	34,38,42,42	0
4	GOL	A	503	6/6	0.92	0.10	45,55,58,61	0
2	PLP	A	501	15/16	0.93	0.12	50,63,69,71	0
2	PLP	E	501	15/16	0.93	0.12	45,47,53,54	0
2	PLP	D	501	15/16	0.95	0.09	33,37,48,50	0
2	PLP	C	501	15/16	0.95	0.09	45,57,64,70	0
3	ZN	C	502	1/1	0.99	0.05	93,93,93,93	0
3	ZN	D	502	1/1	0.99	0.03	61,61,61,61	0
3	ZN	A	502	1/1	0.99	0.07	69,69,69,69	0
3	ZN	E	502	1/1	1.00	0.04	61,61,61,61	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.

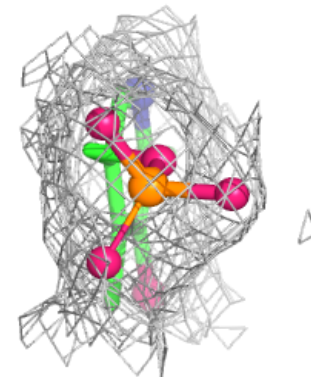
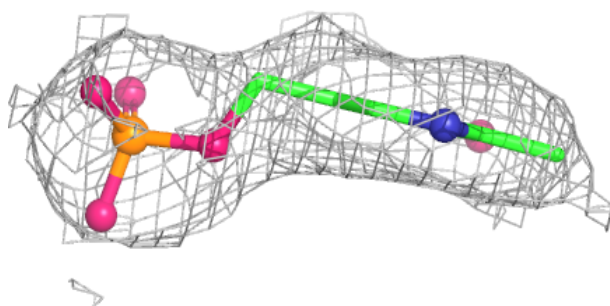
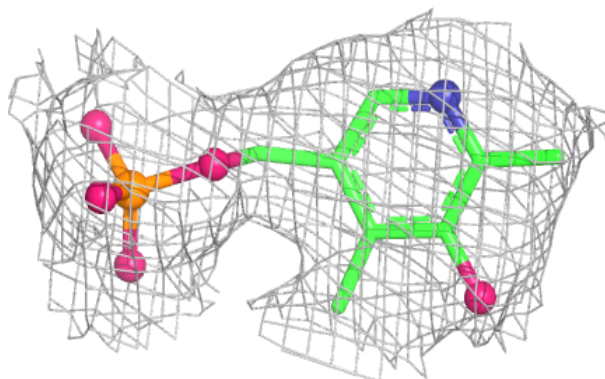


Electron density around PLP E 501:

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

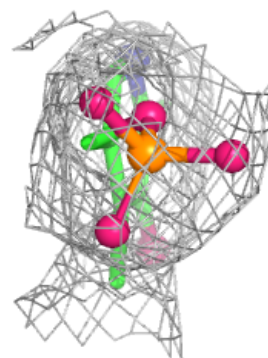
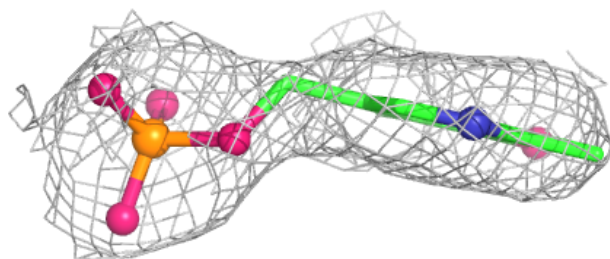
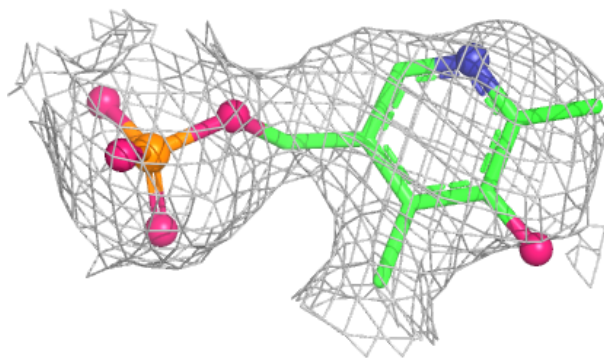
**Electron density around PLP D 501:**

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



Electron density around PLP C 501:

$2mF_o-DF_c$ (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.