



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:26 PM UTC

PDB ID : 8X0P / pdb_00008x0p
Title : Crystal structure of Tyrosine decarboxylase in complex with the cofactor PLP and inhibitor carbidopa
Authors : Wang, H.; Yu, J.; Yao, M.
Deposited on : 2023-11-05
Resolution : 3.35 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:

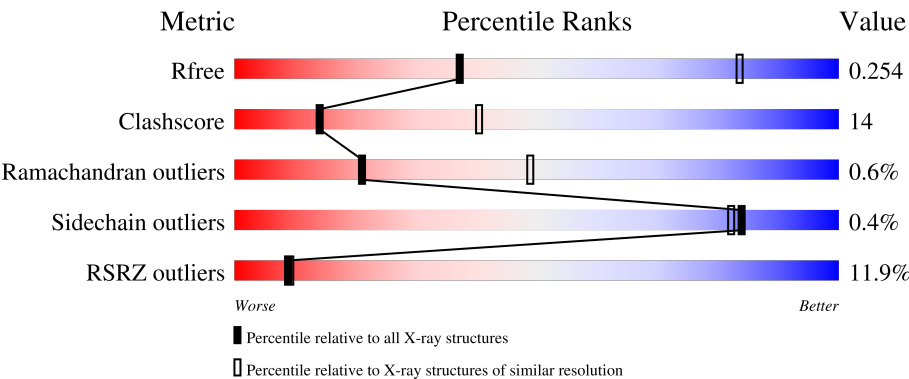
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	531	71%19%• 9%
1	B	531	% 71%19%• 9%
1	C	531	71%20%9%
1	D	531	68%23%• 9%
1	E	531	31% 50%39%• 10%

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Mol	Chain	Length	Quality of chain
1	F	531	

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:

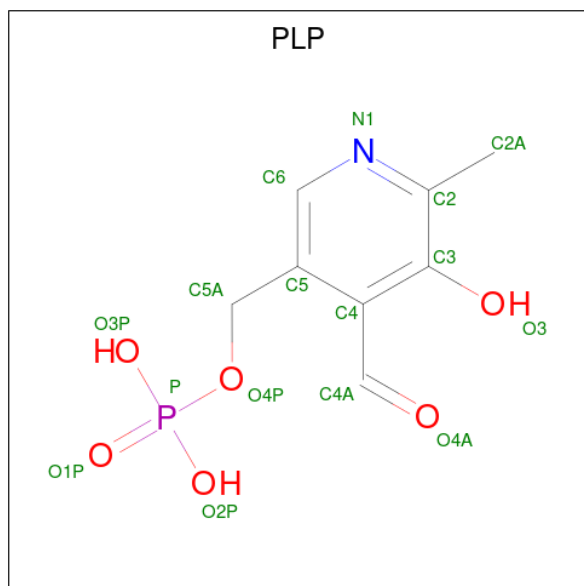
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	E	601	-	-	X	-
2	PLP	F	602	-	-	X	-

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 Tyrosine/DOPA decarboxylase 2.

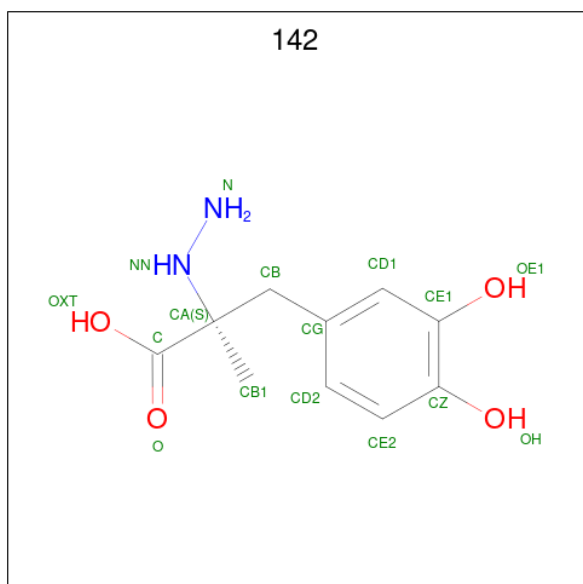
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total 3825	C 2456	N 642	O 703	S 24	0	0	0
1	B	483	Total 3808	C 2446	N 638	O 700	S 24	0	0	0
1	C	485	Total 3825	C 2456	N 642	O 703	S 24	0	0	0
1	D	483	Total 3808	C 2446	N 638	O 700	S 24	0	0	0
1	E	479	Total 3787	C 2434	N 634	O 695	S 24	0	0	0
1	F	474	Total 3732	C 2402	N 624	O 682	S 24	0	0	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $\text{C}_8\text{H}_{10}\text{NO}_6\text{P}$) (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	B	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		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CARBIDOPA (CCD ID: 142) (formula: $C_{10}H_{14}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	10	2	4		
3	B	1	Total	C	N	O	0	0
			16	10	2	4		
3	C	1	Total	C	N	O	0	0
			16	10	2	4		
3	D	1	Total	C	N	O	0	0
			16	10	2	4		
3	F	1	Total	C	N	O	0	0
			16	10	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			16	10	2	4		

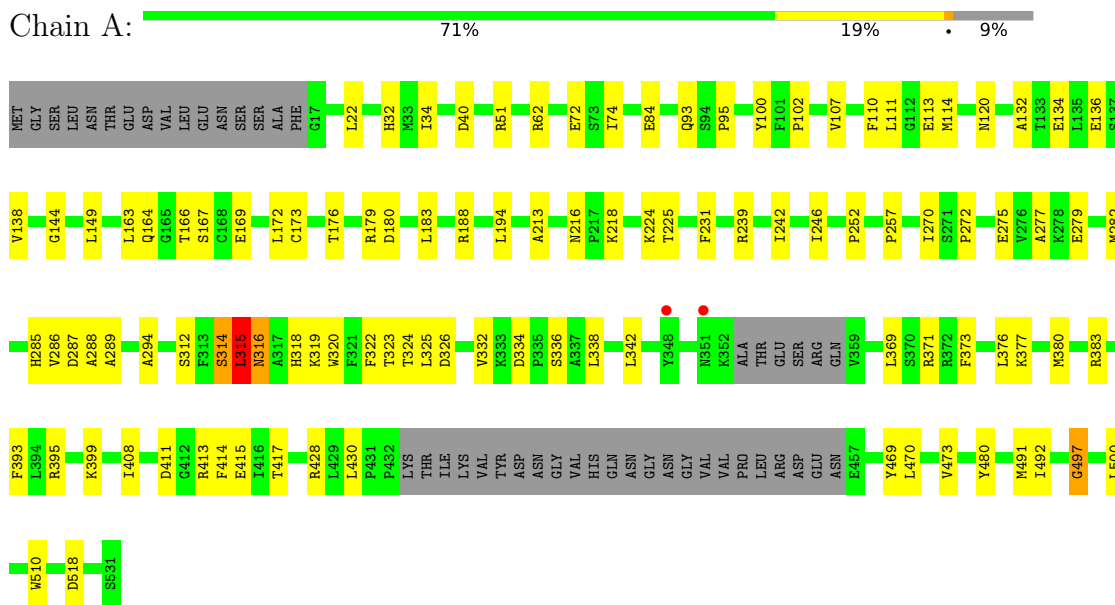
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	5	Total	O	0	0
			5	5		
4	C	3	Total	O	0	0
			3	3		
4	D	2	Total	O	0	0
			2	2		

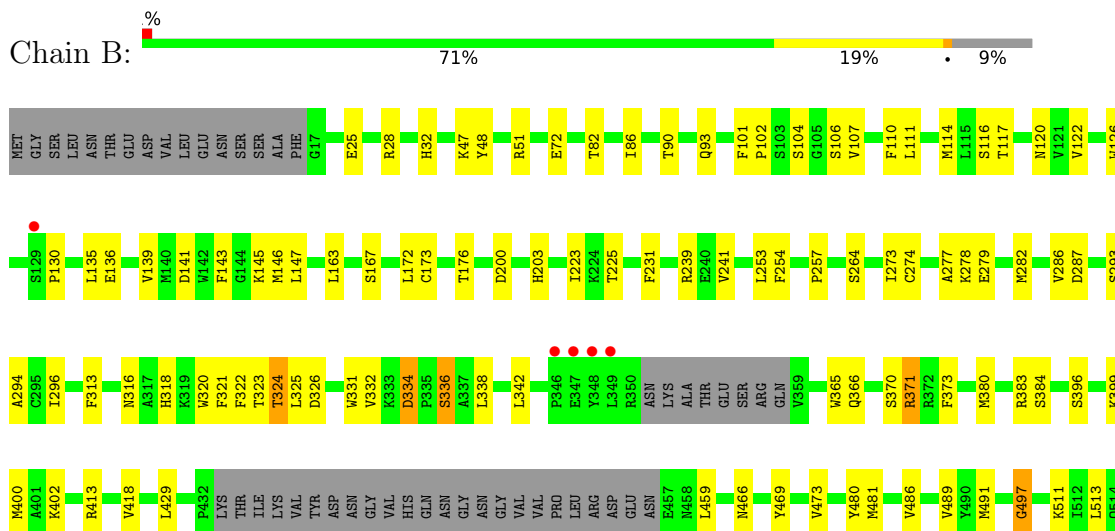
3 Residue-property plots [i](#)

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: Tyrosine/DOPA decarboxylase 2

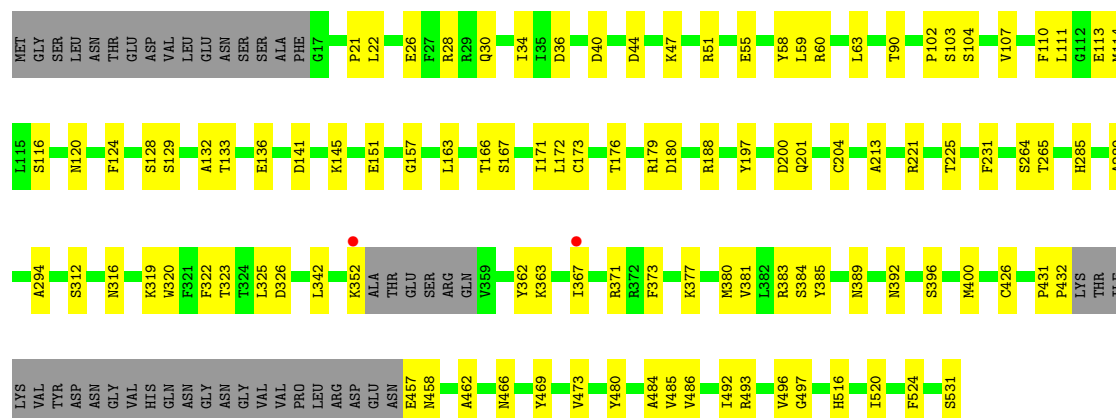


• Molecule 1: Tyrosine/DOPA decarboxylase 2



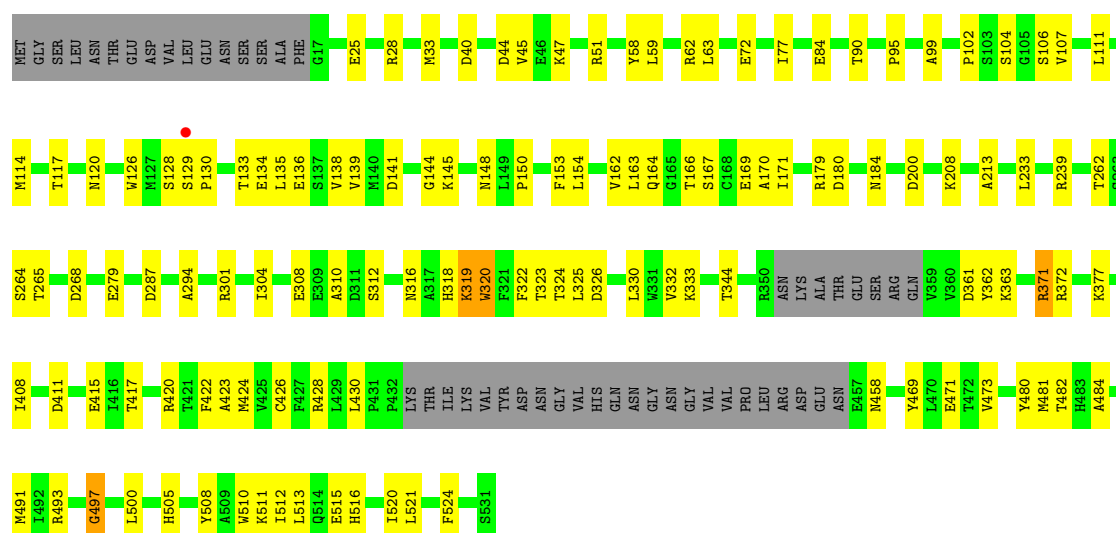
- Molecule 1: Tyrosine/DOPA decarboxylase 2

Chain C: 71% 20% 9%

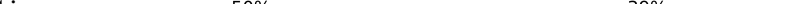


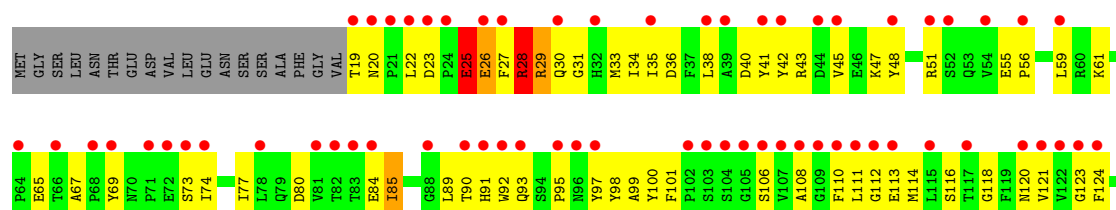
- Molecule 1: Tyrosine/DOPA decarboxylase 2

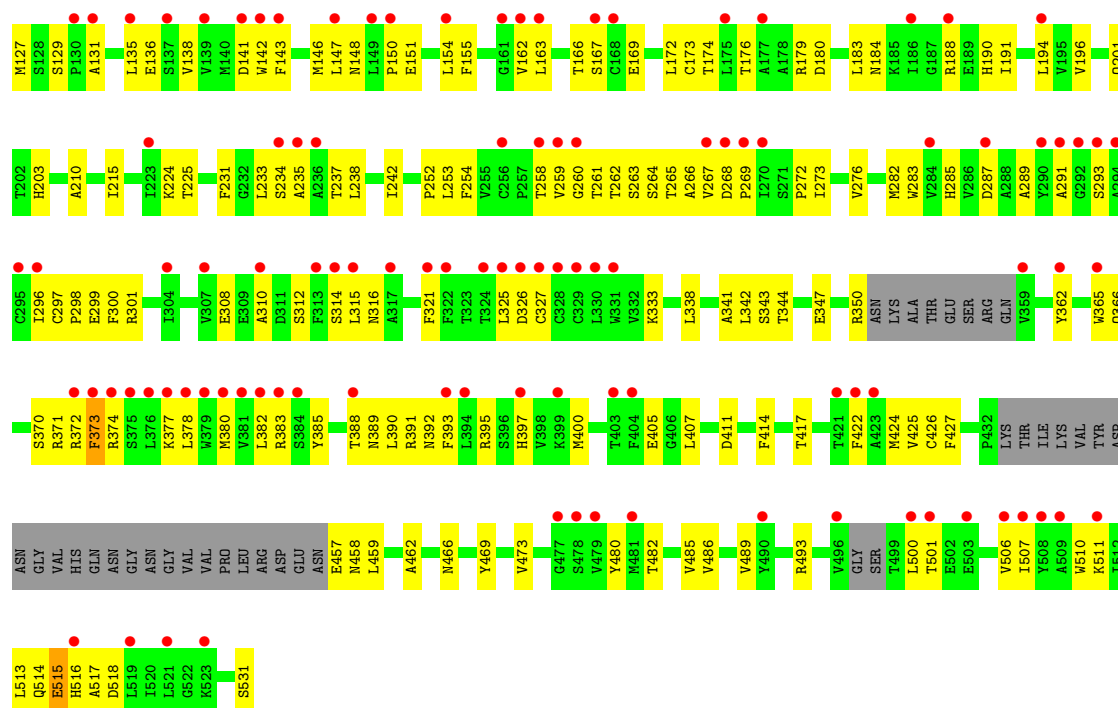
Chain D: 68% 23% 9%



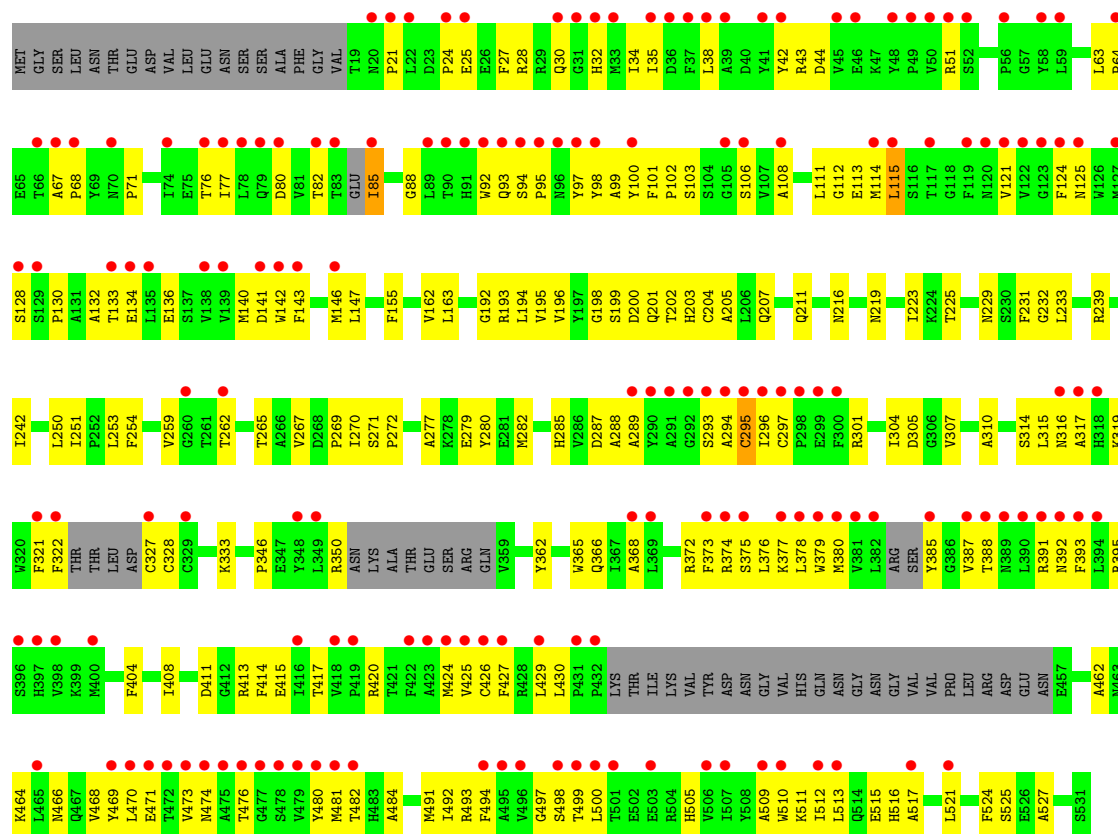
- Molecule 1: Tyrosine/DOPA decarboxylase 2

Chain E:  31% 50% 39% 10%





• Molecule 1: Tyrosine/DOPA decarboxylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	219.54Å 118.98Å 182.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.35 49.84 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.84-3.35) 99.7 (49.84-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.214 , 0.251 0.217 , 0.254	Depositor DCC
R_{free} test set	3470 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22985	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.37 % 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 3.2056e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 142, PLP

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	0.37	7/3919 (0.2%)	0.36	0/5321
1	B	0.28	2/3902 (0.1%)	0.37	0/5299
1	C	0.14	0/3919	0.33	0/5321
1	D	0.25	0/3902	0.40	0/5299
1	E	0.25	1/3880 (0.0%)	0.47	2/5268 (0.0%)
1	F	0.19	0/3822	0.46	0/5185
All	All	0.26	10/23344 (0.0%)	0.40	2/31693 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	ARG	C-O	-6.59	1.16	1.23
1	B	334	ASP	C-O	-6.58	1.18	1.24
1	A	287	ASP	C-O	-6.24	1.16	1.23
1	A	314	SER	C-O	-6.06	1.17	1.24
1	A	286	VAL	C-O	-5.90	1.17	1.24
1	A	289	ALA	CA-C	-5.84	1.45	1.52
1	A	315	LEU	C-O	-5.68	1.16	1.23
1	A	286	VAL	CA-CB	-5.41	1.48	1.54
1	E	25	GLU	CA-C	-5.07	1.46	1.52
1	A	289	ALA	C-O	-5.04	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	85	ILE	CA-C-N	5.02	123.40	120.24
1	E	85	ILE	C-N-CA	5.02	123.40	120.24

There are no chirality outliers.

There are no planarity outliers.

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	3825	0	3778	75	0
1	B	3808	0	3759	82	0
1	C	3825	0	3778	78	0
1	D	3808	0	3759	92	0
1	E	3787	0	3738	198	0
1	F	3732	0	3676	181	0
2	A	15	0	7	2	0
2	B	15	0	6	2	0
2	C	15	0	6	2	0
2	D	15	0	6	5	0
2	E	15	0	7	7	0
2	F	15	0	6	9	0
3	A	16	0	11	3	0
3	B	16	0	9	2	0
3	C	16	0	9	4	0
3	D	16	0	9	6	0
3	F	32	0	20	11	0
4	A	4	0	0	1	0
4	B	5	0	0	0	0
4	C	3	0	0	1	0
4	D	2	0	0	0	0
All	All	22985	0	22584	653	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 14.

All (653) 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:A:166:THR:HB	2:A:601:PLP:O3P	1.58	1.03
1:F:34:ILE:HG22	1:F:38:LEU:HD12	1.39	1.02
1:D:316:ASN:HD22	1:D:318:HIS:CE1	1.81	0.98
1:E:166:THR:OG1	1:E:169:GLU:HB2	1.66	0.95
1:E:385:TYR:HB3	1:E:389:ASN:HB2	1.50	0.93
1:F:34:ILE:HG22	1:F:38:LEU:CD1	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:LEU:HD11	1:E:84:GLU:HG3	1.56	0.88
1:F:101:PHE:O	3:F:603:142:HE2	1.74	0.87
1:F:317:ALA:HB3	1:F:327:CYS:HB3	1.57	0.86
1:F:285:HIS:HE2	1:F:314:SER:HG	1.10	0.85
1:B:116:SER:HB2	1:B:373:PHE:HB3	1.58	0.85
1:D:166:THR:HB	2:D:601:PLP:O3P	1.77	0.83
1:F:203:HIS:NE2	2:F:602:PLP:C4A	2.41	0.83
1:D:316:ASN:ND2	1:D:318:HIS:CE1	2.47	0.82
1:E:383:ARG:HG2	1:F:68:PRO:HG2	1.60	0.82
1:E:424:MET:SD	1:E:493:ARG:NH2	2.54	0.80
1:A:415:GLU:HB3	1:A:430:LEU:HD11	1.62	0.80
1:E:142:TRP:HB3	1:F:67:ALA:HB2	1.64	0.80
1:E:183:LEU:HG	1:E:188:ARG:HA	1.64	0.80
1:E:100:TYR:HE1	1:E:482:THR:HG21	1.48	0.79
1:F:100:TYR:HE1	1:F:482:THR:HG21	1.49	0.79
1:C:457:GLU:HG2	1:C:458:ASN:H	1.47	0.78
1:F:481:MET:HE3	1:F:494:PHE:HD1	1.51	0.76
1:A:288:ALA:O	1:A:315:LEU:HA	1.85	0.76
1:F:481:MET:HE2	1:F:492:ILE:HG12	1.68	0.76
1:D:415:GLU:HB3	1:D:430:LEU:HD11	1.66	0.75
1:F:387:VAL:HG12	1:F:391:ARG:HH22	1.50	0.75
1:E:51:ARG:HA	1:E:90:THR:HG23	1.69	0.75
1:E:388:THR:O	1:E:392:ASN:ND2	2.20	0.74
1:C:116:SER:HB2	1:C:373:PHE:HB3	1.69	0.74
1:F:470:LEU:HD23	1:F:474:ASN:HD21	1.52	0.74
1:A:120:ASN:HB3	1:B:93:GLN:HE21	1.53	0.73
1:E:343:SER:O	1:E:350:ARG:NH2	2.20	0.73
1:F:391:ARG:HB2	1:F:395:ARG:HH11	1.53	0.73
1:C:28:ARG:NH2	1:D:40:ASP:OD1	2.21	0.73
1:E:300:PHE:HE2	1:E:422:PHE:HB3	1.54	0.73
1:E:28:ARG:O	1:E:31:GLY:N	2.23	0.72
1:E:299:GLU:HG2	1:E:300:PHE:HD1	1.54	0.72
1:A:239:ARG:NH2	1:A:279:GLU:OE1	2.20	0.70
1:E:344:THR:HG21	1:F:204:CYS:HB2	1.72	0.70
1:E:459:LEU:HD11	1:E:489:VAL:HG12	1.73	0.70
1:E:25:GLU:O	1:E:27:PHE:N	2.25	0.70
1:E:203:HIS:HD2	1:E:262:THR:HG21	1.57	0.70
1:F:388:THR:O	1:F:392:ASN:ND2	2.25	0.70
1:B:136:GLU:CD	1:B:371:ARG:HH12	2.00	0.69
1:E:262:THR:CG2	2:E:601:PLP:O3	2.41	0.69
1:E:391:ARG:HD3	1:E:395:ARG:HH21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:ASP:O	1:E:377:LYS:NZ	2.26	0.69
1:E:366:GLN:HE22	1:E:371:ARG:HG3	1.57	0.69
1:E:191:ILE:HA	1:E:194:LEU:HD12	1.76	0.68
1:A:285:HIS:ND1	1:A:312:SER:OG	2.23	0.68
1:F:97:TYR:HE2	1:F:99:ALA:HB3	1.57	0.68
1:B:51:ARG:HA	1:B:90:THR:HG23	1.76	0.67
1:A:179:ARG:NH1	1:A:213:ALA:O	2.26	0.67
1:A:316:ASN:OD1	1:A:318:HIS:CE1	2.48	0.67
1:F:289:ALA:HA	1:F:315:LEU:HA	1.75	0.67
1:F:277:ALA:HA	1:F:282:MET:HE3	1.77	0.67
1:C:383:ARG:NH2	1:D:72:GLU:OE1	2.27	0.66
1:D:106:SER:HB3	1:D:322:PHE:HB3	1.77	0.66
1:E:23:ASP:OD2	1:E:25:GLU:HB2	1.95	0.66
1:E:233:LEU:HD23	1:E:273:ILE:HD11	1.78	0.66
1:E:462:ALA:O	1:E:466:ASN:ND2	2.28	0.66
1:A:239:ARG:HA	1:A:242:ILE:HD12	1.77	0.65
1:F:141:ASP:OD1	1:F:155:PHE:N	2.29	0.65
1:F:297:CYS:SG	1:F:395:ARG:NH2	2.65	0.65
1:A:113:GLU:HG2	1:A:377:LYS:HD3	1.77	0.65
1:F:108:ALA:HB1	1:F:380:MET:HB3	1.78	0.65
1:E:28:ARG:O	1:E:29:ARG:C	2.39	0.65
1:E:55:GLU:HG3	1:E:56:PRO:HD2	1.77	0.65
1:F:317:ALA:N	1:F:327:CYS:O	2.29	0.65
1:F:203:HIS:CD2	2:F:602:PLP:C4A	2.80	0.64
1:A:136:GLU:OE1	1:A:371:ARG:NH2	2.20	0.64
1:A:166:THR:CB	2:A:601:PLP:O3P	2.42	0.64
1:F:205:ALA:HB2	2:F:602:PLP:H5A2	1.79	0.64
1:D:426:CYS:HB3	1:D:491:MET:HE3	1.80	0.64
1:E:25:GLU:O	1:E:26:GLU:C	2.41	0.64
1:B:413:ARG:NH2	1:B:518:ASP:OD1	2.26	0.64
1:C:103:SER:OG	1:D:120:ASN:ND2	2.31	0.63
1:E:180:ASP:O	1:E:184:ASN:N	2.29	0.63
1:B:28:ARG:HG3	1:B:32:HIS:HE1	1.64	0.63
1:E:92:TRP:HD1	1:F:121:VAL:CG2	2.12	0.63
1:E:194:LEU:HD22	1:E:253:LEU:HD22	1.81	0.63
1:E:233:LEU:H	1:E:268:ASP:HB3	1.62	0.63
1:F:462:ALA:O	1:F:466:ASN:ND2	2.31	0.62
1:B:146:MET:HB3	1:B:296:ILE:HD12	1.81	0.62
1:E:19:THR:HG22	1:E:20:ASN:H	1.64	0.62
1:C:179:ARG:NH1	1:C:213:ALA:O	2.32	0.62
1:D:316:ASN:ND2	1:D:318:HIS:HE1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:ASN:HA	1:F:328:CYS:HA	1.82	0.62
1:B:239:ARG:NH2	1:B:279:GLU:OE2	2.20	0.62
1:C:166:THR:HB	2:C:601:PLP:O1P	2.00	0.62
1:B:287:ASP:OD2	2:B:601:PLP:N1	2.32	0.62
1:C:102:PRO:HG2	1:C:319:LYS:O	1.99	0.62
1:F:470:LEU:HD23	1:F:474:ASN:ND2	2.15	0.62
1:E:77:ILE:HA	1:E:80:ASP:HB2	1.80	0.62
1:E:325:LEU:O	1:F:372:ARG:NH2	2.30	0.62
1:F:470:LEU:O	1:F:474:ASN:ND2	2.33	0.62
1:E:92:TRP:HD1	1:F:121:VAL:HG22	1.63	0.62
1:F:112:GLY:HA3	1:F:377:LYS:HA	1.81	0.62
1:F:196:VAL:HG22	1:F:254:PHE:HB3	1.80	0.62
1:C:457:GLU:N	1:C:457:GLU:OE1	2.34	0.61
1:E:114:MET:HG2	1:F:34:ILE:HG21	1.81	0.61
1:E:258:THR:HG22	1:E:287:ASP:HB3	1.81	0.61
1:E:298:PRO:HD3	1:E:391:ARG:HH21	1.64	0.61
1:E:100:TYR:CE1	1:E:482:THR:HG21	2.33	0.61
1:F:521:LEU:HA	1:F:524:PHE:HB2	1.81	0.61
1:F:203:HIS:CD2	2:F:602:PLP:C4	2.84	0.61
1:D:481:MET:HE1	1:D:513:LEU:HD21	1.81	0.61
1:B:106:SER:HB3	1:B:322:PHE:HB3	1.84	0.60
1:E:174:THR:HG22	1:E:254:PHE:HE2	1.66	0.60
1:E:151:GLU:HG2	1:E:154:LEU:HD12	1.84	0.60
1:E:261:THR:HG22	1:E:266:ALA:H	1.65	0.60
1:C:285:HIS:ND1	1:C:312:SER:OG	2.34	0.60
1:B:143:PHE:O	1:B:147:LEU:HD12	2.01	0.60
1:C:484:ALA:HB2	1:C:493:ARG:HD2	1.83	0.60
1:F:498:SER:O	1:F:500:LEU:N	2.31	0.60
1:E:80:ASP:O	1:E:84:GLU:OE2	2.20	0.59
1:B:122:VAL:CG1	1:B:370:SER:HB2	2.33	0.59
1:E:85:ILE:HG22	1:E:89:LEU:HD23	1.84	0.59
1:F:132:ALA:HA	1:F:373:PHE:CZ	2.38	0.59
1:C:51:ARG:HA	1:C:90:THR:HG23	1.85	0.59
1:E:343:SER:HB3	1:E:350:ARG:HE	1.67	0.59
1:E:385:TYR:CD1	1:E:393:PHE:HE2	2.20	0.59
1:C:133:THR:HG23	1:C:362:TYR:HD2	1.68	0.59
1:F:375:SER:O	1:F:379:TRP:N	2.36	0.59
1:D:422:PHE:O	1:D:424:MET:N	2.35	0.59
1:E:234:SER:HG	1:E:237:THR:HG1	1.51	0.58
1:F:427:PHE:CZ	1:F:481:MET:HE1	2.38	0.58
1:A:34:ILE:HG13	1:B:111:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:PHE:CZ	1:E:513:LEU:HD21	2.39	0.58
1:F:271:SER:OG	1:F:305:ASP:O	2.21	0.58
1:D:233:LEU:N	1:D:268:ASP:OD1	2.35	0.58
1:E:61:LYS:NZ	1:E:65:GLU:OE2	2.31	0.58
1:A:167:SER:OG	1:A:316:ASN:ND2	2.36	0.58
1:F:100:TYR:CE1	1:F:482:THR:HG21	2.35	0.57
1:F:280:TYR:HB2	1:F:282:MET:HE2	1.84	0.57
1:E:135:LEU:HD22	1:F:85:ILE:HD11	1.87	0.57
1:F:310:ALA:O	1:F:333:LYS:HD2	2.05	0.57
1:F:387:VAL:HG12	1:F:391:ARG:NH2	2.19	0.57
1:F:375:SER:HA	1:F:378:LEU:HB3	1.86	0.57
1:C:400:MET:HE3	1:C:496:VAL:HG11	1.86	0.57
1:E:123:GLY:O	1:E:371:ARG:NH2	2.37	0.57
1:D:287:ASP:OD2	2:D:601:PLP:N1	2.38	0.57
1:F:259:VAL:HB	1:F:288:ALA:HB2	1.85	0.57
1:B:25:GLU:OE2	1:B:28:ARG:NH1	2.38	0.57
1:C:462:ALA:O	1:C:466:ASN:ND2	2.37	0.57
1:C:167:SER:HB2	1:C:316:ASN:OD1	2.03	0.57
1:E:34:ILE:HG12	1:F:111:LEU:HB3	1.86	0.57
1:A:32:HIS:ND1	1:B:32:HIS:HD2	2.04	0.56
1:B:143:PHE:HE1	1:B:296:ILE:HD11	1.70	0.56
1:D:104:SER:HB3	1:D:322:PHE:H	1.69	0.56
1:E:121:VAL:HG21	1:E:129:SER:HB2	1.87	0.56
1:E:269:PRO:HB2	1:E:272:PRO:HD2	1.85	0.56
1:E:108:ALA:HB1	1:E:380:MET:HB3	1.86	0.56
1:F:471:GLU:HA	1:F:474:ASN:HD22	1.70	0.56
1:B:257:PRO:HG3	1:B:273:ILE:HG21	1.88	0.56
1:A:288:ALA:O	1:A:314:SER:O	2.23	0.56
1:E:138:VAL:HG22	1:E:142:TRP:HE1	1.71	0.56
1:E:300:PHE:CE2	1:E:422:PHE:HB3	2.40	0.56
1:F:99:ALA:O	1:F:493:ARG:NH1	2.39	0.56
1:D:25:GLU:OE1	1:D:28:ARG:NH1	2.39	0.56
1:F:265:THR:HG23	1:F:424:MET:HE3	1.88	0.56
1:C:289:ALA:HA	1:C:316:ASN:H	1.70	0.56
1:D:420:ARG:HG3	1:D:424:MET:O	2.05	0.56
1:F:25:GLU:OE1	1:F:28:ARG:NE	2.37	0.56
1:A:332:VAL:HG11	1:A:338:LEU:HD11	1.88	0.55
1:D:239:ARG:NH2	1:D:279:GLU:OE1	2.32	0.55
1:E:378:LEU:O	1:E:382:LEU:HD12	2.07	0.55
1:A:395:ARG:O	1:A:399:LYS:HG3	2.07	0.55
1:E:136:GLU:OE2	1:E:163:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ASN:ND2	2:C:601:PLP:O2P	2.40	0.55
1:E:457:GLU:HG3	1:E:458:ASN:H	1.71	0.55
1:E:95:PRO:HB3	1:E:500:LEU:HB3	1.90	0.55
1:C:136:GLU:HG3	1:C:163:LEU:HD12	1.89	0.54
1:F:239:ARG:NH1	1:F:279:GLU:OE1	2.38	0.54
1:C:180:ASP:OD2	1:C:188:ARG:NH1	2.41	0.54
1:E:131:ALA:HB1	1:F:85:ILE:HD13	1.87	0.54
1:E:196:VAL:HG13	1:E:254:PHE:HB3	1.87	0.54
1:A:120:ASN:HD21	1:B:324:THR:HA	1.72	0.54
1:B:277:ALA:HB1	1:B:282:MET:HB2	1.90	0.54
1:C:485:VAL:HB	1:E:531:SER:HA	1.89	0.54
1:D:361:ASP:OD1	1:D:363:LYS:NZ	2.41	0.54
1:E:285:HIS:HE2	1:E:314:SER:HB2	1.71	0.54
1:E:166:THR:HB	2:E:601:PLP:O3P	2.08	0.54
1:F:262:THR:HB	2:F:602:PLP:O3	2.07	0.54
1:F:473:VAL:O	1:F:476:THR:OG1	2.25	0.54
1:F:140:MET:HE3	1:F:163:LEU:HD11	1.90	0.54
1:A:114:MET:HG2	1:B:110:PHE:HZ	1.72	0.54
1:E:114:MET:HE2	1:F:114:MET:HE2	1.90	0.54
1:E:469:TYR:O	1:E:473:VAL:HG23	2.08	0.54
1:E:97:TYR:HE1	1:E:99:ALA:HB3	1.73	0.54
1:A:180:ASP:OD1	1:A:188:ARG:NH1	2.39	0.54
1:F:420:ARG:HG3	1:F:425:VAL:HB	1.90	0.54
1:A:72:GLU:OE2	1:B:383:ARG:NE	2.28	0.53
1:A:114:MET:HG3	1:B:114:MET:SD	2.48	0.53
1:C:120:ASN:HD21	1:D:324:THR:HA	1.74	0.53
1:C:516:HIS:O	1:C:520:ILE:HG12	2.08	0.53
1:C:60:ARG:NH2	1:D:141:ASP:OD2	2.42	0.53
1:C:319:LYS:HZ2	3:C:602:142:CE1	2.22	0.53
1:A:40:ASP:OD1	1:B:28:ARG:NH2	2.42	0.53
1:B:107:VAL:O	1:B:111:LEU:HG	2.09	0.53
1:B:325:LEU:HG	1:B:326:ASP:HB3	1.91	0.53
1:E:98:TYR:HE2	1:E:501:THR:HG21	1.73	0.53
1:F:99:ALA:HB1	1:F:482:THR:HG23	1.91	0.52
1:A:114:MET:HG2	1:B:110:PHE:CZ	2.44	0.52
1:B:173:CYS:SG	1:B:366:GLN:HA	2.49	0.52
1:E:289:ALA:HA	1:E:316:ASN:H	1.75	0.52
1:A:34:ILE:HD11	1:A:74:ILE:HD11	1.90	0.52
1:E:35:ILE:HD11	1:F:35:ILE:HD11	1.90	0.52
1:F:162:VAL:HB	1:F:365:TRP:HE3	1.74	0.52
1:C:323:THR:HG22	1:C:381:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:LEU:HD11	1:F:115:LEU:HA	1.91	0.52
1:E:106:SER:O	1:E:110:PHE:N	2.43	0.52
1:E:147:LEU:HG	1:E:296:ILE:HG22	1.90	0.52
1:F:143:PHE:HE1	1:F:296:ILE:HD11	1.75	0.52
1:A:408:ILE:HD13	1:A:510:TRP:HZ3	1.74	0.52
1:E:111:LEU:HD11	1:F:30:GLN:HB3	1.92	0.52
1:F:203:HIS:CE1	2:F:602:PLP:C4A	2.92	0.52
1:B:172:LEU:O	1:B:176:THR:HG23	2.10	0.52
1:C:325:LEU:HG	1:C:326:ASP:HB3	1.92	0.52
1:B:318:HIS:HB3	1:B:324:THR:O	2.10	0.52
1:C:172:LEU:O	1:C:176:THR:HG23	2.10	0.52
1:D:417:THR:HG21	1:D:491:MET:HG2	1.92	0.52
1:E:42:TYR:HB2	1:F:24:PRO:HG3	1.91	0.52
1:E:112:GLY:HA2	1:E:380:MET:HE3	1.92	0.52
1:E:172:LEU:O	1:E:176:THR:OG1	2.24	0.52
1:E:457:GLU:CG	1:E:458:ASN:H	2.22	0.52
1:F:63:LEU:HB2	1:F:64:PRO:HD2	1.92	0.52
1:D:415:GLU:HG2	1:D:428:ARG:HG2	1.91	0.52
1:F:92:TRP:C	1:F:94:SER:H	2.16	0.52
1:F:198:GLY:O	1:F:223:ILE:HG12	2.09	0.52
1:B:51:ARG:HD3	1:B:480:TYR:CE1	2.44	0.51
1:F:34:ILE:CG2	1:F:38:LEU:CD1	2.84	0.51
1:F:51:ARG:HE	1:F:474:ASN:HB3	1.76	0.51
1:D:310:ALA:O	1:D:333:LYS:HD2	2.10	0.51
1:D:508:TYR:CZ	1:D:512:ILE:HD11	2.46	0.51
1:A:120:ASN:ND2	4:A:701:HOH:O	2.42	0.51
1:B:82:THR:HA	1:B:86:ILE:HD12	1.91	0.51
1:E:233:LEU:O	1:E:269:PRO:HD2	2.10	0.51
1:E:92:TRP:HE1	1:F:128:SER:HB3	1.76	0.51
1:E:297:CYS:HB3	1:E:299:GLU:OE2	2.11	0.51
1:F:43:ARG:HG3	1:F:44:ASP:H	1.76	0.51
1:D:58:TYR:OH	1:D:84:GLU:O	2.20	0.51
1:F:103:SER:O	1:F:103:SER:OG	2.28	0.51
1:F:415:GLU:HB2	1:F:430:LEU:HD22	1.93	0.51
1:E:25:GLU:O	1:E:28:ARG:N	2.43	0.51
1:D:144:GLY:HA3	1:D:154:LEU:HD21	1.93	0.51
1:E:162:VAL:HG23	1:E:362:TYR:HD1	1.76	0.51
1:C:264:SER:HB3	1:C:486:VAL:HG21	1.92	0.51
1:E:259:VAL:HG22	1:E:267:VAL:HG13	1.92	0.51
1:F:225:THR:HB	1:F:231:PHE:HA	1.93	0.51
1:A:324:THR:HG21	1:B:117:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:O	1:B:32:HIS:ND1	2.44	0.50
1:E:393:PHE:CE2	1:F:21:PRO:HG3	2.47	0.50
1:F:408:ILE:HG22	1:F:510:TRP:CZ3	2.46	0.50
1:B:135:LEU:O	1:B:139:VAL:HG22	2.12	0.50
1:C:342:LEU:O	1:D:208:LYS:NZ	2.42	0.50
1:D:51:ARG:HD3	1:D:480:TYR:CE1	2.47	0.50
1:B:28:ARG:HG3	1:B:32:HIS:CE1	2.45	0.50
1:E:42:TYR:O	1:E:45:VAL:HG22	2.12	0.50
1:E:47:LYS:HE3	1:E:48:TYR:CE2	2.47	0.50
1:E:225:THR:HB	1:E:231:PHE:HA	1.92	0.50
1:F:411:ASP:OD1	1:F:413:ARG:HD3	2.11	0.50
1:C:36:ASP:OD1	1:D:28:ARG:NE	2.43	0.50
1:E:188:ARG:O	1:F:216:ASN:ND2	2.45	0.50
1:E:310:ALA:O	1:E:333:LYS:HD2	2.10	0.50
1:F:113:GLU:N	1:F:377:LYS:HB3	2.27	0.50
1:F:162:VAL:HB	1:F:365:TRP:CE3	2.47	0.50
1:A:51:ARG:HD3	1:A:480:TYR:CE1	2.46	0.50
1:B:106:SER:OG	1:B:322:PHE:O	2.20	0.50
1:D:148:ASN:HB3	1:D:301:ARG:HE	1.77	0.50
1:E:321:PHE:CZ	1:E:390:LEU:HD13	2.47	0.50
1:C:377:LYS:O	1:C:381:VAL:HG23	2.12	0.50
1:D:95:PRO:HB2	1:D:505:HIS:CD2	2.46	0.50
1:D:126:TRP:CE2	1:D:130:PRO:HB3	2.47	0.50
1:E:111:LEU:HD22	1:F:34:ILE:HG12	1.94	0.50
1:C:200:ASP:OD1	1:C:200:ASP:N	2.43	0.49
1:E:143:PHE:O	1:E:147:LEU:HD12	2.12	0.49
1:E:264:SER:OG	1:E:264:SER:O	2.27	0.49
1:E:25:GLU:OE2	1:E:25:GLU:HA	2.11	0.49
1:A:323:THR:O	1:A:377:LYS:HD2	2.12	0.49
1:E:268:ASP:OD1	1:E:268:ASP:N	2.38	0.49
1:C:110:PHE:CE1	1:D:117:THR:HB	2.48	0.49
1:E:176:THR:HG23	1:E:179:ARG:NH2	2.28	0.49
1:E:366:GLN:NE2	1:E:371:ARG:HG3	2.25	0.49
1:F:97:TYR:CE2	1:F:99:ALA:HB3	2.44	0.49
1:A:272:PRO:HA	1:A:275:GLU:HB2	1.93	0.49
1:A:242:ILE:O	1:A:246:ILE:HG13	2.13	0.49
1:E:385:TYR:HB3	1:E:389:ASN:CB	2.34	0.49
1:B:126:TRP:CE2	1:B:130:PRO:HB3	2.48	0.49
1:B:167:SER:OG	1:B:316:ASN:OD1	2.22	0.49
1:B:200:ASP:OD1	1:B:225:THR:OG1	2.28	0.49
1:E:114:MET:CG	1:F:34:ILE:HG21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:SER:OG	1:E:316:ASN:OD1	2.31	0.49
1:E:283:TRP:HZ2	1:E:312:SER:HB3	1.78	0.49
1:F:269:PRO:HB2	1:F:272:PRO:HD2	1.94	0.49
3:C:602:142:CD1	3:C:602:142:NN	2.76	0.49
1:C:265:THR:HG21	4:C:701:HOH:O	2.12	0.49
1:E:40:ASP:OD1	1:E:43:ARG:NH2	2.46	0.49
1:F:147:LEU:O	1:F:301:ARG:NH1	2.42	0.49
1:E:146:MET:HE1	1:E:382:LEU:HD22	1.95	0.48
1:A:110:PHE:CE2	1:A:114:MET:HE2	2.49	0.48
1:B:223:ILE:HG23	1:B:241:VAL:HG21	1.94	0.48
1:D:128:SER:O	1:D:129:SER:OG	2.30	0.48
1:D:312:SER:HB3	1:D:332:VAL:HG12	1.95	0.48
1:C:44:ASP:O	1:C:47:LYS:HG2	2.13	0.48
1:C:326:ASP:O	1:C:377:LYS:NZ	2.46	0.48
1:E:25:GLU:C	1:E:27:PHE:N	2.70	0.48
1:F:239:ARG:O	1:F:242:ILE:HG22	2.13	0.48
1:F:388:THR:HA	1:F:391:ARG:HH21	1.78	0.48
1:C:385:TYR:O	1:C:389:ASN:HB2	2.14	0.48
1:D:200:ASP:N	1:D:200:ASP:OD1	2.45	0.48
1:E:27:PHE:O	1:E:28:ARG:O	2.31	0.48
1:A:225:THR:HB	1:A:231:PHE:HA	1.95	0.48
1:C:104:SER:HB3	1:C:322:PHE:H	1.79	0.48
1:C:289:ALA:HB1	1:C:319:LYS:HE2	1.96	0.48
1:D:319:LYS:HG3	3:D:602:142:OH	2.13	0.48
1:E:338:LEU:HB3	1:E:365:TRP:HA	1.95	0.48
1:E:469:TYR:OH	1:E:513:LEU:O	2.22	0.48
1:F:192:GLY:O	1:F:219:ASN:ND2	2.44	0.48
1:F:287:ASP:OD2	2:F:602:PLP:N1	2.46	0.48
1:F:466:ASN:O	1:F:470:LEU:HB2	2.14	0.48
1:A:408:ILE:HD13	1:A:510:TRP:CZ3	2.48	0.48
1:B:264:SER:HB2	1:B:418:VAL:HG21	1.94	0.48
1:D:319:LYS:HZ1	2:D:601:PLP:C4A	2.27	0.48
1:E:85:ILE:HG22	1:E:89:LEU:CD2	2.44	0.48
1:A:172:LEU:O	1:A:176:THR:HG23	2.14	0.48
1:A:144:GLY:HA2	1:A:149:LEU:HD12	1.95	0.48
1:E:174:THR:HG22	1:E:254:PHE:CE2	2.46	0.48
1:F:143:PHE:HA	1:F:146:MET:HE3	1.96	0.48
1:C:380:MET:O	1:C:384:SER:OG	2.29	0.47
3:D:602:142:NN	3:D:602:142:CD1	2.76	0.47
1:E:124:PHE:CD2	1:F:100:TYR:HE2	2.32	0.47
1:C:110:PHE:HE1	1:D:117:THR:HB	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASP:O	1:D:47:LYS:HG2	2.14	0.47
1:F:194:LEU:O	1:F:219:ASN:ND2	2.47	0.47
1:E:113:GLU:HG3	1:E:377:LYS:HE3	1.95	0.47
1:E:116:SER:OG	1:E:373:PHE:HB3	2.13	0.47
1:E:183:LEU:HD11	1:E:190:HIS:H	1.80	0.47
1:E:203:HIS:NE2	2:E:601:PLP:C4A	2.77	0.47
1:A:102:PRO:HG3	1:A:497:GLY:HA3	1.95	0.47
1:D:134:GLU:O	1:D:138:VAL:HG23	2.14	0.47
1:E:511:LYS:HA	1:E:514:GLN:HB3	1.95	0.47
1:E:262:THR:HG23	2:E:601:PLP:O3	2.11	0.47
1:E:391:ARG:O	1:E:395:ARG:NE	2.46	0.47
1:F:481:MET:SD	1:F:513:LEU:HD21	2.55	0.47
1:E:391:ARG:HD3	1:E:395:ARG:NH2	2.27	0.47
1:A:113:GLU:CG	1:A:377:LYS:HD3	2.43	0.47
1:A:136:GLU:HG3	1:A:163:LEU:HD12	1.96	0.47
1:B:511:LYS:O	1:B:515:GLU:HG3	2.15	0.47
1:E:101:PHE:O	3:F:601:142:HE2	2.14	0.47
1:E:263:SER:HB3	1:E:486:VAL:HG21	1.97	0.47
1:E:289:ALA:HA	1:E:315:LEU:HA	1.95	0.47
1:A:415:GLU:OE1	1:A:428:ARG:NH2	2.41	0.47
1:B:225:THR:HB	1:B:231:PHE:HA	1.97	0.47
1:F:199:SER:HB3	1:F:233:LEU:HD13	1.95	0.47
1:F:294:ALA:O	1:F:296:ILE:N	2.48	0.47
3:F:603:142:NN	3:F:603:142:CD1	2.77	0.47
1:E:69:TYR:HA	1:F:387:VAL:HB	1.97	0.47
1:E:97:TYR:CE1	1:E:99:ALA:HB3	2.49	0.47
1:F:229:ASN:ND2	1:F:232:GLY:O	2.47	0.47
1:A:325:LEU:HA	1:A:326:ASP:HA	1.60	0.47
1:B:111:LEU:HB2	1:B:380:MET:HE2	1.96	0.47
1:B:136:GLU:HG3	1:B:163:LEU:HD12	1.97	0.47
1:C:432:PRO:HD2	1:C:524:PHE:CE2	2.50	0.47
1:E:383:ARG:HB3	1:F:77:ILE:HD12	1.97	0.47
1:F:133:THR:HB	1:F:362:TYR:HD2	1.80	0.47
1:C:114:MET:HG3	1:D:114:MET:SD	2.55	0.46
1:C:128:SER:O	1:D:90:THR:HB	2.15	0.46
1:D:408:ILE:HD13	1:D:510:TRP:CZ3	2.50	0.46
1:E:111:LEU:HD22	1:F:34:ILE:CG1	2.45	0.46
1:E:347:GLU:HA	1:E:350:ARG:HD2	1.98	0.46
1:F:203:HIS:CG	2:F:602:PLP:C4	2.98	0.46
1:F:417:THR:HG21	1:F:491:MET:HB2	1.98	0.46
1:A:107:VAL:O	1:A:111:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LEU:HD12	1:F:295:CYS:HB2	1.98	0.46
1:F:376:LEU:HD23	1:F:376:LEU:HA	1.75	0.46
1:A:242:ILE:HD13	1:A:282:MET:HE1	1.97	0.46
1:E:150:PRO:HG3	1:E:308:GLU:HA	1.98	0.46
1:E:285:HIS:NE2	1:E:314:SER:HB2	2.30	0.46
1:F:509:ALA:HA	1:F:512:ILE:HG13	1.97	0.46
1:F:517:ALA:O	1:F:521:LEU:HB2	2.16	0.46
1:D:319:LYS:HD2	3:D:602:142:CZ	2.46	0.46
1:E:41:TYR:O	1:E:45:VAL:HG13	2.14	0.46
1:E:238:LEU:O	1:E:242:ILE:HG13	2.16	0.46
1:E:252:PRO:HB2	1:E:282:MET:SD	2.55	0.46
1:A:62:ARG:HD2	1:A:84:GLU:OE1	2.16	0.46
1:A:322:PHE:CZ	1:A:393:PHE:HB3	2.51	0.46
1:E:148:ASN:O	1:E:301:ARG:NH2	2.48	0.46
1:D:411:ASP:HB2	1:D:510:TRP:HH2	1.80	0.46
1:E:73:SER:O	1:E:77:ILE:HD13	2.16	0.46
1:B:104:SER:HB3	1:B:322:PHE:H	1.81	0.46
1:B:136:GLU:OE2	1:B:371:ARG:NH1	2.49	0.46
1:C:294:ALA:HB2	1:C:320:TRP:CZ3	2.50	0.46
1:C:380:MET:SD	1:D:77:ILE:HG21	2.56	0.46
1:A:369:LEU:HD13	1:B:203:HIS:HE1	1.81	0.45
1:C:26:GLU:OE2	1:C:30:GLN:NE2	2.49	0.45
1:E:405:GLU:HB2	1:E:425:VAL:HG21	1.98	0.45
1:F:391:ARG:HB2	1:F:395:ARG:NH1	2.27	0.45
1:D:408:ILE:HD13	1:D:510:TRP:HZ3	1.81	0.45
1:E:347:GLU:HG3	1:E:350:ARG:NH1	2.31	0.45
1:A:383:ARG:NE	1:B:72:GLU:OE1	2.41	0.45
1:D:136:GLU:HG3	1:D:163:LEU:HD12	1.97	0.45
1:D:294:ALA:HB2	1:D:320:TRP:CZ3	2.51	0.45
1:E:385:TYR:CE1	1:E:393:PHE:HE2	2.33	0.45
1:F:374:ARG:HE	1:F:374:ARG:HB3	1.45	0.45
1:D:511:LYS:O	1:D:515:GLU:HG3	2.17	0.45
1:E:27:PHE:O	1:E:28:ARG:C	2.58	0.45
1:E:67:ALA:HB2	1:F:142:TRP:HB3	1.97	0.45
1:F:111:LEU:HA	1:F:114:MET:HB2	1.97	0.45
1:B:167:SER:HB2	2:B:601:PLP:O4P	2.16	0.45
1:C:51:ARG:HD3	1:C:480:TYR:CE1	2.51	0.45
1:D:179:ARG:NH1	1:D:213:ALA:O	2.48	0.45
1:B:173:CYS:HB3	1:B:342:LEU:HD11	1.98	0.45
1:D:99:ALA:HB1	1:D:482:THR:HG23	1.99	0.45
1:D:319:LYS:NZ	3:D:602:142:N	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ARG:O	1:E:30:GLN:N	2.49	0.45
1:E:372:ARG:O	1:E:374:ARG:N	2.49	0.45
1:B:399:LYS:HD2	1:B:402:LYS:HE3	1.98	0.45
1:C:133:THR:HG23	1:C:362:TYR:CD2	2.49	0.45
1:D:141:ASP:O	1:D:145:LYS:HG3	2.17	0.45
1:D:319:LYS:NZ	2:D:601:PLP:C4A	2.80	0.45
1:F:77:ILE:HA	1:F:80:ASP:HB2	1.99	0.45
1:A:95:PRO:HB3	1:A:500:LEU:O	2.17	0.45
1:C:124:PHE:O	1:C:363:LYS:HD3	2.17	0.45
1:E:201:GLN:O	1:E:261:THR:OG1	2.35	0.45
1:E:261:THR:HG22	1:E:266:ALA:N	2.32	0.45
1:C:40:ASP:OD1	1:D:28:ARG:NH2	2.49	0.45
1:E:411:ASP:HB3	1:E:414:PHE:HD1	1.82	0.45
1:E:516:HIS:O	1:E:517:ALA:C	2.60	0.45
1:F:424:MET:HA	1:F:494:PHE:O	2.16	0.45
1:A:257:PRO:HD2	1:A:285:HIS:O	2.17	0.44
1:A:413:ARG:NH1	1:A:518:ASP:OD2	2.45	0.44
1:D:51:ARG:NH2	1:D:471:GLU:OE1	2.46	0.44
1:D:521:LEU:HA	1:D:524:PHE:HB2	1.99	0.44
1:E:138:VAL:HG22	1:E:142:TRP:NE1	2.31	0.44
1:A:470:LEU:HD13	1:A:492:ILE:HG23	2.00	0.44
1:C:167:SER:O	1:C:171:ILE:HG13	2.18	0.44
1:F:464:LYS:O	1:F:468:VAL:HG23	2.17	0.44
1:F:525:SER:O	1:F:527:ALA:N	2.41	0.44
1:B:325:LEU:HA	1:B:326:ASP:HA	1.64	0.44
1:C:128:SER:O	1:C:129:SER:OG	2.36	0.44
1:E:233:LEU:N	1:E:268:ASP:HB3	2.32	0.44
1:E:370:SER:OG	3:F:603:142:OE1	2.32	0.44
1:F:51:ARG:HD3	1:F:480:TYR:CZ	2.52	0.44
1:F:102:PRO:HG3	1:F:497:GLY:HA3	1.99	0.44
1:F:223:ILE:HB	1:F:233:LEU:HD11	2.00	0.44
1:F:512:ILE:HA	1:F:515:GLU:HG2	1.99	0.44
1:A:277:ALA:HB1	1:A:282:MET:HB2	2.00	0.44
1:F:92:TRP:HZ3	1:F:101:PHE:O	2.01	0.44
1:A:102:PRO:HG2	1:A:319:LYS:O	2.17	0.44
1:E:293:SER:HB3	1:E:321:PHE:CD1	2.52	0.44
1:E:506:VAL:HG12	1:E:507:ILE:HD13	1.98	0.44
1:F:207:GLN:O	1:F:211:GLN:HG3	2.17	0.44
1:F:366:GLN:HG3	1:F:368:ALA:H	1.82	0.44
3:F:603:142:HNN	3:F:603:142:HD1	1.83	0.44
1:B:143:PHE:CE1	1:B:296:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:CYS:SG	1:C:367:ILE:HG13	2.58	0.44
1:E:29:ARG:HD3	1:E:33:MET:HE2	2.00	0.44
1:E:210:ALA:HB1	1:E:215:ILE:HB	1.98	0.44
1:F:259:VAL:HG13	1:F:267:VAL:HG12	1.99	0.44
1:B:380:MET:O	1:B:384:SER:OG	2.35	0.44
1:E:51:ARG:HG3	1:E:480:TYR:CE1	2.52	0.44
1:E:407:LEU:HD13	1:E:510:TRP:CD1	2.53	0.44
1:B:396:SER:O	1:B:400:MET:HG3	2.18	0.44
1:C:59:LEU:HG	1:C:63:LEU:HD12	1.99	0.44
1:D:136:GLU:CD	1:D:371:ARG:HH12	2.26	0.44
1:D:516:HIS:O	1:D:520:ILE:HG12	2.17	0.44
1:E:146:MET:HB2	1:E:146:MET:HE3	1.41	0.44
1:F:515:GLU:HG3	1:F:516:HIS:ND1	2.32	0.44
3:C:602:142:HD1	3:C:602:142:HNN	1.82	0.43
1:E:174:THR:HG21	1:E:285:HIS:ND1	2.33	0.43
1:F:130:PRO:O	1:F:134:GLU:HG3	2.18	0.43
1:B:286:VAL:HB	1:B:313:PHE:HD1	1.83	0.43
1:B:459:LEU:HD11	1:B:489:VAL:HG22	1.99	0.43
1:D:45:VAL:HG13	1:D:95:PRO:HD3	2.00	0.43
1:A:100:TYR:HB3	3:A:602:142:HB1	2.00	0.43
1:A:417:THR:HG21	1:A:491:MET:HB3	2.01	0.43
1:B:294:ALA:HB2	1:B:320:TRP:CZ3	2.54	0.43
1:C:225:THR:HB	1:C:231:PHE:HA	2.00	0.43
1:C:325:LEU:HA	1:C:326:ASP:HA	1.59	0.43
1:C:431:PRO:HA	1:C:432:PRO:HD3	1.88	0.43
3:D:602:142:HNN	3:D:602:142:HD1	1.83	0.43
1:E:162:VAL:HG23	1:E:362:TYR:CD1	2.52	0.43
1:E:259:VAL:HA	1:E:267:VAL:HG22	2.01	0.43
1:F:34:ILE:O	1:F:38:LEU:N	2.49	0.43
1:B:102:PRO:HG3	1:B:497:GLY:HA3	1.99	0.43
1:B:332:VAL:HG11	1:B:338:LEU:HD11	1.99	0.43
1:C:136:GLU:OE1	1:C:371:ARG:NH2	2.51	0.43
1:C:325:LEU:O	1:D:372:ARG:NH2	2.50	0.43
1:E:176:THR:HG22	1:E:341:ALA:HB1	2.00	0.43
1:F:24:PRO:HA	1:F:27:PHE:HB3	2.00	0.43
1:F:106:SER:HB2	1:F:385:TYR:OH	2.18	0.43
1:F:420:ARG:HG2	1:F:424:MET:O	2.18	0.43
1:A:183:LEU:HD21	1:A:194:LEU:HD11	2.01	0.43
1:E:22:LEU:HD13	1:F:42:TYR:HE1	1.84	0.43
1:E:260:GLY:HA3	1:E:291:ALA:HB2	2.01	0.43
1:E:299:GLU:HG2	1:E:300:PHE:CD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ILE:HD12	1:F:304:ILE:HA	2.01	0.43
1:E:397:HIS:HA	1:E:400:MET:HE3	1.99	0.43
1:C:107:VAL:O	1:C:111:LEU:HG	2.19	0.43
1:C:113:GLU:OE2	1:D:372:ARG:NH2	2.52	0.43
1:C:151:GLU:HG2	1:C:157:GLY:HA3	2.01	0.43
1:D:170:ALA:HB1	1:D:330:LEU:HD13	1.99	0.43
1:D:264:SER:O	1:D:265:THR:C	2.61	0.43
1:F:404:PHE:HE2	1:F:494:PHE:CZ	2.36	0.43
1:B:274:CYS:O	1:B:278:LYS:HG2	2.19	0.43
1:C:141:ASP:O	1:C:145:LYS:HG3	2.18	0.43
1:E:111:LEU:HA	1:E:114:MET:HE3	1.99	0.43
3:F:601:142:HD1	3:F:601:142:HNN	1.84	0.43
1:B:141:ASP:O	1:B:145:LYS:HG3	2.19	0.43
1:C:392:ASN:O	1:C:396:SER:OG	2.31	0.43
1:D:301:ARG:NH1	1:D:304:ILE:HG13	2.34	0.43
1:E:141:ASP:OD2	1:E:155:PHE:HB2	2.18	0.43
1:F:304:ILE:O	1:F:307:VAL:HG12	2.19	0.43
1:E:22:LEU:HD23	1:E:22:LEU:HA	1.85	0.43
1:E:163:LEU:HD22	1:E:327:CYS:SG	2.59	0.43
1:F:143:PHE:CE1	1:F:296:ILE:HD11	2.53	0.43
1:F:417:THR:OG1	1:F:426:CYS:HB2	2.18	0.43
1:B:47:LYS:HE2	1:B:48:TYR:CE1	2.54	0.42
1:B:293:SER:O	1:B:296:ILE:HG12	2.18	0.42
1:D:484:ALA:HB2	1:D:493:ARG:HD2	2.01	0.42
1:E:124:PHE:HD2	1:F:100:TYR:HE2	1.65	0.42
1:F:193:ARG:HA	1:F:250:LEU:HD22	2.01	0.42
1:F:346:PRO:O	1:F:350:ARG:HG3	2.19	0.42
1:F:484:ALA:HB2	1:F:493:ARG:HD2	2.01	0.42
1:E:100:TYR:HB3	3:F:601:142:HB1	2.00	0.42
1:F:51:ARG:HE	1:F:474:ASN:CB	2.31	0.42
1:E:262:THR:HG22	2:E:601:PLP:O3	2.19	0.42
1:E:407:LEU:HD11	1:E:507:ILE:HD12	2.00	0.42
1:F:293:SER:HB3	1:F:321:PHE:CE1	2.54	0.42
1:F:373:PHE:CZ	1:F:376:LEU:HG	2.55	0.42
1:F:404:PHE:CD1	1:F:404:PHE:C	2.98	0.42
1:D:102:PRO:HG3	1:D:497:GLY:HA3	2.02	0.42
1:D:458:ASN:OD1	1:D:458:ASN:N	2.52	0.42
1:E:33:MET:O	1:E:36:ASP:HB3	2.19	0.42
1:A:93:GLN:NE2	1:B:120:ASN:HB3	2.34	0.42
1:A:134:GLU:O	1:A:138:VAL:HG23	2.19	0.42
1:A:216:ASN:OD1	1:A:218:LYS:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:MET:HE3	1:B:380:MET:HB3	1.94	0.42
1:D:107:VAL:O	1:D:111:LEU:HG	2.19	0.42
1:F:28:ARG:HG3	1:F:32:HIS:HD2	1.84	0.42
3:A:602:142:CD1	3:A:602:142:NN	2.83	0.42
1:F:481:MET:HE3	1:F:494:PHE:CD1	2.42	0.42
3:F:601:142:NN	3:F:601:142:CD1	2.83	0.42
1:A:132:ALA:HA	1:A:373:PHE:CE1	2.54	0.42
1:A:164:GLN:OE1	1:A:169:GLU:HG2	2.19	0.42
1:D:325:LEU:HA	1:D:326:ASP:HA	1.63	0.42
1:E:407:LEU:HB3	1:E:510:TRP:NE1	2.34	0.42
1:F:76:THR:O	1:F:80:ASP:HB2	2.20	0.42
1:F:201:GLN:HE21	1:F:225:THR:HG1	1.66	0.42
1:A:173:CYS:HB3	1:A:342:LEU:HD11	2.01	0.42
1:B:102:PRO:CG	1:B:497:GLY:HA3	2.50	0.42
1:C:22:LEU:HD23	1:D:500:LEU:HD11	2.01	0.42
1:D:323:THR:O	1:D:377:LYS:HD2	2.20	0.42
1:E:203:HIS:CD2	2:E:601:PLP:C4	3.03	0.42
1:E:417:THR:OG1	1:E:426:CYS:HB3	2.20	0.42
1:C:352:LYS:HD2	1:C:352:LYS:HA	1.79	0.42
1:B:101:PHE:HB2	3:B:602:142:HB12	2.02	0.42
1:B:399:LYS:HD2	1:B:399:LYS:HA	1.84	0.42
1:B:486:VAL:HB	1:B:491:MET:HE3	2.02	0.42
1:C:469:TYR:O	1:C:473:VAL:HG23	2.20	0.42
3:C:602:142:CD1	3:C:602:142:HNN	2.33	0.42
3:D:602:142:CD1	3:D:602:142:HNN	2.33	0.42
1:E:101:PHE:O	3:F:601:142:HD2	2.20	0.42
1:E:124:PHE:CD2	1:F:100:TYR:CE2	3.08	0.42
1:F:469:TYR:CE1	1:F:473:VAL:HG21	2.54	0.42
1:A:224:LYS:HA	1:A:224:LYS:HD3	1.80	0.41
1:B:253:LEU:HG	1:B:254:PHE:HB2	2.01	0.41
1:B:332:VAL:HG21	1:B:338:LEU:CD1	2.50	0.41
1:C:204:CYS:O	1:D:344:THR:HG21	2.20	0.41
1:D:62:ARG:HA	1:D:62:ARG:HD2	1.91	0.41
1:D:469:TYR:O	1:D:473:VAL:HG23	2.20	0.41
1:F:136:GLU:HG2	1:F:375:SER:HB3	2.02	0.41
1:F:293:SER:HB3	1:F:321:PHE:CD1	2.55	0.41
1:F:404:PHE:C	1:F:404:PHE:HD1	2.28	0.41
1:B:101:PHE:O	3:B:602:142:HE2	2.20	0.41
1:B:143:PHE:HB3	1:B:331:TRP:HZ2	1.85	0.41
1:B:365:TRP:CD1	1:B:365:TRP:N	2.89	0.41
1:C:34:ILE:HG12	1:D:111:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:HG23	1:D:362:TYR:HD2	1.85	0.41
1:A:111:LEU:HB2	1:A:380:MET:CE	2.50	0.41
1:B:481:MET:HE1	1:B:513:LEU:HD21	2.02	0.41
1:E:166:THR:CB	2:E:601:PLP:O3P	2.68	0.41
1:E:224:LYS:HD2	1:E:224:LYS:HA	1.81	0.41
1:E:510:TRP:O	1:E:514:GLN:N	2.50	0.41
1:F:98:TYR:HB3	1:F:494:PHE:HA	2.02	0.41
1:D:319:LYS:HZ1	2:D:601:PLP:C4	2.34	0.41
1:E:118:GLY:HA3	1:F:38:LEU:HD22	2.03	0.41
1:F:200:ASP:OD1	1:F:200:ASP:N	2.54	0.41
1:A:252:PRO:HB2	1:A:282:MET:HE2	2.01	0.41
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.84	0.41
3:A:602:142:HNN	3:A:602:142:HD1	1.84	0.41
1:B:334:ASP:OD2	1:B:336:SER:CB	2.69	0.41
1:D:308:GLU:O	1:D:333:LYS:NZ	2.52	0.41
1:F:92:TRP:CH2	1:F:100:TYR:CD2	3.09	0.41
1:D:33:MET:HE2	1:D:33:MET:HB3	1.82	0.41
1:E:173:CYS:HB3	1:E:342:LEU:HD11	2.01	0.41
1:A:22:LEU:HD12	1:A:22:LEU:HA	1.88	0.41
1:B:469:TYR:O	1:B:473:VAL:HG23	2.21	0.41
1:C:197:TYR:CE2	1:C:221:ARG:HG3	2.55	0.41
1:D:164:GLN:OE1	1:D:169:GLU:HG2	2.21	0.41
1:E:73:SER:OG	1:E:74:ILE:N	2.54	0.41
1:E:90:THR:O	1:E:92:TRP:N	2.53	0.41
1:E:93:GLN:O	1:E:93:GLN:HG2	2.19	0.41
1:F:322:PHE:CZ	1:F:393:PHE:HD1	2.38	0.41
3:F:603:142:CD1	3:F:603:142:HNN	2.33	0.41
1:A:334:ASP:OD1	1:A:336:SER:OG	2.39	0.41
1:A:411:ASP:HB3	1:A:414:PHE:HD1	1.85	0.41
1:B:321:PHE:O	1:B:323:THR:HG23	2.21	0.41
1:C:201:GLN:HE22	1:C:486:VAL:HG13	1.86	0.41
1:D:162:VAL:HG23	1:D:362:TYR:CD1	2.56	0.41
1:D:167:SER:O	1:D:171:ILE:HG13	2.20	0.41
1:E:127:MET:HE3	1:F:51:ARG:HB3	2.01	0.41
1:E:263:SER:HB3	1:E:486:VAL:CG2	2.51	0.41
1:E:298:PRO:HD3	1:E:391:ARG:NH2	2.34	0.41
1:F:125:ASN:OD1	1:F:125:ASN:N	2.54	0.41
1:C:132:ALA:HA	1:C:373:PHE:CE1	2.56	0.41
1:D:150:PRO:HG2	1:D:153:PHE:HD2	1.86	0.41
1:F:85:ILE:O	1:F:88:GLY:N	2.52	0.41
1:A:294:ALA:HB2	1:A:320:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:SER:N	1:B:318:HIS:O	2.52	0.40
1:C:531:SER:HA	1:E:485:VAL:HB	2.03	0.40
1:E:235:ALA:HB1	1:E:276:VAL:HG21	2.03	0.40
1:E:515:GLU:O	1:E:518:ASP:HB2	2.20	0.40
1:F:95:PRO:HB2	1:F:505:HIS:CD2	2.57	0.40
1:D:59:LEU:HG	1:D:63:LEU:HD12	2.02	0.40
1:F:34:ILE:CG2	1:F:38:LEU:HD11	2.49	0.40
1:F:115:LEU:HD13	1:F:376:LEU:HD13	2.02	0.40
1:F:199:SER:N	1:F:202:THR:OG1	2.52	0.40
1:F:203:HIS:CE1	2:F:602:PLP:H5A1	2.55	0.40
1:F:511:LYS:O	1:F:515:GLU:N	2.51	0.40
1:A:469:TYR:O	1:A:473:VAL:HG23	2.21	0.40
1:C:55:GLU:O	1:C:58:TYR:HB3	2.21	0.40
1:C:426:CYS:HA	1:C:492:ILE:O	2.22	0.40
1:D:180:ASP:O	1:D:184:ASN:ND2	2.54	0.40
1:E:42:TYR:CB	1:F:24:PRO:HG3	2.50	0.40
1:F:124:PHE:CD1	1:F:124:PHE:C	3.00	0.40
1:F:195:VAL:HG23	1:F:251:ILE:O	2.20	0.40
1:F:316:ASN:OD1	1:F:319:LYS:HD2	2.21	0.40
1:F:414:PHE:CE1	1:F:429:LEU:HD23	2.56	0.40
1:C:21:PRO:O	1:D:107:VAL:HG23	2.21	0.40
1:D:126:TRP:CZ2	1:D:130:PRO:HB3	2.57	0.40
1:E:258:THR:HA	1:E:287:ASP:O	2.22	0.40
1:F:194:LEU:HD13	1:F:253:LEU:HD22	2.02	0.40
1:F:285:HIS:NE2	1:F:314:SER:OG	2.20	0.40
1:F:481:MET:CE	1:F:494:PHE:HD1	2.29	0.40
1:A:110:PHE:HE2	1:A:114:MET:HE2	1.85	0.40
1:A:270:ILE:H	1:A:270:ILE:HG13	1.70	0.40
1:B:429:LEU:N	1:B:466:ASN:OD1	2.47	0.40
1:D:135:LEU:O	1:D:139:VAL:HG22	2.21	0.40
1:E:389:ASN:OD1	1:F:71:PRO:HG3	2.22	0.40
1:F:92:TRP:CZ3	3:F:603:142:CD2	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/531 (90%)	455 (95%)	23 (5%)	1 (0%)	43	70
1	B	477/531 (90%)	458 (96%)	17 (4%)	2 (0%)	30	58
1	C	479/531 (90%)	455 (95%)	23 (5%)	1 (0%)	43	70
1	D	477/531 (90%)	452 (95%)	22 (5%)	3 (1%)	21	49
1	E	471/531 (89%)	442 (94%)	21 (4%)	8 (2%)	7	27
1	F	462/531 (87%)	417 (90%)	42 (9%)	3 (1%)	21	49
All	All	2845/3186 (89%)	2679 (94%)	148 (5%)	18 (1%)	21	49

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	423	ALA
1	D	320	TRP
1	E	28	ARG
1	E	91	HIS
1	F	499	THR
1	A	497	GLY
1	B	497	GLY
1	E	25	GLU
1	E	26	GLU
1	E	373	PHE
1	F	295	CYS
1	D	497	GLY
1	E	29	ARG
1	B	324	THR
1	E	120	ASN
1	E	265	THR
1	F	93	GLN
1	C	497	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/456 (91%)	414 (100%)	2 (0%)	81	80
1	B	414/456 (91%)	413 (100%)	1 (0%)	87	85
1	C	416/456 (91%)	416 (100%)	0	100	100
1	D	414/456 (91%)	411 (99%)	3 (1%)	76	77
1	E	412/456 (90%)	410 (100%)	2 (0%)	81	80
1	F	403/456 (88%)	400 (99%)	3 (1%)	76	77
All	All	2475/2736 (90%)	2464 (100%)	11 (0%)	84	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	LEU
1	A	316	ASN
1	B	336	SER
1	D	262	THR
1	D	319	LYS
1	D	371	ARG
1	E	28	ARG
1	E	515	GLU
1	F	82	THR
1	F	85	ILE
1	F	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	201	GLN
1	A	211	GLN
1	A	318	HIS
1	A	474	ASN
1	A	483	HIS
1	B	32	HIS
1	B	93	GLN
1	B	229	ASN
1	B	316	ASN
1	C	30	GLN
1	C	203	HIS

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Mol	Chain	Res	Type
1	C	219	ASN
1	C	514	GLN
1	D	96	ASN
1	D	316	ASN
1	D	318	HIS
1	E	366	GLN
1	E	392	ASN
1	F	70	ASN
1	F	474	ASN
1	F	505	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](#)

12 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	142	D	602	2	14,16,16	1.60	1 (7%)	20,23,23	1.43	3 (15%)
2	PLP	B	601	3	15,15,16	2.99	3 (20%)	21,22,23	1.18	1 (4%)
2	PLP	D	601	3	15,15,16	3.01	3 (20%)	21,22,23	1.18	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	142	C	602	2	14,16,16	1.60	1 (7%)	20,23,23	1.43	3 (15%)
2	PLP	E	601	3	15,15,16	2.02	4 (26%)	21,22,23	1.67	3 (14%)
3	142	B	602	2	14,16,16	1.59	1 (7%)	20,23,23	1.44	3 (15%)
2	PLP	C	601	3	15,15,16	3.00	3 (20%)	21,22,23	1.19	1 (4%)
3	142	A	602	2	14,16,16	1.33	1 (7%)	20,23,23	1.49	2 (10%)
3	142	F	601	2	14,16,16	1.33	1 (7%)	20,23,23	1.49	2 (10%)
2	PLP	A	601	3	15,15,16	2.02	4 (26%)	21,22,23	1.67	3 (14%)
2	PLP	F	602	3	15,15,16	2.99	3 (20%)	21,22,23	1.18	1 (4%)
3	142	F	603	2	14,16,16	1.59	1 (7%)	20,23,23	1.43	3 (15%)

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	142	D	602	2	-	3/11/14/14	0/1/1/1
2	PLP	B	601	3	-	4/6/6/8	0/1/1/1
2	PLP	D	601	3	-	4/6/6/8	0/1/1/1
3	142	C	602	2	-	3/11/14/14	0/1/1/1
2	PLP	E	601	3	-	3/6/6/8	0/1/1/1
3	142	B	602	2	-	1/11/14/14	0/1/1/1
2	PLP	C	601	3	-	4/6/6/8	0/1/1/1
3	142	A	602	2	-	7/11/14/14	0/1/1/1
3	142	F	601	2	-	7/11/14/14	0/1/1/1
2	PLP	A	601	3	-	3/6/6/8	0/1/1/1
2	PLP	F	602	3	-	4/6/6/8	0/1/1/1
3	142	F	603	2	-	3/11/14/14	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	PLP	C3-C2	7.65	1.48	1.41
2	F	602	PLP	C3-C2	7.62	1.48	1.41
2	C	601	PLP	C3-C2	7.61	1.48	1.41
2	B	601	PLP	C3-C2	7.59	1.48	1.41
2	D	601	PLP	C5-C4	7.28	1.48	1.40
2	C	601	PLP	C5-C4	7.26	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PLP	C5-C4	7.24	1.48	1.40
2	F	602	PLP	C5-C4	7.20	1.48	1.40
3	D	602	142	CZ-CE1	5.25	1.48	1.40
3	C	602	142	CZ-CE1	5.25	1.48	1.40
3	B	602	142	CZ-CE1	5.23	1.48	1.40
3	F	603	142	CZ-CE1	5.22	1.48	1.40
2	C	601	PLP	C3-C4	4.40	1.48	1.40
2	D	601	PLP	C3-C4	4.36	1.48	1.40
2	F	602	PLP	C3-C4	4.36	1.48	1.40
2	B	601	PLP	C3-C4	4.34	1.48	1.40
2	E	601	PLP	C3-C2	-4.02	1.36	1.41
2	A	601	PLP	C3-C2	-4.02	1.36	1.41
2	A	601	PLP	P-O1P	3.57	1.61	1.50
2	E	601	PLP	P-O1P	3.57	1.61	1.50
2	A	601	PLP	P-O2P	-3.20	1.42	1.54
2	E	601	PLP	P-O2P	-3.20	1.42	1.54
2	E	601	PLP	P-O3P	-3.04	1.43	1.54
2	A	601	PLP	P-O3P	-3.04	1.43	1.54
3	F	601	142	CB-CA	-2.13	1.52	1.55
3	A	602	142	CB-CA	-2.12	1.52	1.55

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	142	CA-NN-N	5.08	121.82	113.78
3	F	601	142	CA-NN-N	5.07	121.81	113.78
2	A	601	PLP	C2A-C2-C3	-4.55	115.47	120.80
2	E	601	PLP	C2A-C2-C3	-4.55	115.47	120.80
3	C	602	142	CA-NN-N	3.94	120.02	113.78
3	F	603	142	CA-NN-N	3.94	120.01	113.78
3	D	602	142	CA-NN-N	3.94	120.01	113.78
3	B	602	142	CA-NN-N	3.91	119.97	113.78
3	B	602	142	CA-CB-CG	-2.96	109.48	115.05
3	D	602	142	CA-CB-CG	-2.94	109.52	115.05
3	F	603	142	CA-CB-CG	-2.93	109.53	115.05
3	C	602	142	CA-CB-CG	-2.92	109.55	115.05
2	A	601	PLP	O3P-P-O4P	2.80	113.98	106.67
2	E	601	PLP	O3P-P-O4P	2.79	113.95	106.67
3	B	602	142	O-C-CA	-2.42	118.44	122.78
3	D	602	142	O-C-CA	-2.40	118.47	122.78
3	F	603	142	O-C-CA	-2.37	118.53	122.78
3	C	602	142	O-C-CA	-2.36	118.55	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	PLP	C6-N1-C2	2.24	123.27	119.20
2	B	601	PLP	C6-N1-C2	2.21	123.20	119.20
2	D	601	PLP	C6-N1-C2	2.20	123.19	119.20
2	F	602	PLP	C6-N1-C2	2.20	123.18	119.20
3	A	602	142	OXT-C-CA	2.14	120.19	113.77
3	F	601	142	OXT-C-CA	2.14	120.17	113.77
2	A	601	PLP	C2A-C2-N1	2.00	121.41	117.64
2	E	601	PLP	C2A-C2-N1	2.00	121.41	117.64

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PLP	C5A-O4P-P-O1P
2	A	601	PLP	C5A-O4P-P-O2P
2	A	601	PLP	C5A-O4P-P-O3P
2	B	601	PLP	C4-C5-C5A-O4P
2	B	601	PLP	C5A-O4P-P-O2P
2	B	601	PLP	C5A-O4P-P-O3P
2	C	601	PLP	C4-C5-C5A-O4P
2	C	601	PLP	C5A-O4P-P-O2P
2	C	601	PLP	C5A-O4P-P-O3P
2	D	601	PLP	C4-C5-C5A-O4P
2	D	601	PLP	C5A-O4P-P-O1P
2	D	601	PLP	C5A-O4P-P-O2P
2	D	601	PLP	C5A-O4P-P-O3P
2	E	601	PLP	C5A-O4P-P-O1P
2	E	601	PLP	C5A-O4P-P-O2P
2	E	601	PLP	C5A-O4P-P-O3P
2	F	602	PLP	C4-C5-C5A-O4P
2	F	602	PLP	C5A-O4P-P-O2P
2	F	602	PLP	C5A-O4P-P-O3P
3	A	602	142	OXT-C-CA-CB1
3	F	601	142	OXT-C-CA-CB1
2	B	601	PLP	C5A-O4P-P-O1P
2	C	601	PLP	C5A-O4P-P-O1P
2	F	602	PLP	C5A-O4P-P-O1P
3	A	602	142	OXT-C-CA-CB
3	D	602	142	OXT-C-CA-CB
3	F	601	142	OXT-C-CA-CB
3	D	602	142	OXT-C-CA-CB1
3	A	602	142	CB1-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	F	601	142	CB1-CA-CB-CG
3	C	602	142	O-C-CA-CB1
3	F	603	142	O-C-CA-CB1
3	A	602	142	O-C-CA-CB
3	C	602	142	OXT-C-CA-CB
3	D	602	142	O-C-CA-CB
3	F	601	142	O-C-CA-CB
3	F	603	142	OXT-C-CA-CB
3	A	602	142	O-C-CA-CB1
3	F	601	142	O-C-CA-CB1
3	A	602	142	NN-CA-CB-CG
3	F	601	142	NN-CA-CB-CG
3	A	602	142	C-CA-CB-CG
3	F	601	142	C-CA-CB-CG
3	B	602	142	O-C-CA-CB1
3	C	602	142	OXT-C-CA-CB1
3	F	603	142	OXT-C-CA-CB1

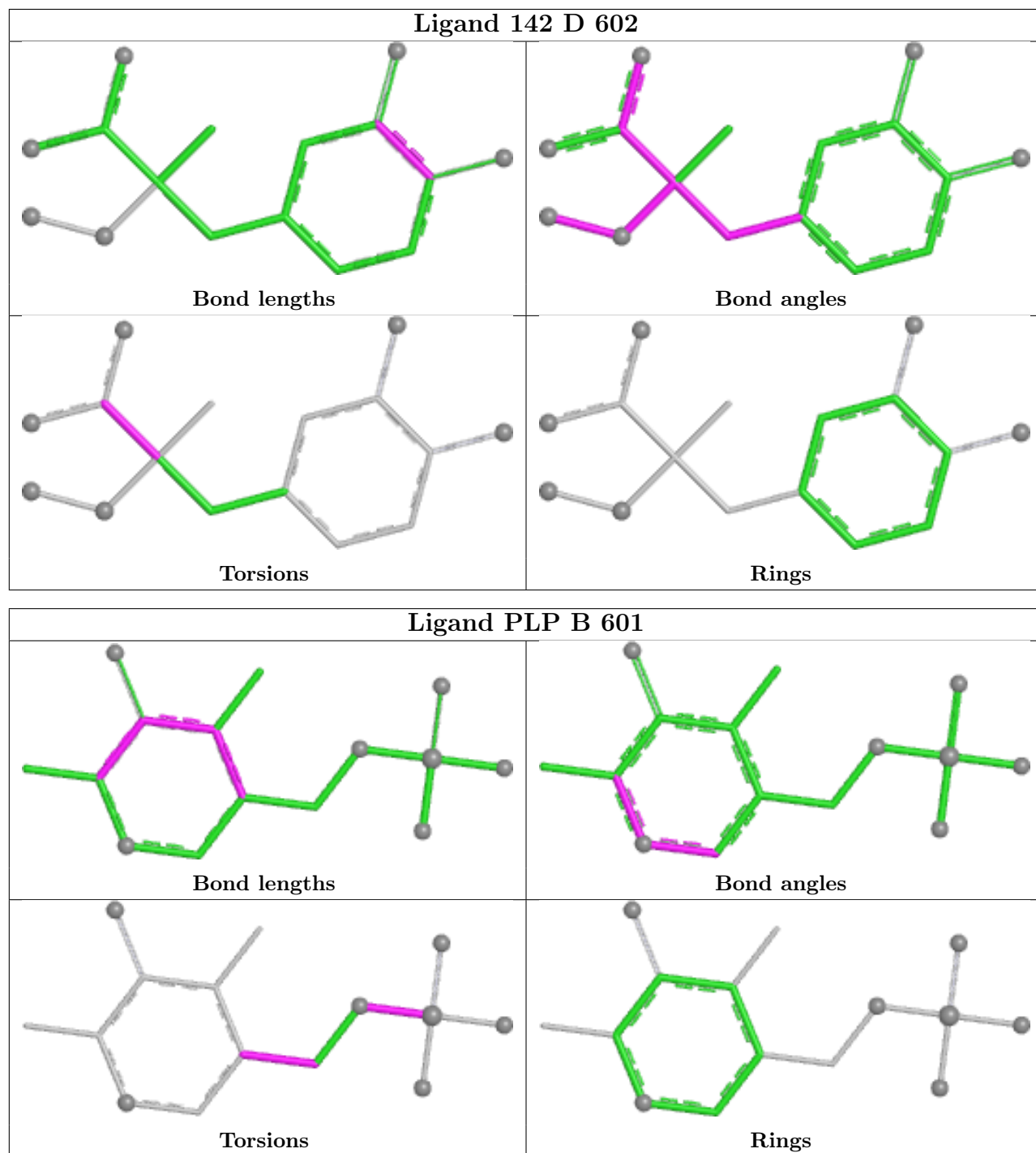
There are no ring outliers.

12 monomers are involved in 53 short contacts:

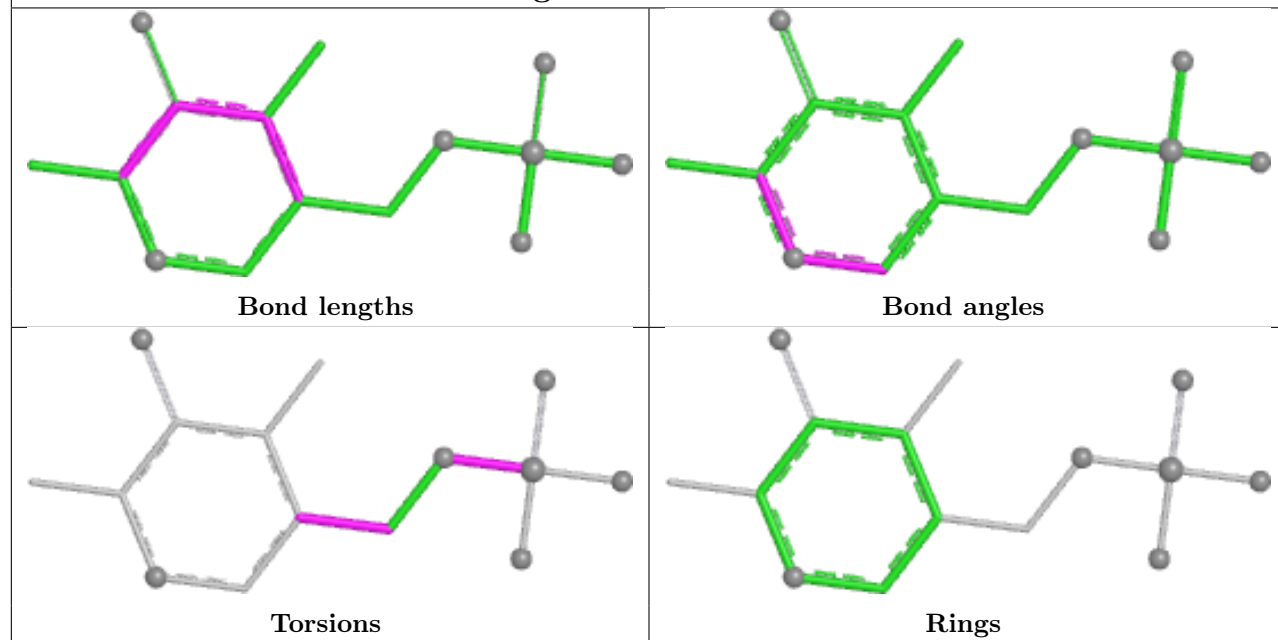
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	142	6	0
2	B	601	PLP	2	0
2	D	601	PLP	5	0
3	C	602	142	4	0
2	E	601	PLP	7	0
3	B	602	142	2	0
2	C	601	PLP	2	0
3	A	602	142	3	0
3	F	601	142	5	0
2	A	601	PLP	2	0
2	F	602	PLP	9	0
3	F	603	142	6	0

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

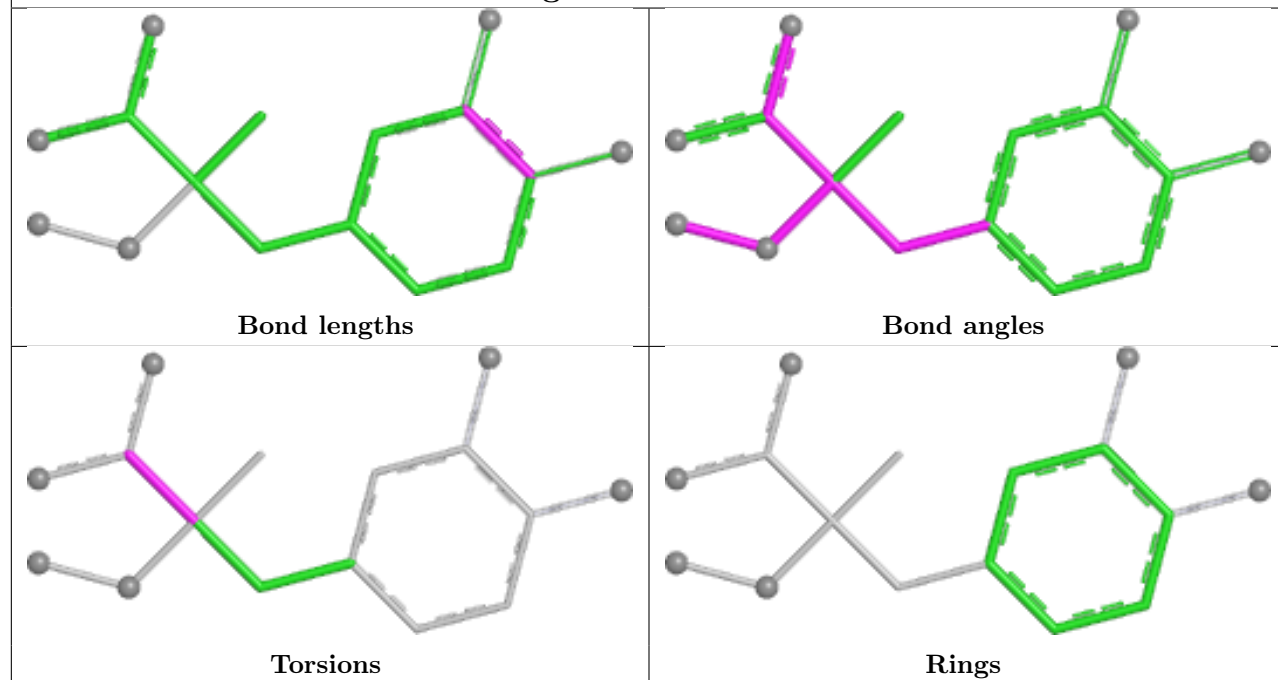
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



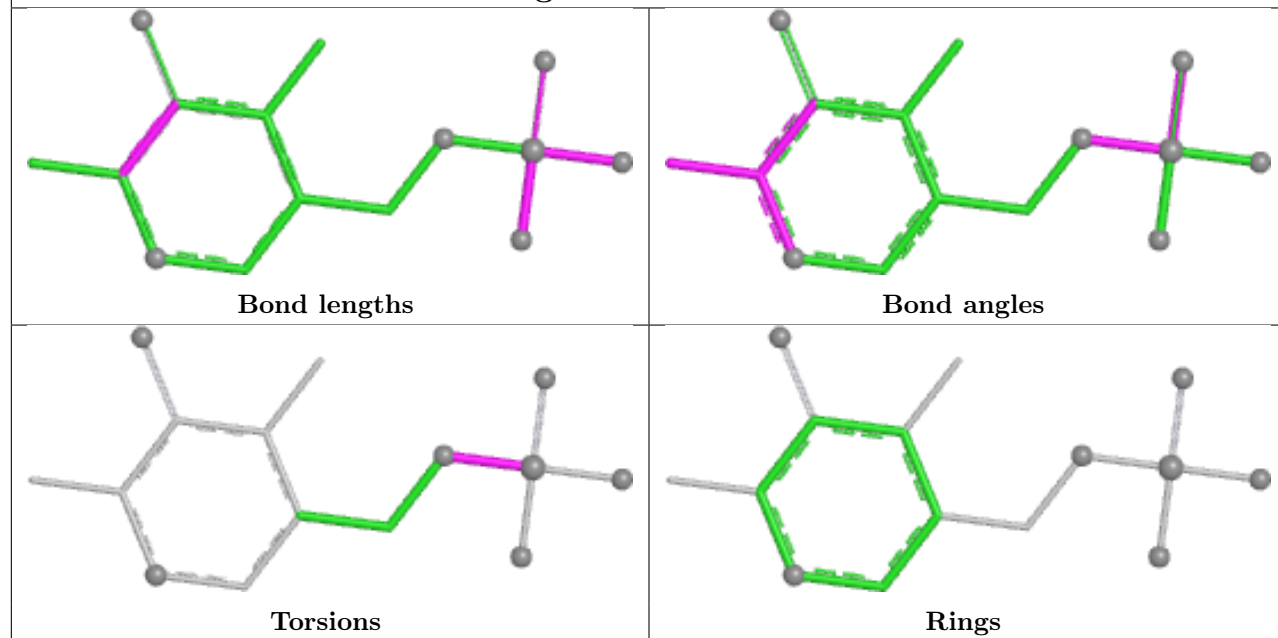
Ligand PLP D 601



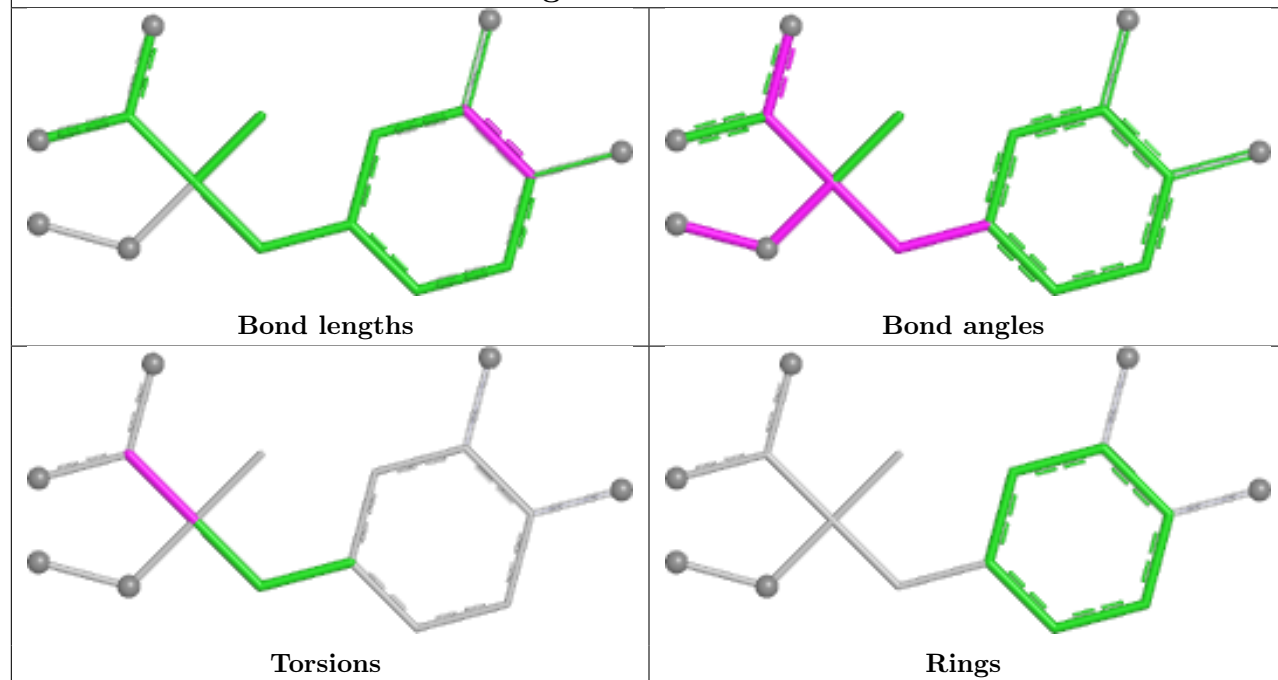
Ligand 142 C 602



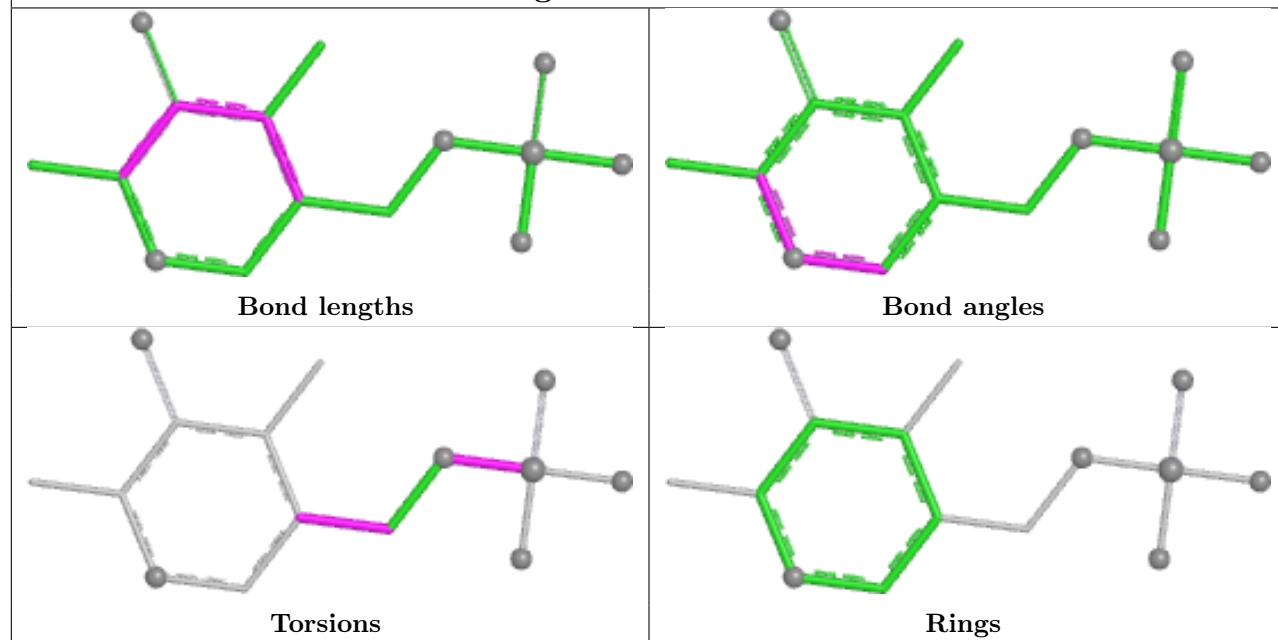
Ligand PLP E 601



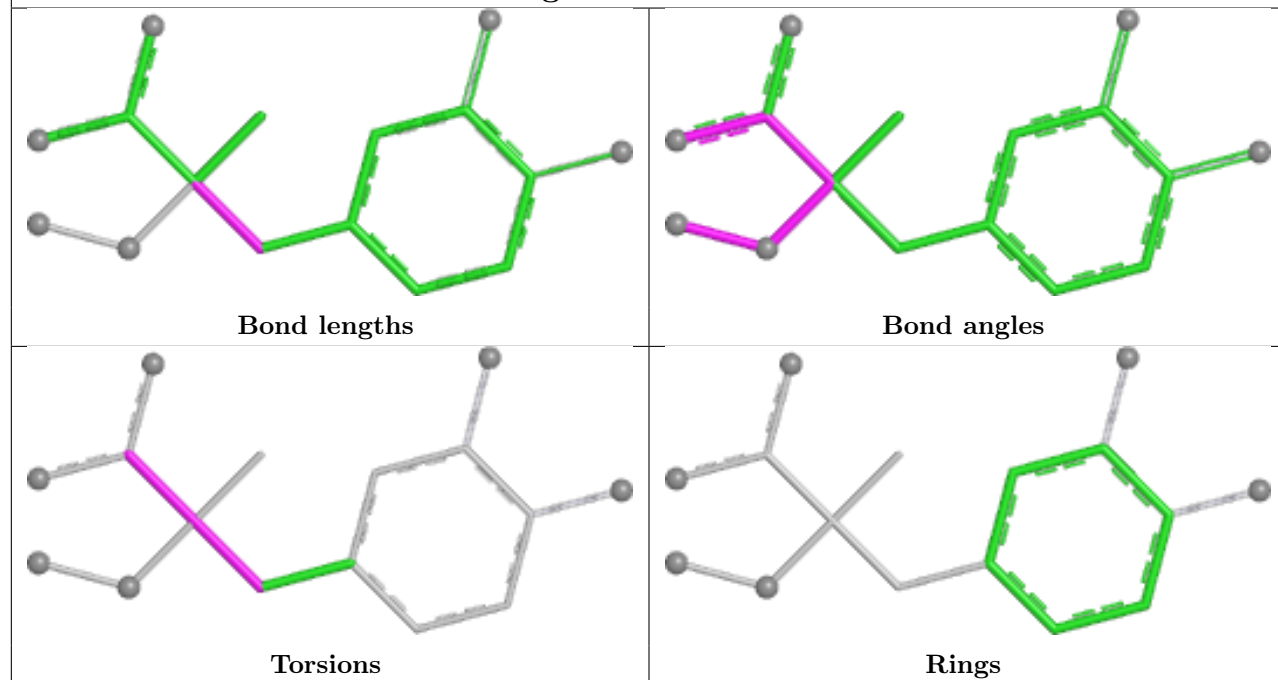
Ligand 142 B 602



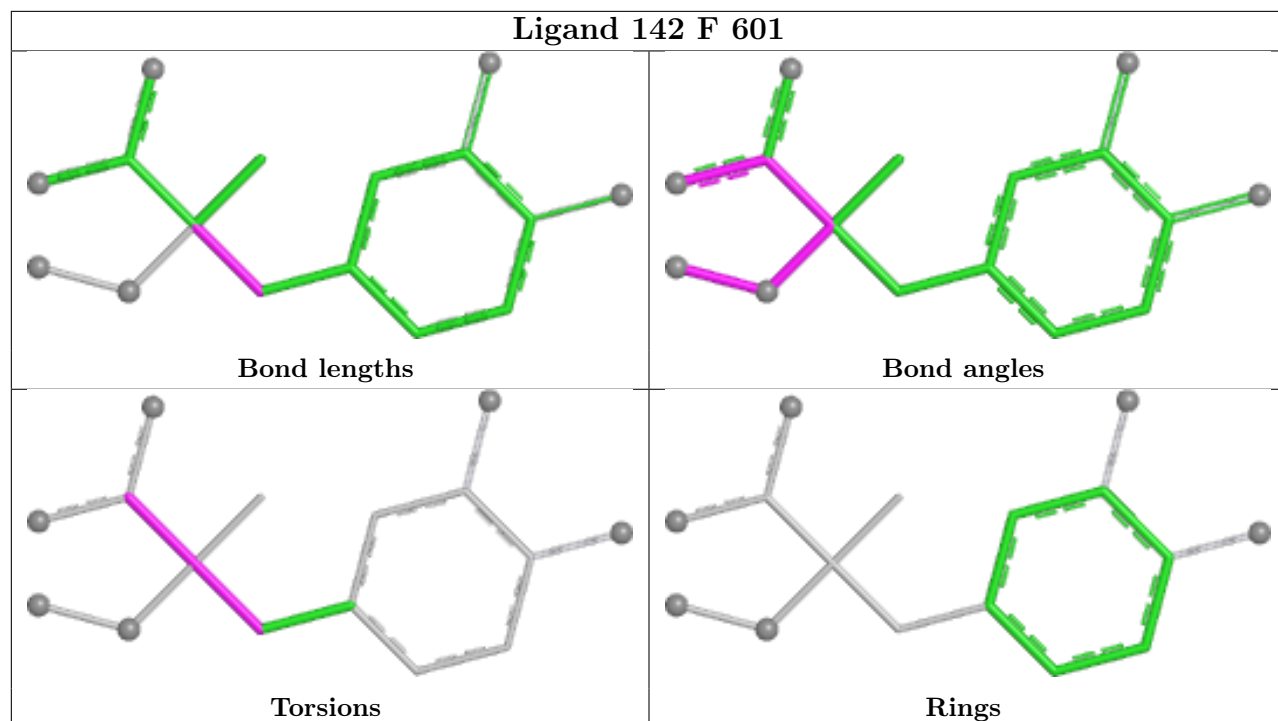
Ligand PLP C 601



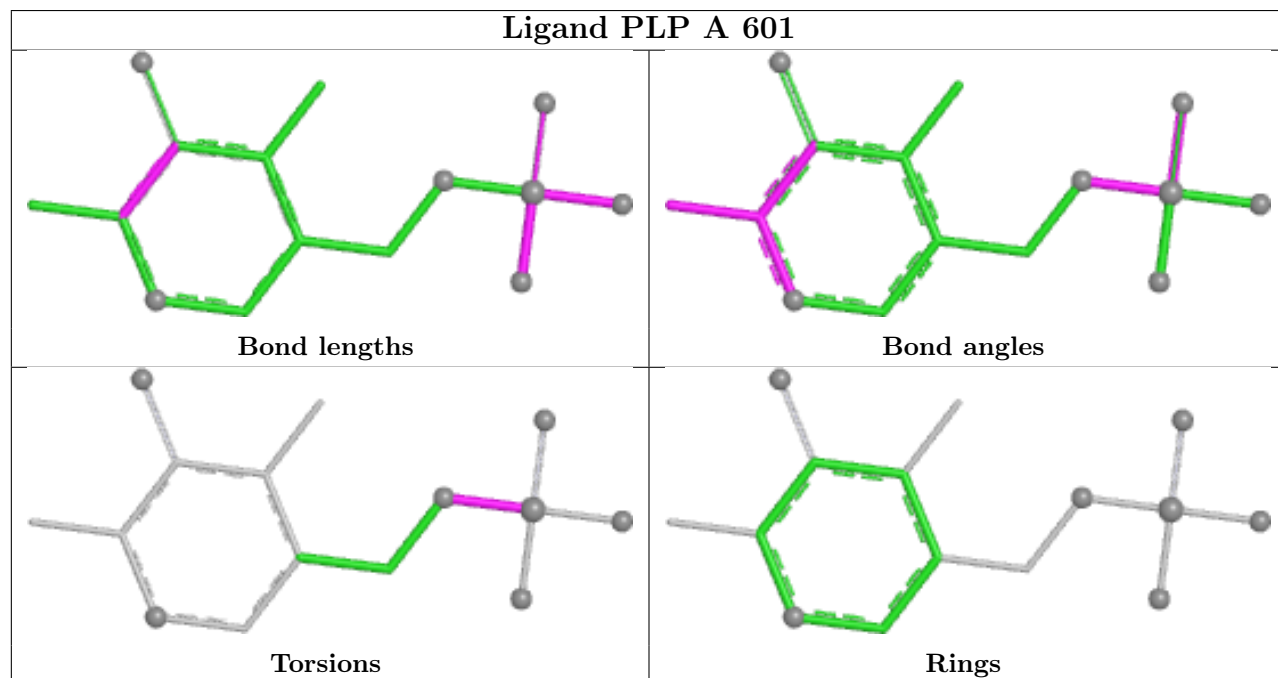
Ligand 142 A 602

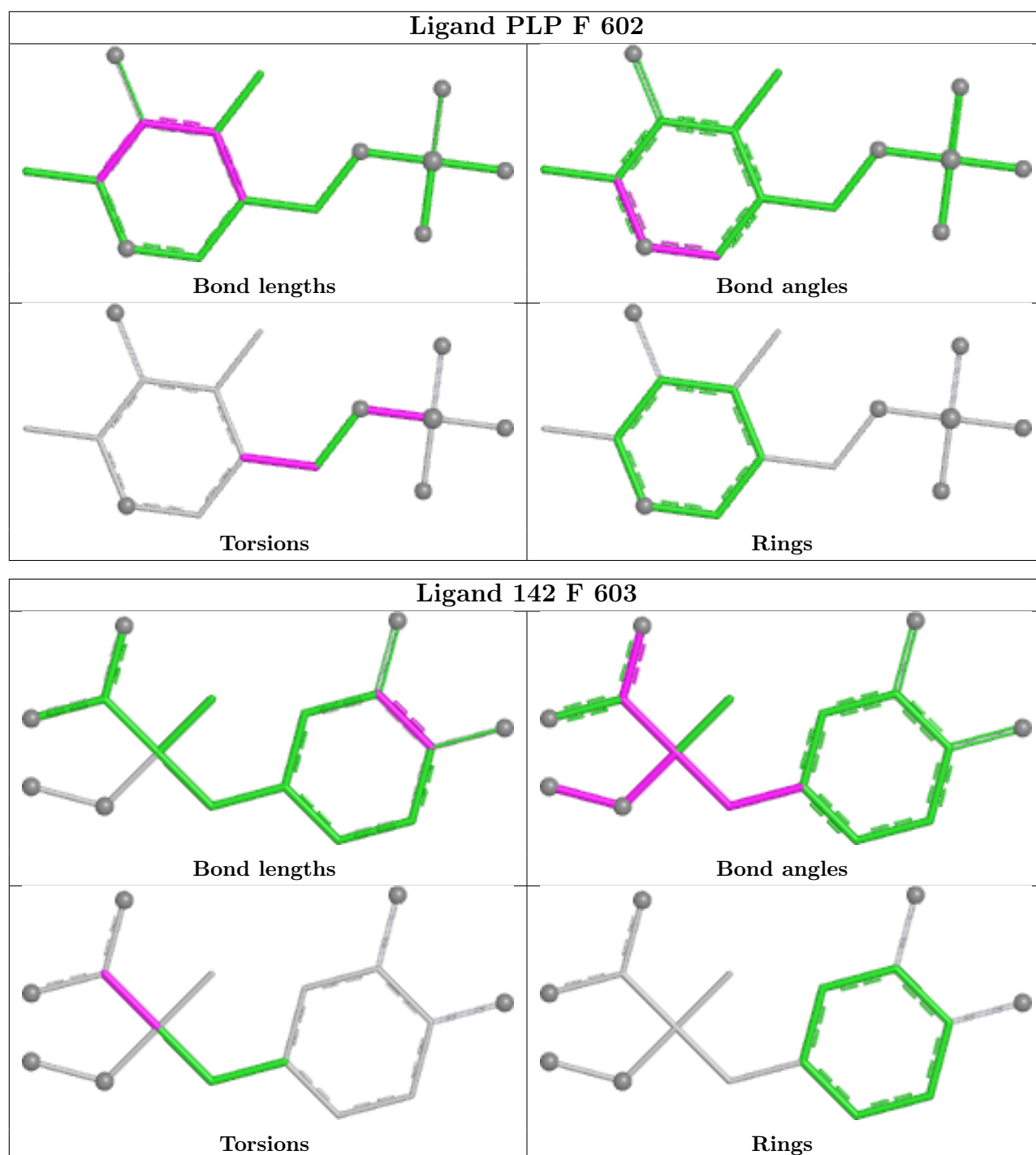


Ligand 142 F 601



Ligand PLP A 601





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	485/531 (91%)	-0.09	2 (0%) 88 81	19, 36, 57, 94	0
1	B	483/531 (90%)	-0.18	5 (1%) 79 66	20, 33, 54, 98	0
1	C	485/531 (91%)	-0.05	2 (0%) 88 81	21, 37, 63, 101	0
1	D	483/531 (90%)	-0.13	1 (0%) 91 87	18, 34, 55, 82	0
1	E	479/531 (90%)	1.71	167 (34%) 1 1	60, 92, 113, 126	0
1	F	474/531 (89%)	1.66	166 (35%) 1 1	41, 89, 116, 128	0
All	All	2889/3186 (90%)	0.48	343 (11%) 9 9	18, 42, 107, 128	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	22	LEU	7.4
1	F	379	TRP	6.1
1	F	318	HIS	5.8
1	F	380	MET	5.7
1	E	500	LEU	5.7
1	F	479	VAL	5.6
1	F	90	THR	5.4
1	F	41	TYR	5.1
1	E	121	VAL	5.0
1	F	92	TRP	5.0
1	F	96	ASN	5.0
1	F	77	ILE	4.9
1	F	423	ALA	4.9
1	E	122	VAL	4.9
1	E	20	ASN	4.8
1	F	327	CYS	4.8
1	E	105	GLY	4.8
1	F	477	GLY	4.8
1	F	89	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	83	THR	4.7
1	F	24	PRO	4.7
1	E	143	PHE	4.6
1	F	393	PHE	4.5
1	F	37	PHE	4.4
1	F	95	PRO	4.4
1	F	480	TYR	4.4
1	E	24	PRO	4.3
1	F	382	LEU	4.3
1	F	298	PRO	4.2
1	F	296	ILE	4.2
1	F	50	VAL	4.2
1	F	42	TYR	4.2
1	F	122	VAL	4.2
1	F	513	LEU	4.2
1	F	128	SER	4.2
1	E	68	PRO	4.2
1	F	74	ILE	4.2
1	F	59	LEU	4.1
1	E	378	LEU	4.1
1	E	27	PHE	4.1
1	E	478	SER	4.0
1	F	498	SER	4.0
1	E	292	GLY	4.0
1	F	121	VAL	4.0
1	F	506	VAL	4.0
1	F	22	LEU	4.0
1	F	120	ASN	4.0
1	F	507	ILE	4.0
1	F	499	THR	3.8
1	F	369	LEU	3.8
1	E	509	ALA	3.8
1	E	328	CYS	3.8
1	F	135	LEU	3.8
1	E	268	ASP	3.8
1	F	348	TYR	3.8
1	E	51	ARG	3.8
1	F	45	VAL	3.8
1	E	93	GLN	3.7
1	E	383	ARG	3.7
1	F	38	LEU	3.7
1	F	387	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	85	ILE	3.7
1	F	142	TRP	3.7
1	E	163	LEU	3.7
1	E	167	SER	3.7
1	E	324	THR	3.7
1	F	478	SER	3.7
1	E	382	LEU	3.7
1	E	103	SER	3.6
1	F	494	PHE	3.6
1	E	88	GLY	3.6
1	E	379	TRP	3.6
1	F	129	SER	3.6
1	E	507	ILE	3.6
1	F	97	TYR	3.6
1	F	64	PRO	3.6
1	F	48	TYR	3.5
1	E	377	LYS	3.5
1	F	49	PRO	3.5
1	F	52	SER	3.5
1	E	294	ALA	3.5
1	E	72	GLU	3.5
1	E	97	TYR	3.5
1	E	59	LEU	3.5
1	E	74	ILE	3.5
1	E	329	CYS	3.4
1	E	106	SER	3.4
1	F	123	GLY	3.4
1	F	394	LEU	3.4
1	E	365	TRP	3.4
1	F	297	CYS	3.3
1	F	373	PHE	3.3
1	E	394	LEU	3.3
1	F	106	SER	3.3
1	E	19	THR	3.3
1	F	143	PHE	3.3
1	E	393	PHE	3.3
1	F	500	LEU	3.3
1	E	503	GLU	3.3
1	F	294	ALA	3.3
1	E	71	PRO	3.2
1	E	142	TRP	3.2
1	E	380	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	94	SER	3.2
1	E	326	ASP	3.2
1	E	381	VAL	3.2
1	E	479	VAL	3.2
1	F	30	GLN	3.2
1	F	425	VAL	3.2
1	F	300	PHE	3.2
1	E	44	ASP	3.2
1	F	133	THR	3.2
1	F	299	GLU	3.2
1	F	322	PHE	3.2
1	F	93	GLN	3.2
1	E	423	ALA	3.2
1	E	422	PHE	3.1
1	E	373	PHE	3.1
1	E	258	THR	3.1
1	E	260	GLY	3.1
1	E	90	THR	3.1
1	E	109	GLY	3.1
1	B	347	GLU	3.1
1	E	124	PHE	3.1
1	E	269	PRO	3.1
1	E	388	THR	3.1
1	E	331	TRP	3.1
1	E	327	CYS	3.1
1	F	390	LEU	3.0
1	E	91	HIS	3.0
1	F	67	ALA	3.0
1	E	147	LEU	3.0
1	F	119	PHE	3.0
1	B	346	PRO	3.0
1	F	295	CYS	3.0
1	E	304	ILE	3.0
1	E	104	SER	2.9
1	F	374	ARG	2.9
1	F	66	THR	2.9
1	E	310	ALA	2.9
1	E	45	VAL	2.9
1	E	290	TYR	2.9
1	E	73	SER	2.9
1	E	293	SER	2.9
1	F	481	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	511	LYS	2.9
1	E	95	PRO	2.9
1	F	389	ASN	2.9
1	F	329	CYS	2.9
1	E	110	PHE	2.9
1	E	397	HIS	2.9
1	E	317	ALA	2.9
1	E	359	VAL	2.9
1	E	48	TYR	2.9
1	F	32	HIS	2.8
1	F	51	ARG	2.8
1	F	260	GLY	2.8
1	E	150	PRO	2.8
1	E	256	CYS	2.8
1	E	481	MET	2.8
1	F	91	HIS	2.8
1	F	521	LEU	2.8
1	E	137	SER	2.8
1	E	92	TRP	2.8
1	E	141	ASP	2.8
1	F	510	TRP	2.8
1	F	474	ASN	2.8
1	E	39	ALA	2.8
1	E	66	THR	2.8
1	E	82	THR	2.8
1	E	123	GLY	2.7
1	E	52	SER	2.7
1	F	82	THR	2.7
1	F	501	THR	2.7
1	F	36	ASP	2.7
1	F	58	TYR	2.7
1	E	54	VAL	2.7
1	E	81	VAL	2.7
1	F	432	PRO	2.7
1	F	78	LEU	2.7
1	F	115	LEU	2.7
1	F	292	GLY	2.7
1	E	149	LEU	2.7
1	E	108	ALA	2.7
1	E	69	TYR	2.7
1	E	107	VAL	2.7
1	F	100	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	385	TYR	2.7
1	E	296	ILE	2.6
1	F	46	GLU	2.6
1	F	396	SER	2.6
1	E	372	ARG	2.6
1	E	267	VAL	2.6
1	F	509	ALA	2.6
1	F	21	PRO	2.6
1	F	68	PRO	2.6
1	F	424	MET	2.6
1	F	381	VAL	2.6
1	F	418	VAL	2.6
1	F	512	ILE	2.6
1	E	477	GLY	2.6
1	E	325	LEU	2.6
1	F	378	LEU	2.6
1	F	496	VAL	2.6
1	E	384	SER	2.6
1	E	307	VAL	2.6
1	E	421	THR	2.6
1	F	400	MET	2.5
1	E	259	VAL	2.5
1	F	368	ALA	2.5
1	F	503	GLU	2.5
1	F	397	HIS	2.5
1	F	291	ALA	2.5
1	F	316	ASN	2.5
1	F	472	THR	2.5
1	E	362	TYR	2.5
1	E	78	LEU	2.5
1	E	284	VAL	2.5
1	E	162	VAL	2.5
1	F	416	ILE	2.5
1	F	471	GLU	2.5
1	E	96	ASN	2.5
1	E	38	LEU	2.5
1	E	508	TYR	2.5
1	F	317	ALA	2.4
1	F	495	ALA	2.4
1	E	168	CYS	2.4
1	E	26	GLU	2.4
1	F	134	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	422	PHE	2.4
1	E	519	LEU	2.4
1	F	470	LEU	2.4
1	E	41	TYR	2.4
1	E	314	SER	2.4
1	E	501	THR	2.4
1	F	20	ASN	2.4
1	F	125	ASN	2.4
1	F	392	ASN	2.4
1	E	32	HIS	2.4
1	E	270	ILE	2.4
1	E	42	TYR	2.4
1	E	161	GLY	2.4
1	C	352	LYS	2.4
1	F	419	PRO	2.4
1	F	431	PRO	2.4
1	A	348	TYR	2.4
1	E	287	ASP	2.4
1	E	236	ALA	2.4
1	E	234	SER	2.4
1	E	496	VAL	2.4
1	F	482	THR	2.3
1	B	348	TYR	2.3
1	F	39	ALA	2.3
1	E	30	GLN	2.3
1	E	322	PHE	2.3
1	E	330	LEU	2.3
1	E	506	VAL	2.3
1	E	117	THR	2.3
1	E	403	THR	2.3
1	F	76	THR	2.3
1	E	490	TYR	2.3
1	E	135	LEU	2.3
1	F	124	PHE	2.3
1	F	25	GLU	2.3
1	E	139	VAL	2.3
1	F	388	THR	2.3
1	F	517	ALA	2.3
1	F	98	TYR	2.3
1	A	351	ASN	2.3
1	E	154	LEU	2.3
1	F	79	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	367	ILE	2.3
1	F	31	GLY	2.3
1	F	377	LYS	2.3
1	F	391	ARG	2.3
1	E	175	LEU	2.3
1	E	321	PHE	2.3
1	E	375	SER	2.3
1	F	105	GLY	2.2
1	E	313	PHE	2.2
1	E	516	HIS	2.2
1	D	129	SER	2.2
1	E	399	LYS	2.2
1	F	426	CYS	2.2
1	E	223	ILE	2.2
1	E	130	PRO	2.2
1	F	56	PRO	2.2
1	F	475	ALA	2.2
1	E	83	THR	2.2
1	F	476	THR	2.2
1	B	129	SER	2.2
1	E	84	GLU	2.2
1	F	35	ILE	2.2
1	B	349	LEU	2.2
1	E	21	PRO	2.2
1	E	115	LEU	2.2
1	F	427	PHE	2.2
1	F	138	VAL	2.2
1	E	194	LEU	2.2
1	E	177	ALA	2.2
1	F	33	MET	2.2
1	F	139	VAL	2.2
1	F	398	VAL	2.2
1	F	469	TYR	2.2
1	F	465	LEU	2.2
1	F	114	MET	2.2
1	E	120	ASN	2.2
1	E	131	ALA	2.2
1	F	141	ASP	2.2
1	F	473	VAL	2.1
1	E	35	ILE	2.1
1	E	376	LEU	2.1
1	E	521	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	64	PRO	2.1
1	F	321	PHE	2.1
1	F	127	MET	2.1
1	E	188	ARG	2.1
1	F	108	ALA	2.1
1	E	56	PRO	2.1
1	F	293	SER	2.1
1	F	80	ASP	2.1
1	E	291	ALA	2.1
1	F	70	ASN	2.1
1	E	523	LYS	2.1
1	E	295	CYS	2.1
1	E	102	PRO	2.1
1	E	113	GLU	2.1
1	F	349	LEU	2.1
1	F	117	THR	2.1
1	F	262	THR	2.1
1	F	290	TYR	2.1
1	F	289	ALA	2.1
1	E	112	GLY	2.1
1	E	404	PHE	2.1
1	E	186	ILE	2.0
1	E	315	LEU	2.0
1	E	374	ARG	2.0
1	F	429	LEU	2.0
1	E	111	LEU	2.0
1	F	375	SER	2.0
1	F	146	MET	2.0
1	E	235	ALA	2.0
1	E	23	ASP	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

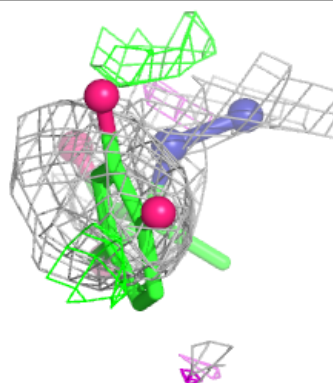
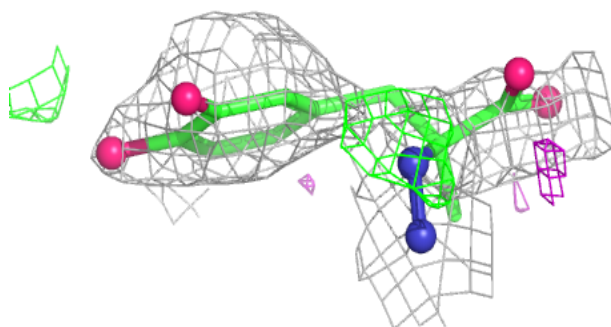
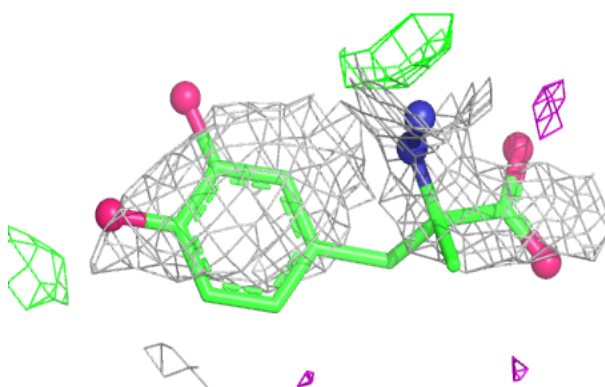
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	142	F	601	16/16	0.60	0.28	89,106,117,119	0
3	142	F	603	16/16	0.72	0.21	88,109,115,117	0
2	PLP	E	601	15/16	0.84	0.15	74,89,109,124	0
2	PLP	F	602	15/16	0.86	0.18	41,61,90,95	0
3	142	D	602	16/16	0.86	0.19	26,38,49,50	0
3	142	A	602	16/16	0.90	0.16	24,45,61,67	0
3	142	B	602	16/16	0.90	0.15	25,33,45,50	0
3	142	C	602	16/16	0.90	0.15	31,37,50,53	0
2	PLP	C	601	15/16	0.93	0.11	28,35,50,56	0
2	PLP	D	601	15/16	0.94	0.11	22,27,43,45	0
2	PLP	A	601	15/16	0.95	0.10	23,35,50,53	0
2	PLP	B	601	15/16	0.95	0.12	27,32,49,55	0

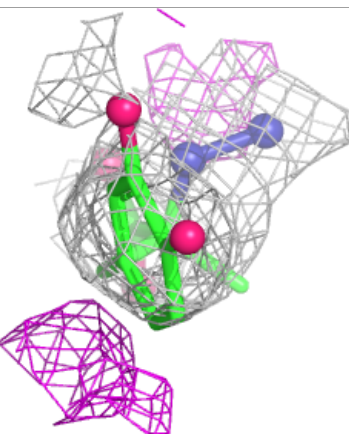
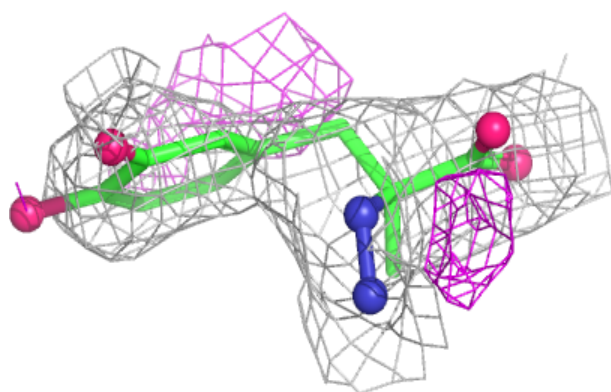
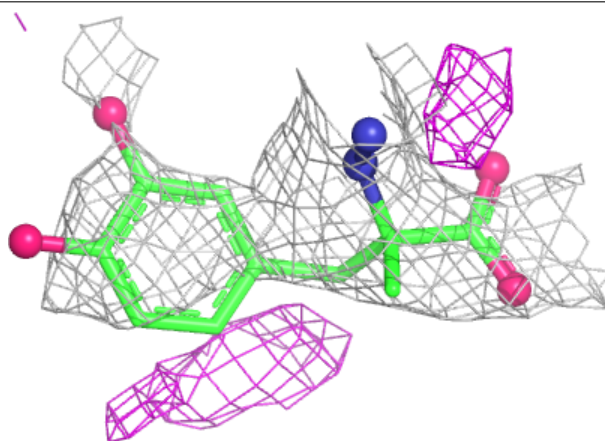
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 142 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)

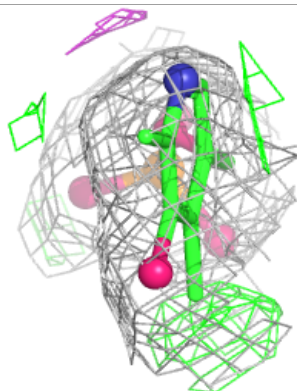
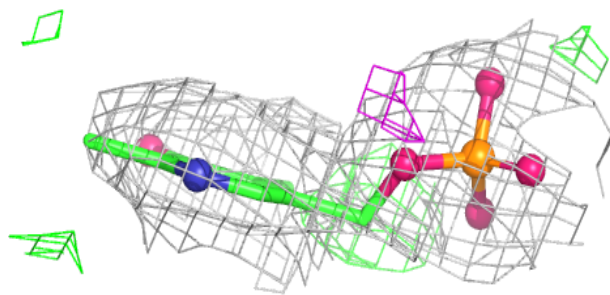
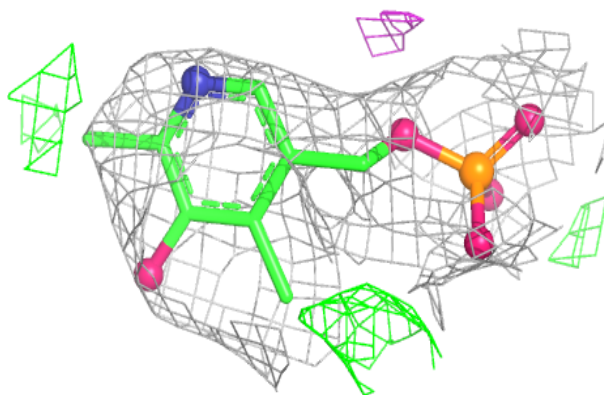
**Electron density around 142 F 603:**

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

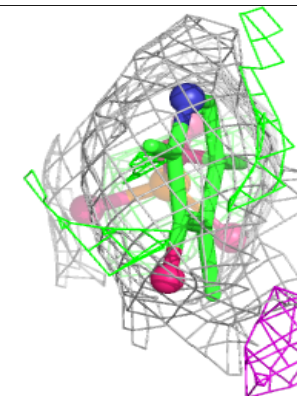
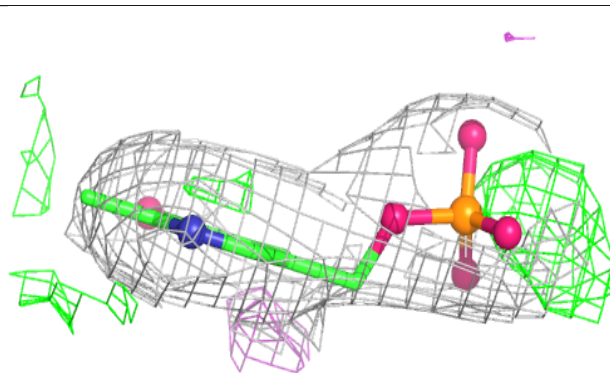
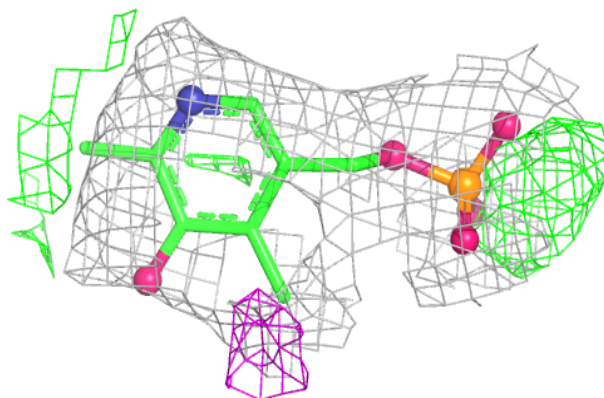


Electron density around PLP E 601:

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

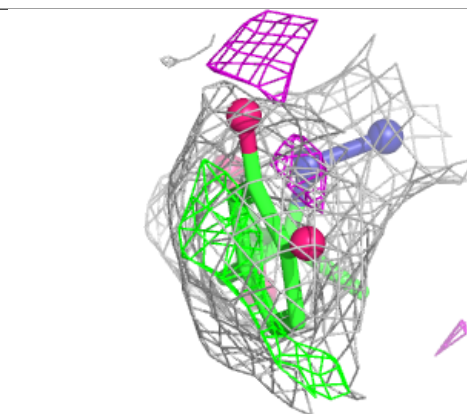
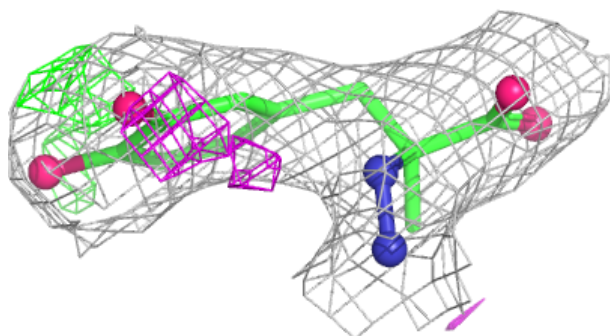
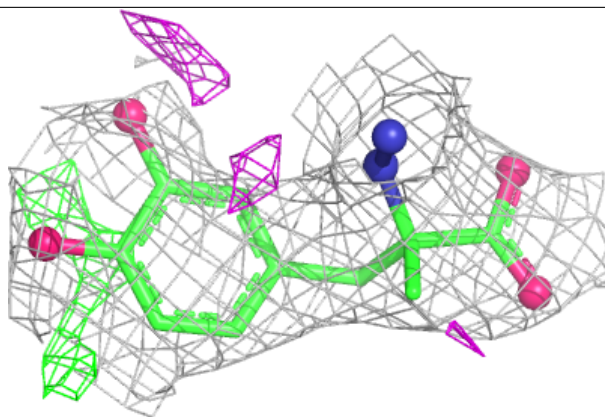
**Electron density around PLP F 602:**

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

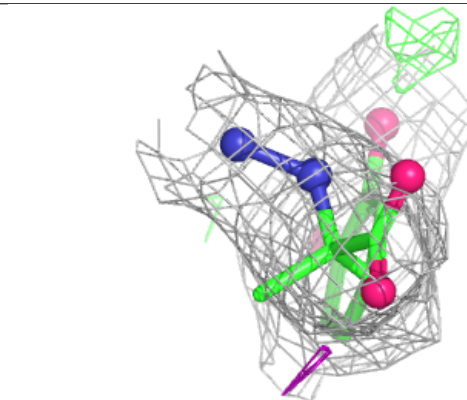
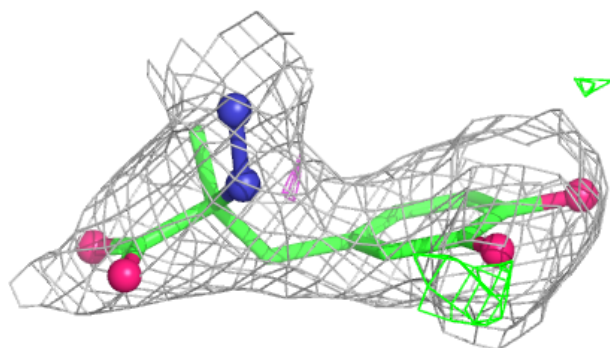
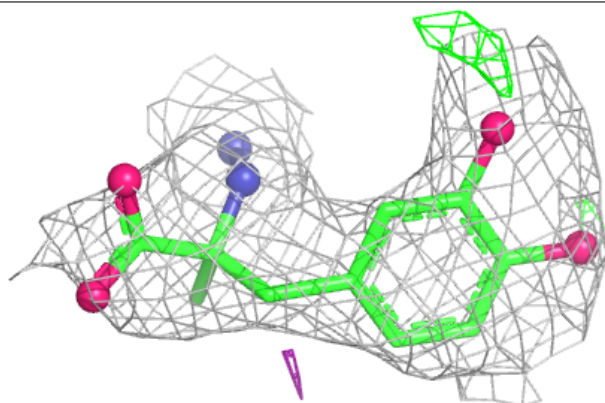


Electron density around 142 D 602:

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

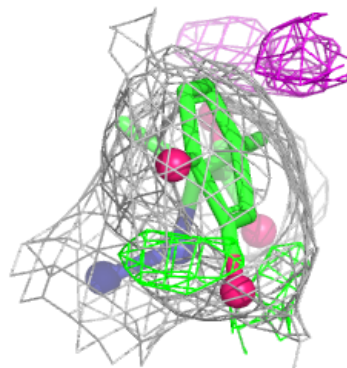
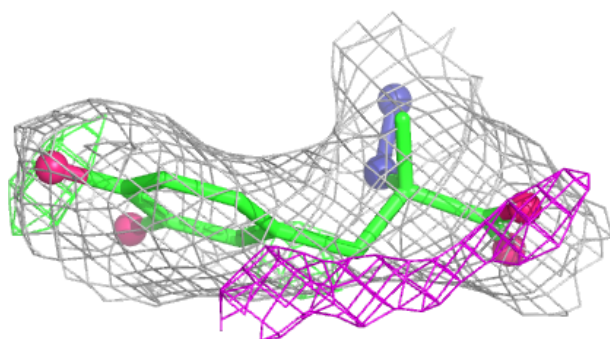
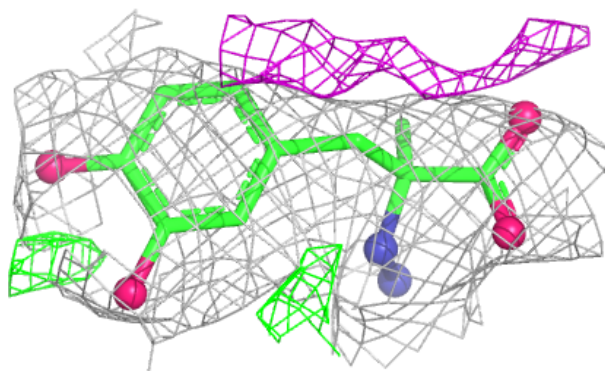
**Electron density around 142 A 602:**

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

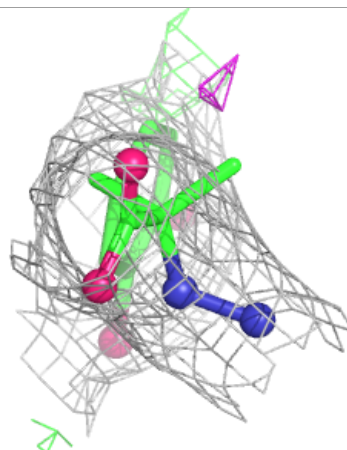
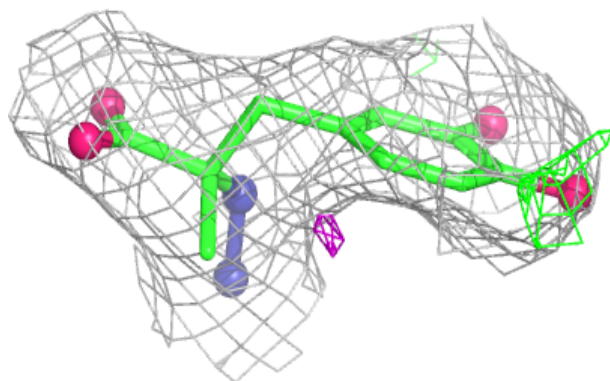
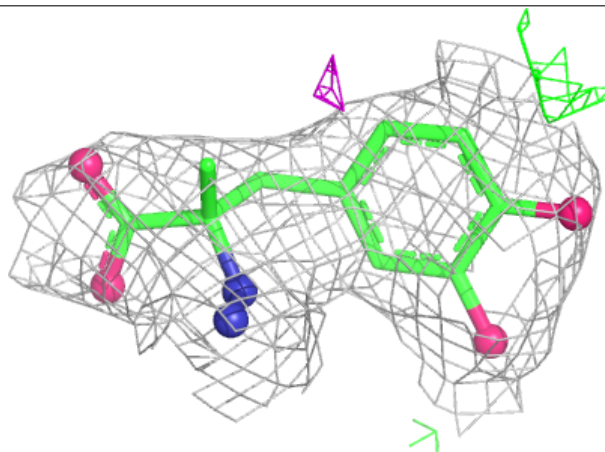


Electron density around 142 B 602:

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

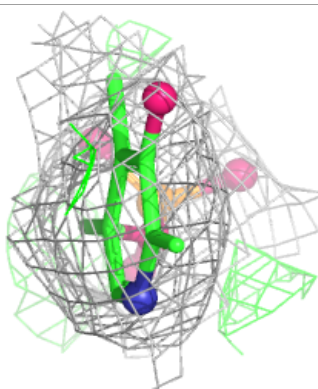
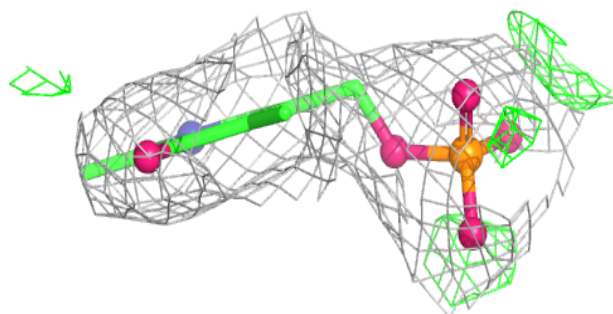
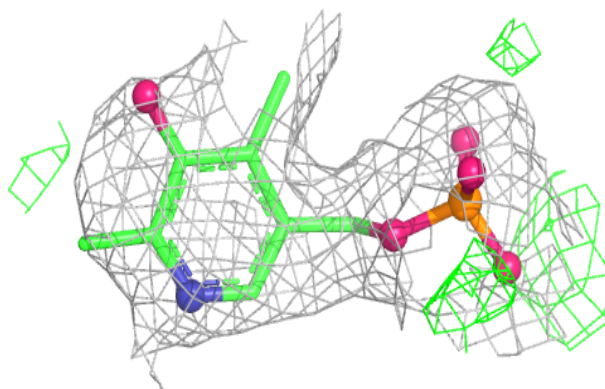
**Electron density around 142 C 602:**

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

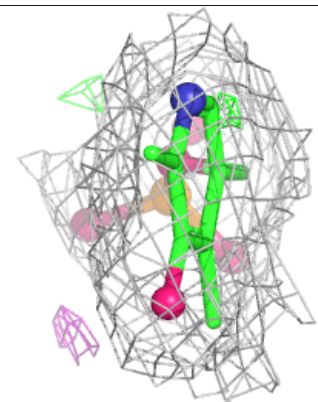
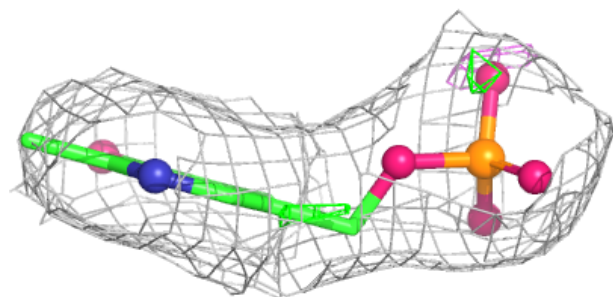
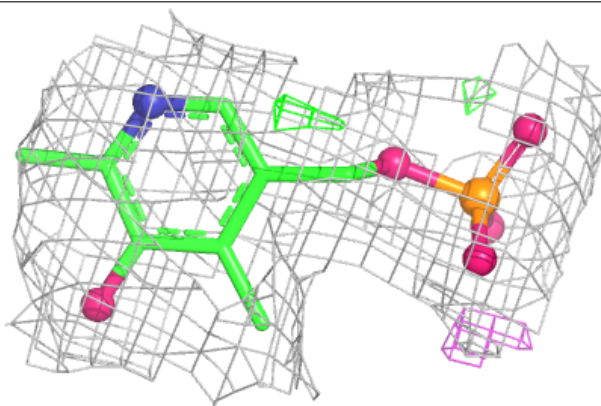


Electron density around PLP C 601:

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

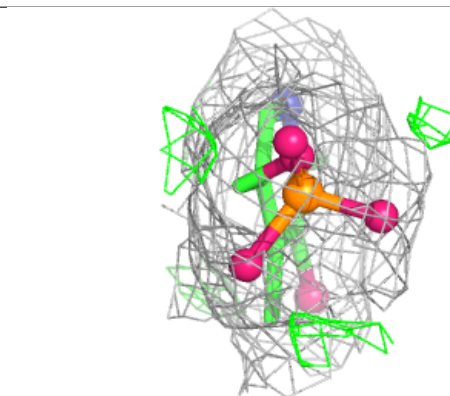
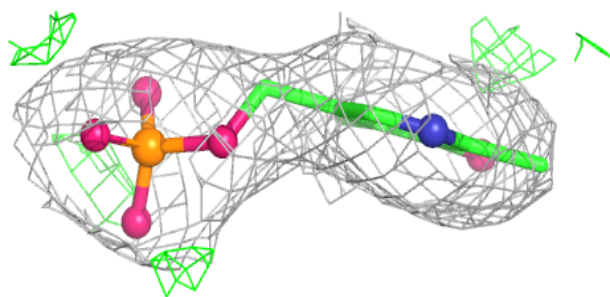
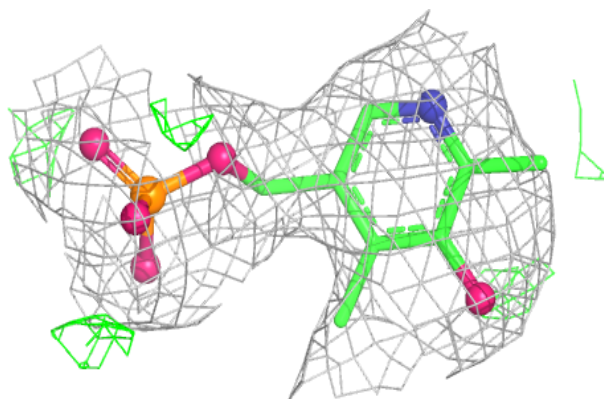
**Electron density around PLP D 601:**

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

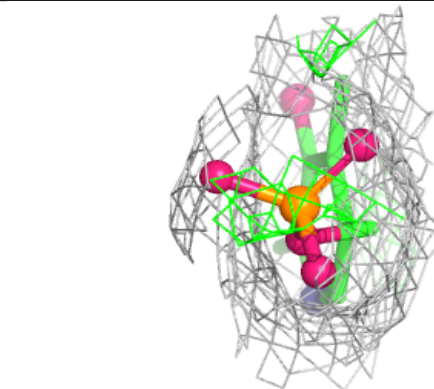
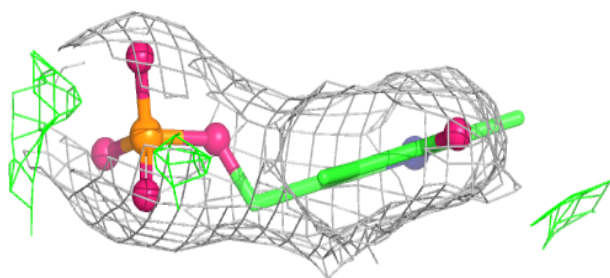
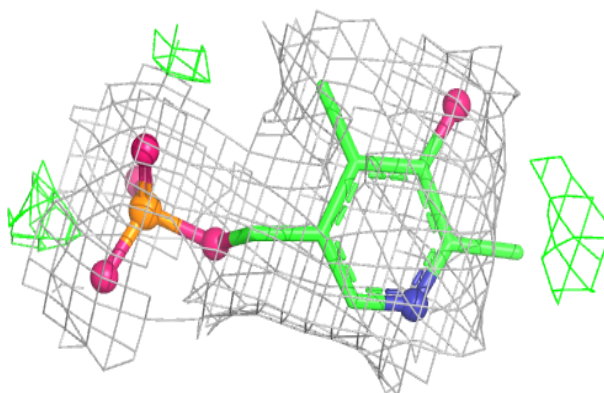


Electron density around PLP A 601:

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

**Electron density around PLP B 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.