



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:20 pm BST

PDB ID : 6RL5
Title : The first crystal structure of the DABA aminotransferase EctB in the ec-toine biosynthesis pathway of the model organism *Chromohalobacter salexi-gens* DSM 3034
Authors : Hillier, H.T.; Altermark, B.; Leiros, I.
Deposited on : 2019-05-01
Resolution : 2.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

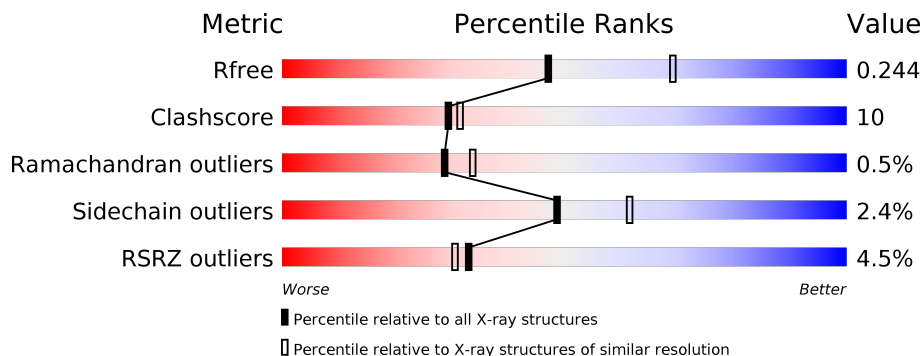
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



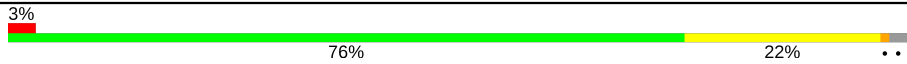

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	429	 2% 78% 19% ..
1	B	429	 3% 75% 21% ..
1	C	429	 5% 77% 21% .
1	D	429	 5% 74% 22% ..
1	E	429	 4% 72% 24% ..
1	F	429	 7% 79% 17% ..

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Mol	Chain	Length	Quality of chain
1	G	429	 <p>3% 76% 22% ..</p>
1	H	429	 <p>4% 74% 21% ..</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26163 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 Diaminobutyrate--2-oxoglutarate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3204	2021	565	603	15	0	0	0
1	B	419	3220	2030	568	607	15	0	0	0
1	C	419	3220	2030	568	607	15	0	0	0
1	D	417	3209	2024	566	604	15	0	0	0
1	E	418	3213	2026	567	605	15	0	0	0
1	F	417	3215	2027	569	604	15	0	1	0
1	G	422	3243	2043	573	612	15	0	0	0
1	H	417	3209	2024	566	604	15	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

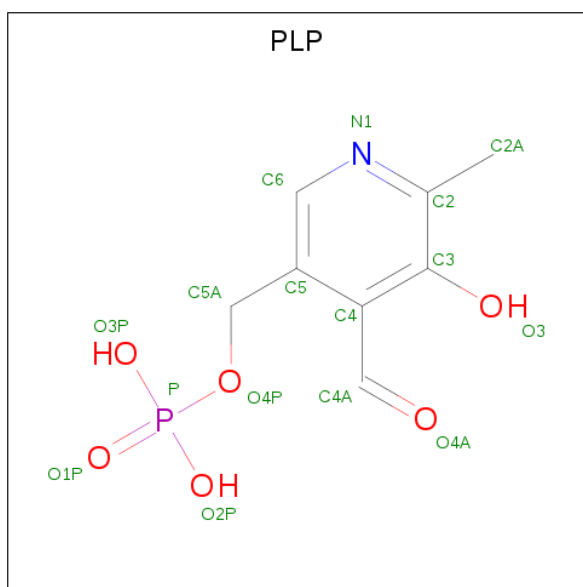
Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP Q9ZEU7
A	425	HIS	-	expression tag	UNP Q9ZEU7
A	426	HIS	-	expression tag	UNP Q9ZEU7
A	427	HIS	-	expression tag	UNP Q9ZEU7
A	428	HIS	-	expression tag	UNP Q9ZEU7
A	429	HIS	-	expression tag	UNP Q9ZEU7
B	424	HIS	-	expression tag	UNP Q9ZEU7
B	425	HIS	-	expression tag	UNP Q9ZEU7
B	426	HIS	-	expression tag	UNP Q9ZEU7
B	427	HIS	-	expression tag	UNP Q9ZEU7
B	428	HIS	-	expression tag	UNP Q9ZEU7
B	429	HIS	-	expression tag	UNP Q9ZEU7
C	424	HIS	-	expression tag	UNP Q9ZEU7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	expression tag	UNP Q9ZEU7
C	426	HIS	-	expression tag	UNP Q9ZEU7
C	427	HIS	-	expression tag	UNP Q9ZEU7
C	428	HIS	-	expression tag	UNP Q9ZEU7
C	429	HIS	-	expression tag	UNP Q9ZEU7
D	424	HIS	-	expression tag	UNP Q9ZEU7
D	425	HIS	-	expression tag	UNP Q9ZEU7
D	426	HIS	-	expression tag	UNP Q9ZEU7
D	427	HIS	-	expression tag	UNP Q9ZEU7
D	428	HIS	-	expression tag	UNP Q9ZEU7
D	429	HIS	-	expression tag	UNP Q9ZEU7
E	424	HIS	-	expression tag	UNP Q9ZEU7
E	425	HIS	-	expression tag	UNP Q9ZEU7
E	426	HIS	-	expression tag	UNP Q9ZEU7
E	427	HIS	-	expression tag	UNP Q9ZEU7
E	428	HIS	-	expression tag	UNP Q9ZEU7
E	429	HIS	-	expression tag	UNP Q9ZEU7
F	424	HIS	-	expression tag	UNP Q9ZEU7
F	425	HIS	-	expression tag	UNP Q9ZEU7
F	426	HIS	-	expression tag	UNP Q9ZEU7
F	427	HIS	-	expression tag	UNP Q9ZEU7
F	428	HIS	-	expression tag	UNP Q9ZEU7
F	429	HIS	-	expression tag	UNP Q9ZEU7
G	424	HIS	-	expression tag	UNP Q9ZEU7
G	425	HIS	-	expression tag	UNP Q9ZEU7
G	426	HIS	-	expression tag	UNP Q9ZEU7
G	427	HIS	-	expression tag	UNP Q9ZEU7
G	428	HIS	-	expression tag	UNP Q9ZEU7
G	429	HIS	-	expression tag	UNP Q9ZEU7
H	424	HIS	-	expression tag	UNP Q9ZEU7
H	425	HIS	-	expression tag	UNP Q9ZEU7
H	426	HIS	-	expression tag	UNP Q9ZEU7
H	427	HIS	-	expression tag	UNP Q9ZEU7
H	428	HIS	-	expression tag	UNP Q9ZEU7
H	429	HIS	-	expression tag	UNP Q9ZEU7

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by author).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total 37	O 37	0	0
3	B	46	Total 46	O 46	0	0
3	C	28	Total 28	O 28	0	0
3	D	25	Total 25	O 25	0	0

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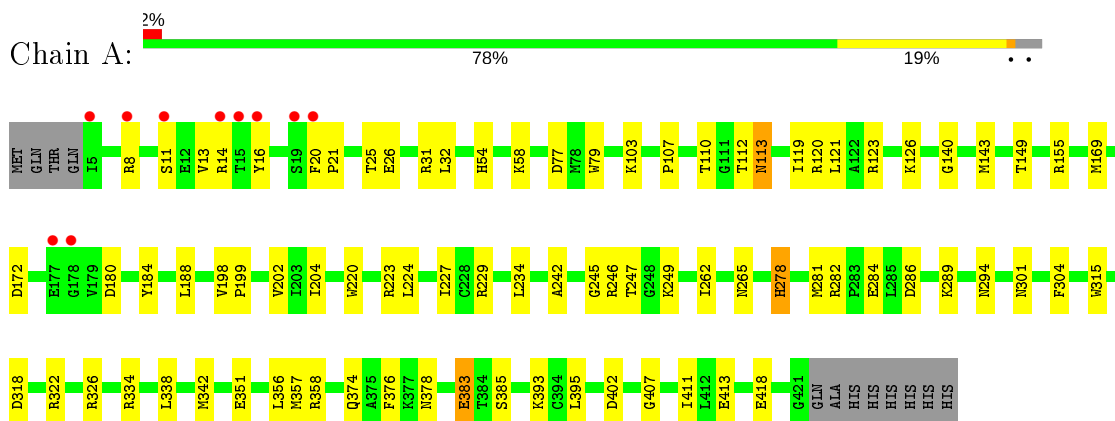
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	50	Total 50	O 50	0	0
3	F	43	Total 43	O 43	0	0
3	G	50	Total 50	O 50	0	0
3	H	31	Total 31	O 31	0	0

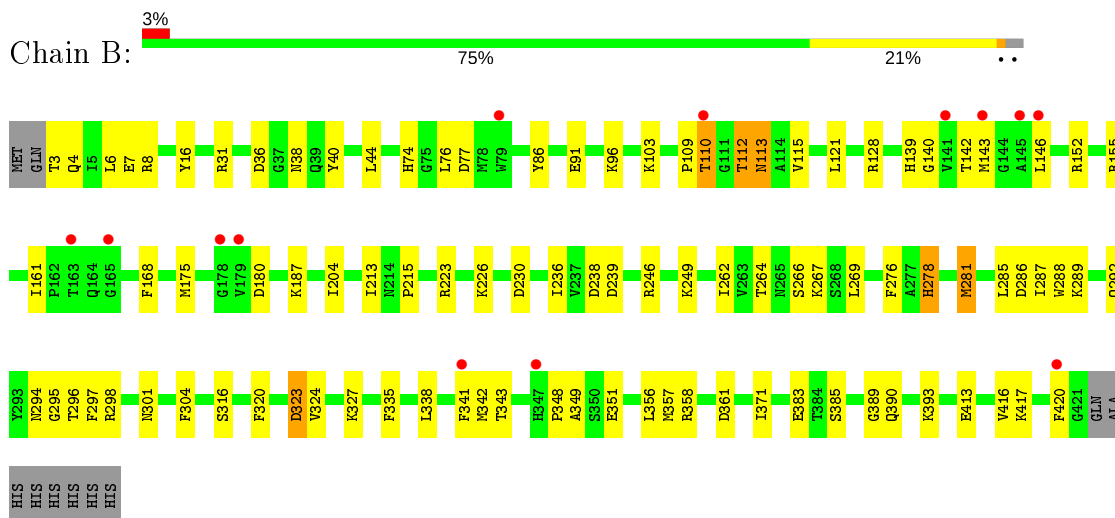
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

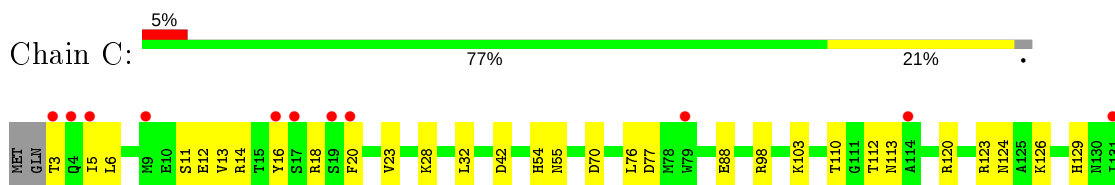
- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

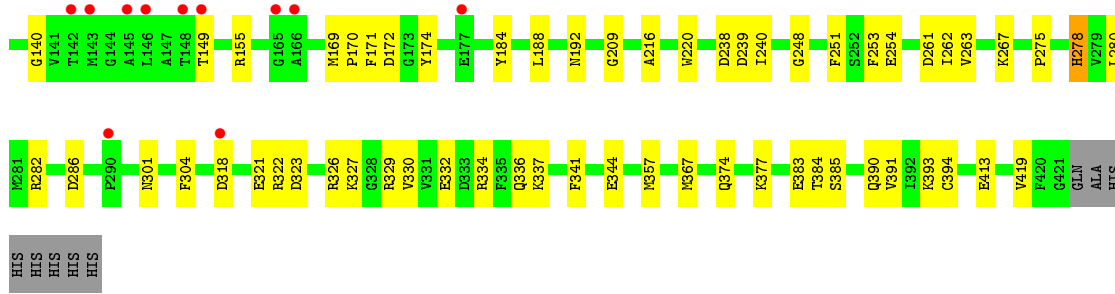


- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

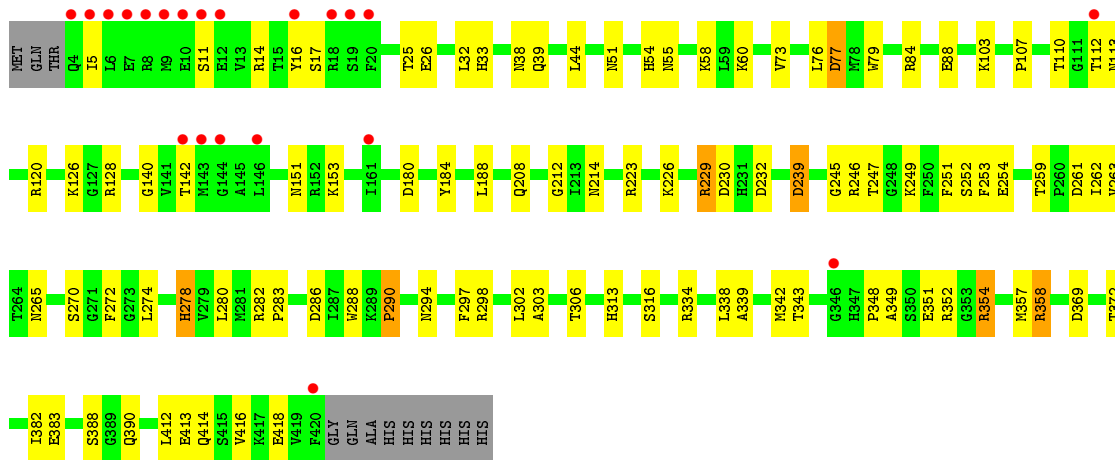
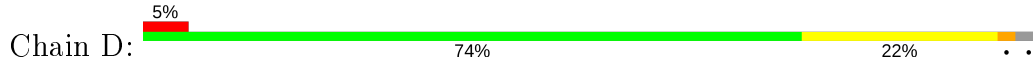


- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

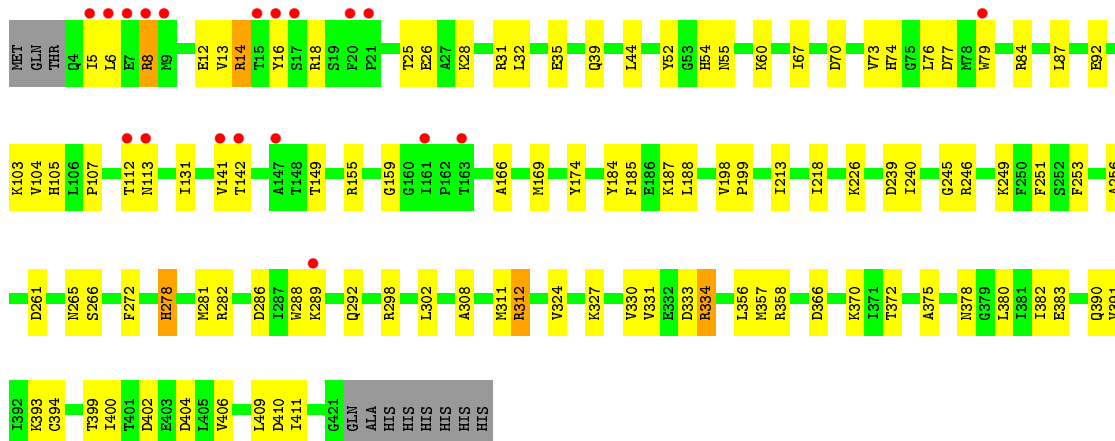




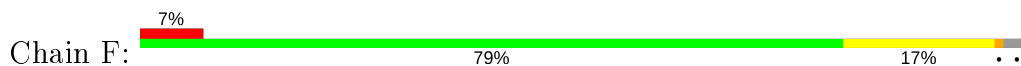
- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

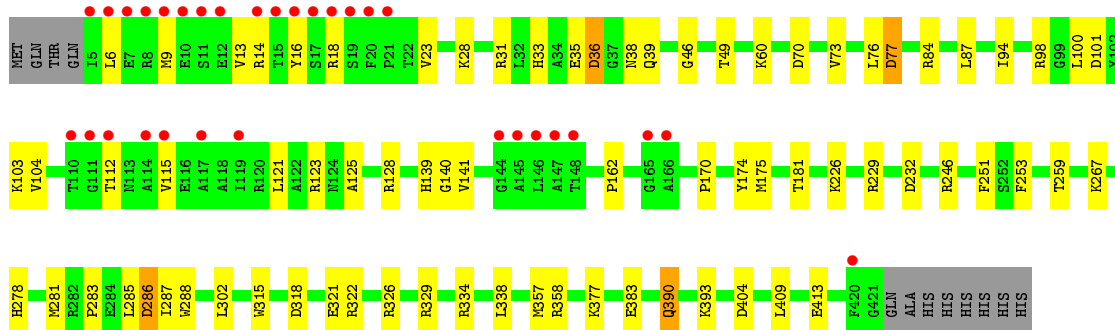


- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

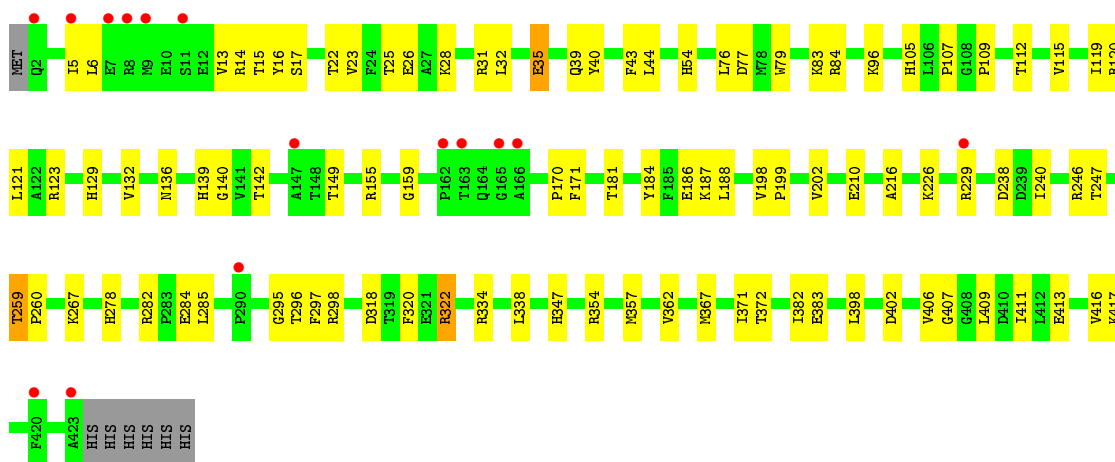
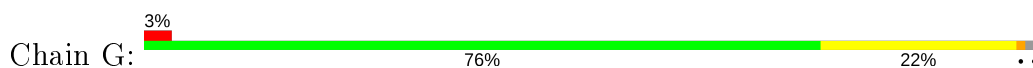


- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

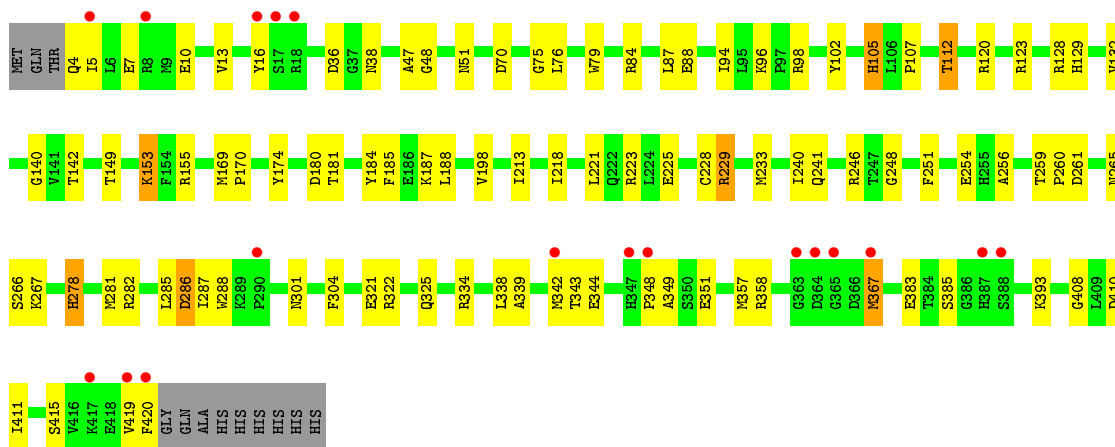
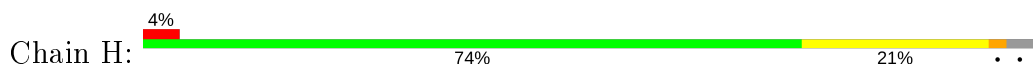




• Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase



• Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.06Å 124.78Å 145.42Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	49.07 – 2.45 49.07 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.07-2.45) 98.8 (49.07-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.185 , 0.243 0.185 , 0.244	Depositor DCC
R_{free} test set	2704 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26163	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: 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	0.49	1/3272 (0.0%)	0.63	1/4419 (0.0%)
1	B	0.47	0/3288	0.60	1/4441 (0.0%)
1	C	0.44	0/3288	0.59	0/4441
1	D	0.43	0/3277	0.60	1/4426 (0.0%)
1	E	0.48	0/3281	0.60	0/4431
1	F	0.49	0/3283	0.62	0/4433
1	G	0.47	0/3311	0.63	0/4472
1	H	0.47	0/3277	0.59	0/4426
All	All	0.47	1/26277 (0.0%)	0.61	3/35489 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	GLU	CG-CD	5.86	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	168	PHE	C-N-CA	5.23	134.78	121.70
1	A	318	ASP	CB-CG-OD1	5.07	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3204	0	3140	62	0
1	B	3220	0	3156	68	0
1	C	3220	0	3155	68	0
1	D	3209	0	3145	73	0
1	E	3213	0	3151	75	0
1	F	3215	0	3153	67	0
1	G	3243	0	3176	68	0
1	H	3209	0	3148	74	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
2	E	15	0	7	0	0
2	F	15	0	7	0	0
2	G	15	0	7	0	0
2	H	15	0	7	0	0
3	A	37	0	0	4	0
3	B	46	0	0	1	0
3	C	28	0	0	4	0
3	D	25	0	0	1	0
3	E	50	0	0	7	0
3	F	43	0	0	2	0
3	G	50	0	0	5	0
3	H	31	0	0	2	0
All	All	26163	0	25280	486	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 10.

All (486) 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:G:417:LYS:NZ	3:G:601:HOH:O	1.81	1.07
1:A:180:ASP:OD2	1:A:223:ARG:NH1	2.03	0.92
1:B:110:THR:OG1	1:B:113:ASN:HB2	1.72	0.90
1:A:112:THR:HG22	1:A:140:GLY:HA3	1.57	0.86
1:B:112:THR:HG23	1:B:140:GLY:HA3	1.57	0.86
1:H:112:THR:HG23	1:H:140:GLY:HA3	1.60	0.82
1:G:372:THR:HG22	1:G:382:ILE:HG23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:TRP:HZ3	1:E:84:ARG:HB2	1.45	0.81
1:D:14:ARG:HD2	1:D:17:SER:OG	1.79	0.81
1:E:265:ASN:HD22	1:E:278:HIS:HE1	1.27	0.79
1:G:282:ARG:NH2	3:G:602:HOH:O	2.14	0.79
1:C:238:ASP:OD1	1:C:240:ILE:HG12	1.84	0.77
1:E:113:ASN:ND2	3:E:601:HOH:O	2.16	0.77
1:C:16:TYR:HB2	1:D:77:ASP:HB2	1.65	0.77
1:G:347:HIS:CE1	1:G:367:MET:HG3	2.22	0.75
1:C:323:ASP:OD1	1:C:326:ARG:NH1	2.20	0.74
1:A:16:TYR:HD2	1:B:77:ASP:HB3	1.52	0.74
1:D:51:ASN:OD1	1:D:246:ARG:NH2	2.17	0.73
1:D:294:ASN:HB2	1:D:298:ARG:HH21	1.54	0.73
1:E:77:ASP:HB2	1:F:16:TYR:HB2	1.71	0.73
1:F:31:ARG:NH2	1:F:404:ASP:OD1	2.21	0.73
1:C:374:GLN:NE2	3:C:602:HOH:O	2.23	0.72
1:E:73:VAL:HG13	1:E:302:LEU:HG	1.70	0.72
1:D:112:THR:HG21	1:D:142:THR:H	1.55	0.71
1:G:334:ARG:HG3	1:G:409:LEU:HD13	1.73	0.70
1:C:124:ASN:OD1	3:C:601:HOH:O	2.09	0.70
1:D:343:THR:HG22	1:D:348:PRO:HA	1.74	0.70
1:H:112:THR:HG21	1:H:142:THR:H	1.55	0.70
1:E:324:VAL:HG13	1:E:356:LEU:HD12	1.72	0.69
1:F:112:THR:HG22	1:F:140:GLY:HA3	1.74	0.69
1:H:265:ASN:HB2	1:H:278:HIS:CE1	2.28	0.68
1:B:385:SER:HB3	1:B:393:LYS:HE2	1.76	0.68
1:E:105:HIS:CE1	1:F:13:VAL:HG11	2.29	0.67
1:G:371:ILE:HD13	1:G:416:VAL:HG22	1.75	0.67
1:G:16:TYR:HE1	1:G:383:GLU:HG3	1.60	0.67
1:H:169:MET:HE3	1:H:170:PRO:HD2	1.76	0.66
1:E:31:ARG:NH1	1:E:39:GLN:OE1	2.29	0.66
1:A:374:GLN:NE2	1:A:418:GLU:OE2	2.27	0.66
1:H:180:ASP:OD2	1:H:223:ARG:NH1	2.27	0.66
1:C:332:GLU:O	1:C:336:GLN:HG3	1.95	0.65
1:C:3:THR:HG23	1:D:84:ARG:HE	1.61	0.65
1:E:12:GLU:OE1	1:E:18:ARG:NH2	2.21	0.65
1:E:87:LEU:HB2	1:F:6:LEU:HD21	1.77	0.65
1:D:180:ASP:OD2	1:D:223:ARG:NH1	2.29	0.65
1:B:323:ASP:OD2	1:B:327:LYS:HE3	1.94	0.65
1:C:322:ARG:O	1:C:322:ARG:HD3	1.97	0.65
1:G:25:THR:HG23	1:G:26:GLU:H	1.62	0.65
1:B:351:GLU:OE2	1:B:358:ARG:NH1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HB	1:B:288:TRP:HB3	1.80	0.64
1:G:282:ARG:NH2	1:G:284:GLU:OE1	2.31	0.64
1:B:383:GLU:HG2	1:B:393:LYS:HE3	1.80	0.64
1:G:347:HIS:HE1	1:G:367:MET:HG3	1.62	0.64
1:H:51:ASN:OD1	1:H:246:ARG:NH2	2.28	0.63
1:A:126:LYS:HE3	1:A:234:LEU:HD21	1.79	0.63
1:C:3:THR:HG21	1:C:23:VAL:HG21	1.81	0.63
1:C:334:ARG:HD2	1:C:413:GLU:OE1	1.99	0.63
1:A:282:ARG:NH2	1:A:284:GLU:OE2	2.31	0.63
1:C:263:VAL:HB	1:C:280:LEU:HB2	1.80	0.63
1:E:6:LEU:HD23	1:F:87:LEU:HD12	1.81	0.62
1:B:77:ASP:HB2	1:B:298:ARG:HH21	1.64	0.62
1:D:261:ASP:HA	1:D:282:ARG:HG3	1.80	0.62
1:E:265:ASN:HD22	1:E:278:HIS:CE1	2.15	0.62
1:E:308:ALA:HA	1:E:311:MET:HE3	1.81	0.62
1:B:295:GLY:O	1:B:298:ARG:NH1	2.32	0.62
1:C:70:ASP:OD1	1:D:60:LYS:NZ	2.32	0.62
1:D:226:LYS:HD2	1:D:229:ARG:HH21	1.63	0.62
1:E:218:ILE:HD12	1:E:256:ALA:HB2	1.82	0.62
1:B:390:GLN:OE1	1:B:390:GLN:N	2.32	0.62
1:E:149:THR:O	1:E:155:ARG:HD2	1.99	0.62
1:C:112:THR:HG22	1:C:140:GLY:HA3	1.81	0.61
1:D:151:ASN:OD1	1:D:153:LYS:HG2	2.00	0.61
1:G:43:PHE:HB3	1:G:382:ILE:HD12	1.83	0.61
1:B:343:THR:HG22	1:B:348:PRO:HA	1.83	0.61
1:D:265:ASN:HB2	1:D:278:HIS:CD2	2.36	0.61
1:E:13:VAL:HG23	1:F:288:TRP:HB3	1.82	0.61
1:H:367:MET:HE3	1:H:420:PHE:CZ	2.35	0.61
1:B:281:MET:HE1	1:B:286:ASP:HA	1.83	0.60
1:E:5:ILE:HD12	1:E:8:ARG:NH1	2.16	0.60
1:G:44:LEU:HD13	1:G:383:GLU:HB2	1.84	0.60
1:C:32:LEU:HD13	1:C:42:ASP:HB2	1.82	0.60
1:D:212:GLY:O	1:D:352:ARG:NH2	2.29	0.60
1:F:174:TYR:CE2	1:G:187:LYS:HD3	2.36	0.60
1:G:112:THR:HG23	1:G:140:GLY:HA3	1.84	0.60
1:H:334:ARG:NH2	1:H:410:ASP:OD1	2.34	0.60
1:D:126:LYS:NZ	1:D:232:ASP:OD1	2.35	0.59
1:A:284:GLU:N	1:A:284:GLU:OE1	2.33	0.59
1:B:341:PHE:CZ	1:B:417:LYS:HG2	2.37	0.59
1:F:103:LYS:NZ	1:F:286:ASP:OD2	2.23	0.59
1:B:112:THR:HG21	1:B:142:THR:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:PHE:HB3	1:E:253:PHE:CE2	2.37	0.59
1:E:31:ARG:NH2	1:E:404:ASP:OD1	2.35	0.59
1:C:98:ARG:HD3	1:C:254:GLU:OE2	2.03	0.59
1:D:351:GLU:OE2	1:D:358:ARG:NH1	2.36	0.58
1:C:374:GLN:HG3	1:C:419:VAL:HG23	1.86	0.58
1:E:246:ARG:HG3	1:E:357:MET:HB2	1.85	0.58
1:E:378:ASN:O	1:E:411:ILE:HD13	2.03	0.58
1:G:149:THR:O	1:G:155:ARG:HD2	2.04	0.58
1:D:343:THR:HG22	1:D:349:ALA:H	1.68	0.58
1:E:240:ILE:HG23	1:E:266:SER:HB3	1.85	0.58
1:G:96:LYS:NZ	3:G:605:HOH:O	2.37	0.58
1:H:343:THR:HG23	1:H:348:PRO:HA	1.84	0.58
1:A:119:ILE:HD12	1:A:123:ARG:NH1	2.19	0.58
1:G:112:THR:CG2	1:G:140:GLY:HA3	2.34	0.58
1:D:25:THR:HG23	1:D:26:GLU:H	1.69	0.58
1:H:351:GLU:OE1	1:H:358:ARG:NH1	2.36	0.57
1:G:171:PHE:CZ	1:G:216:ALA:HB2	2.39	0.57
1:E:74:HIS:CE1	1:F:49:THR:HG21	2.40	0.57
1:G:338:LEU:HD21	1:G:413:GLU:HA	1.87	0.57
1:H:281:MET:HE1	1:H:286:ASP:HA	1.87	0.57
1:E:112:THR:HG21	1:E:142:THR:H	1.70	0.56
1:B:294:ASN:HB2	1:B:298:ARG:NH1	2.20	0.56
1:D:110:THR:OG1	1:D:113:ASN:HB2	2.06	0.56
1:H:246:ARG:HG3	1:H:357:MET:HB2	1.87	0.56
1:B:342:MET:HG2	1:B:420:PHE:CZ	2.40	0.56
1:C:385:SER:HB3	1:C:393:LYS:HD3	1.87	0.56
1:A:351:GLU:OE2	1:A:358:ARG:NH1	2.38	0.56
1:F:16:TYR:CE1	1:F:383:GLU:HG3	2.40	0.56
1:E:390:GLN:HG2	1:E:391:VAL:HG23	1.88	0.55
1:F:94:ILE:O	1:F:98:ARG:HD2	2.06	0.55
1:G:31:ARG:NH1	1:G:39:GLN:HE21	2.04	0.55
1:F:170:PRO:HG2	1:F:181:THR:HB	1.89	0.55
1:G:25:THR:HG23	1:G:26:GLU:HG2	1.88	0.55
1:F:112:THR:CG2	1:F:140:GLY:HA3	2.36	0.55
1:E:76:LEU:HD13	1:F:16:TYR:CE2	2.41	0.55
1:H:285:LEU:O	1:H:287:ILE:N	2.40	0.55
1:E:334:ARG:NH2	1:E:410:ASP:OD1	2.30	0.54
1:D:55:ASN:HA	1:D:272:PHE:CE1	2.43	0.54
1:E:213:ILE:HD11	1:E:393:LYS:HG2	1.88	0.54
1:G:210:GLU:HG2	3:G:616:HOH:O	2.07	0.54
1:A:229:ARG:NH1	3:A:602:HOH:O	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:THR:HG23	1:D:140:GLY:HA3	1.89	0.54
1:A:301:ASN:HA	1:A:304:PHE:CD2	2.43	0.54
1:D:251:PHE:HB2	1:D:254:GLU:HG3	1.89	0.54
1:C:169:MET:HE3	1:C:170:PRO:HD2	1.89	0.54
1:H:385:SER:HB3	1:H:393:LYS:HD3	1.89	0.54
1:A:112:THR:HG22	1:A:140:GLY:CA	2.34	0.54
1:A:13:VAL:HB	1:B:288:TRP:CB	2.37	0.54
1:B:295:GLY:O	1:B:298:ARG:HG3	2.07	0.54
1:C:322:ARG:HH12	1:C:329:ARG:NH1	2.06	0.54
1:G:14:ARG:HH11	1:G:17:SER:HB2	1.72	0.54
1:C:88:GLU:HG3	1:D:5:ILE:HD12	1.90	0.54
1:B:324:VAL:HG13	1:B:356:LEU:HD12	1.90	0.53
1:F:14:ARG:O	1:F:18:ARG:NE	2.42	0.53
1:E:32:LEU:HD21	1:E:54:HIS:NE2	2.23	0.53
1:H:261:ASP:HA	1:H:282:ARG:HG3	1.91	0.53
1:A:246:ARG:HG3	1:A:357:MET:HB2	1.89	0.53
1:B:236:ILE:HG12	1:B:262:ILE:HB	1.90	0.53
1:E:103:LYS:NZ	1:E:286:ASP:OD2	2.24	0.53
1:A:334:ARG:NH2	1:A:413:GLU:OE2	2.41	0.53
1:G:402:ASP:O	1:G:406:VAL:HG23	2.09	0.53
1:A:32:LEU:HD11	1:A:54:HIS:NE2	2.24	0.53
1:A:16:TYR:CD2	1:B:77:ASP:HB3	2.39	0.53
1:C:5:ILE:HD13	1:D:88:GLU:HG2	1.91	0.52
1:D:16:TYR:HE1	1:D:383:GLU:HG3	1.73	0.52
1:E:169:MET:HE1	1:E:185:PHE:HA	1.92	0.52
1:G:296:THR:OG1	1:H:267:LYS:NZ	2.43	0.52
1:D:229:ARG:CZ	1:D:229:ARG:HB2	2.39	0.52
1:C:28:LYS:HE2	1:C:55:ASN:O	2.10	0.52
1:E:92:GLU:HB3	3:E:647:HOH:O	2.08	0.52
1:F:318:ASP:O	1:F:322:ARG:HG3	2.09	0.52
1:E:105:HIS:HE1	1:F:13:VAL:HG11	1.74	0.52
1:F:358:ARG:NH2	3:F:604:HOH:O	2.42	0.52
1:E:289:LYS:O	1:E:292:GLN:HG3	2.09	0.52
1:H:47:ALA:O	1:H:267:LYS:HE3	2.10	0.52
1:A:338:LEU:O	1:A:342:MET:HG3	2.10	0.52
1:B:187:LYS:HE2	1:C:174:TYR:CE1	2.45	0.52
1:C:390:GLN:HG2	1:C:391:VAL:HG23	1.91	0.52
1:D:316:SER:OG	3:D:601:HOH:O	2.18	0.52
1:E:366:ASP:O	1:E:370:LYS:HG3	2.10	0.52
1:G:83:LYS:NZ	1:H:10:GLU:OE1	2.38	0.52
1:D:33:HIS:CD2	1:D:39:GLN:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LYS:HE3	1:E:55:ASN:O	2.10	0.52
1:G:13:VAL:HB	1:H:288:TRP:HB3	1.91	0.51
1:C:172:ASP:HB2	1:C:220:TRP:CE2	2.44	0.51
1:B:115:VAL:HG21	1:B:139:HIS:HB3	1.91	0.51
1:G:25:THR:HG23	1:G:26:GLU:N	2.26	0.51
1:E:184:TYR:CZ	1:E:188:LEU:HD11	2.46	0.51
1:G:247:THR:HB	1:G:354:ARG:HG2	1.92	0.51
1:H:170:PRO:HG2	1:H:181:THR:HB	1.92	0.51
1:A:77:ASP:HB2	1:B:16:TYR:HB2	1.92	0.51
1:D:103:LYS:HE2	1:D:283:PRO:HB3	1.93	0.51
1:G:120:ARG:NH1	3:G:604:HOH:O	2.37	0.51
1:C:248:GLY:O	1:C:321:GLU:HG3	2.11	0.50
1:D:120:ARG:HG2	1:D:288:TRP:HH2	1.75	0.50
1:A:284:GLU:H	1:A:284:GLU:CD	2.10	0.50
1:C:149:THR:O	1:C:155:ARG:HD2	2.10	0.50
1:H:339:ALA:O	1:H:343:THR:OG1	2.22	0.50
1:C:301:ASN:HA	1:C:304:PHE:CD2	2.46	0.50
1:C:275:PRO:HG3	1:D:297:PHE:HB3	1.93	0.50
1:D:44:LEU:HD13	1:D:383:GLU:HB2	1.93	0.50
1:B:187:LYS:HE2	1:C:174:TYR:CZ	2.46	0.50
1:H:112:THR:HG23	1:H:140:GLY:CA	2.35	0.50
1:F:128:ARG:NH2	1:F:232:ASP:O	2.45	0.50
1:C:327:LYS:HA	1:C:330:VAL:HG12	1.93	0.50
1:D:11:SER:O	1:D:14:ARG:HG2	2.11	0.50
1:H:153:LYS:NZ	3:H:601:HOH:O	2.45	0.50
1:C:240:ILE:O	1:C:267:LYS:HB2	2.11	0.50
1:F:390:GLN:O	1:F:390:GLN:HG2	2.11	0.50
1:H:301:ASN:HA	1:H:304:PHE:CD2	2.47	0.50
1:F:162:PRO:HB3	1:G:129:HIS:CE1	2.47	0.50
1:A:223:ARG:HD3	3:A:620:HOH:O	2.11	0.50
1:A:25:THR:HG22	1:A:26:GLU:N	2.27	0.50
1:B:246:ARG:HG3	1:B:357:MET:HB2	1.93	0.50
1:F:23:VAL:HB	1:F:35:GLU:HG3	1.94	0.50
1:H:408:GLY:HA2	1:H:411:ILE:HD12	1.94	0.50
1:A:294:ASN:ND2	3:A:603:HOH:O	2.32	0.49
1:E:35:GLU:OE2	1:F:84:ARG:NH2	2.44	0.49
1:H:218:ILE:HG23	1:H:256:ALA:HA	1.93	0.49
1:A:20:PHE:CZ	1:A:383:GLU:HG2	2.46	0.49
1:D:303:ALA:HA	1:D:306:THR:HG22	1.94	0.49
1:C:377:LYS:HB3	1:G:96:LYS:HD3	1.94	0.49
1:B:213:ILE:O	1:B:215:PRO:HD3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:LYS:HE2	1:E:400:ILE:O	2.12	0.49
3:E:623:HOH:O	1:H:198:VAL:HG22	2.12	0.49
1:H:342:MET:HE2	1:H:349:ALA:HB2	1.94	0.49
1:B:349:ALA:HA	1:B:361:ASP:O	2.13	0.49
1:B:3:THR:O	1:B:7:GLU:HG3	2.11	0.49
1:E:16:TYR:CE2	1:F:76:LEU:HD13	2.47	0.49
1:A:385:SER:HB3	1:A:393:LYS:HD3	1.95	0.49
1:C:322:ARG:HH12	1:C:329:ARG:NH2	2.11	0.49
1:C:322:ARG:HH22	1:C:329:ARG:HH12	1.61	0.49
1:F:87:LEU:HD21	1:F:104:VAL:HG21	1.94	0.49
1:B:86:TYR:OH	1:B:278:HIS:HD2	1.96	0.49
1:D:128:ARG:NH2	1:D:232:ASP:O	2.45	0.48
1:G:28:LYS:HD3	1:H:70:ASP:OD2	2.13	0.48
1:A:184:TYR:CZ	1:A:188:LEU:HD11	2.48	0.48
1:B:36:ASP:OD2	1:B:38:ASN:ND2	2.45	0.48
1:C:172:ASP:HB2	1:C:220:TRP:CD2	2.49	0.48
1:E:281:MET:CE	1:E:286:ASP:HA	2.43	0.48
1:G:170:PRO:HG2	1:G:181:THR:HB	1.95	0.48
1:D:334:ARG:NH2	1:D:413:GLU:OE1	2.43	0.48
1:G:367:MET:O	1:G:371:ILE:HG13	2.13	0.48
1:C:261:ASP:HA	1:C:282:ARG:HD2	1.95	0.48
1:E:55:ASN:HA	1:E:272:PHE:CE1	2.48	0.48
1:E:67:ILE:O	1:F:60:LYS:HE3	2.14	0.48
1:F:125:ALA:HA	1:F:287:ILE:HD13	1.94	0.48
1:A:21:PRO:HD2	1:A:376:PHE:CE2	2.49	0.48
1:E:265:ASN:HB2	1:E:278:HIS:CE1	2.48	0.48
1:H:16:TYR:HE1	1:H:383:GLU:OE2	1.96	0.48
1:G:6:LEU:HD11	1:H:84:ARG:HB2	1.95	0.48
1:E:87:LEU:HB2	1:F:6:LEU:CD2	2.44	0.48
1:F:101:ASP:O	1:F:283:PRO:HD3	2.13	0.48
1:H:321:GLU:O	1:H:325:GLN:HG3	2.14	0.48
1:A:149:THR:O	1:A:155:ARG:HD2	2.14	0.48
1:B:180:ASP:OD2	1:B:223:ARG:NH1	2.42	0.48
1:A:245:GLY:HA2	1:A:249:LYS:O	2.14	0.47
1:G:184:TYR:CZ	1:G:188:LEU:HD11	2.49	0.47
1:G:318:ASP:O	1:G:322:ARG:HD3	2.14	0.47
1:H:225:GLU:O	1:H:229:ARG:HD3	2.13	0.47
1:H:265:ASN:HD22	1:H:278:HIS:HE1	1.61	0.47
1:A:204:ILE:HD11	1:A:220:TRP:HZ3	1.79	0.47
1:A:265:ASN:HB2	1:A:278:HIS:CD2	2.50	0.47
1:B:146:LEU:HD21	1:B:155:ARG:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:ARG:HG2	1:H:129:HIS:HA	1.96	0.47
1:D:32:LEU:HD21	1:D:54:HIS:CE1	2.50	0.47
1:D:58:LYS:HG3	1:D:313:HIS:CE1	2.49	0.47
1:A:407:GLY:O	1:A:411:ILE:HG13	2.15	0.47
1:B:74:HIS:NE2	1:B:296:THR:O	2.44	0.47
1:C:12:GLU:O	1:C:18:ARG:NH2	2.47	0.47
1:G:105:HIS:CD2	1:H:13:VAL:HG11	2.50	0.47
1:H:48:GLY:HA3	1:H:241:GLN:NE2	2.28	0.47
1:B:4:GLN:O	1:B:8:ARG:HD3	2.15	0.47
1:D:226:LYS:HE3	1:D:230:ASP:OD2	2.14	0.47
1:G:31:ARG:HA	1:G:40:TYR:O	2.15	0.47
1:A:20:PHE:HZ	1:A:383:GLU:HG2	1.80	0.47
1:A:172:ASP:HB2	1:A:220:TRP:CD2	2.50	0.47
1:C:18:ARG:HE	1:D:290:PRO:HB3	1.80	0.47
1:D:73:VAL:HG13	1:D:302:LEU:HG	1.96	0.47
1:D:343:THR:CG2	1:D:349:ALA:H	2.28	0.47
1:C:322:ARG:HH12	1:C:329:ARG:CZ	2.28	0.47
1:G:246:ARG:HG3	1:G:357:MET:HB2	1.96	0.46
1:E:13:VAL:HG23	1:F:288:TRP:CB	2.46	0.46
1:H:102:TYR:OH	1:H:260:PRO:O	2.22	0.46
1:A:326:ARG:NH2	1:A:402:ASP:OD1	2.48	0.46
1:D:339:ALA:O	1:D:343:THR:HG23	2.15	0.46
1:E:372:THR:HG23	1:E:382:ILE:O	2.16	0.46
1:G:132:VAL:HB	1:G:202:VAL:HG12	1.97	0.46
1:D:412:LEU:O	1:D:416:VAL:HG23	2.15	0.46
1:H:94:ILE:O	1:H:98:ARG:HD2	2.16	0.46
1:A:110:THR:OG1	1:A:113:ASN:HB2	2.16	0.46
1:A:16:TYR:CE2	1:B:76:LEU:HG	2.50	0.46
1:D:126:LYS:HD3	1:D:126:LYS:HA	1.63	0.46
1:D:414:GLN:NE2	1:D:418:GLU:OE2	2.46	0.46
1:E:331:VAL:HG12	1:E:358:ARG:HD3	1.98	0.46
1:E:60:LYS:NZ	1:F:70:ASP:OD1	2.44	0.46
1:H:240:ILE:HG22	1:H:267:LYS:HD2	1.98	0.46
1:A:79:TRP:CD1	1:B:6:LEU:HD22	2.51	0.46
1:E:77:ASP:OD2	1:E:298:ARG:NH1	2.49	0.46
1:F:285:LEU:O	1:F:287:ILE:N	2.44	0.46
1:F:315:TRP:CZ3	1:F:321:GLU:HG3	2.50	0.46
1:D:76:LEU:CD1	1:D:298:ARG:HH12	2.29	0.45
1:E:131:ILE:O	1:E:166:ALA:HA	2.15	0.45
1:G:238:ASP:OD1	1:G:240:ILE:HD12	2.16	0.45
1:C:32:LEU:CD1	1:C:42:ASP:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:MET:HE2	1:E:286:ASP:HA	1.98	0.45
1:B:285:LEU:O	1:B:287:ILE:N	2.49	0.45
1:H:96:LYS:HA	1:H:96:LYS:HD3	1.68	0.45
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.73	0.45
1:D:372:THR:HG23	1:D:382:ILE:O	2.16	0.45
1:H:415:SER:O	1:H:419:VAL:HG23	2.15	0.45
1:C:367:MET:HA	1:C:367:MET:HE3	1.98	0.45
1:C:112:THR:HG22	1:C:140:GLY:CA	2.45	0.45
1:F:46:GLY:HA3	1:F:49:THR:HG22	1.99	0.45
1:B:342:MET:HE3	1:B:342:MET:HB2	1.55	0.45
1:C:322:ARG:HH12	1:C:329:ARG:HH12	1.63	0.45
1:H:301:ASN:HA	1:H:304:PHE:HD2	1.81	0.45
1:B:121:LEU:HD22	1:B:281:MET:HE3	1.99	0.45
1:C:16:TYR:HD1	1:C:20:PHE:HE2	1.65	0.45
1:F:259:THR:OG1	1:F:259:THR:O	2.32	0.45
1:E:198:VAL:HA	1:E:199:PRO:HD3	1.83	0.44
1:F:73:VAL:HG22	1:F:302:LEU:HD21	1.99	0.44
1:D:14:ARG:HG3	1:D:14:ARG:HH11	1.83	0.44
1:A:172:ASP:HB2	1:A:220:TRP:CE2	2.53	0.44
1:B:44:LEU:HD13	1:B:383:GLU:HB3	1.99	0.44
1:B:152:ARG:HG3	1:C:192:ASN:O	2.17	0.44
1:F:33:HIS:NE2	1:F:39:GLN:OE1	2.49	0.44
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.83	0.44
1:B:371:ILE:HD13	1:B:416:VAL:HG22	1.98	0.44
1:E:375:ALA:HB1	1:E:380:LEU:HB3	1.99	0.44
1:F:31:ARG:HH11	1:F:39:GLN:NE2	2.16	0.44
1:C:110:THR:OG1	1:C:113:ASN:HB2	2.17	0.44
1:D:388:SER:HB3	1:D:390:GLN:HG3	1.98	0.44
1:F:141:VAL:HG22	3:F:641:HOH:O	2.18	0.44
1:G:109:PRO:HD3	1:G:297:PHE:O	2.17	0.44
1:G:23:VAL:HG22	1:G:35:GLU:HB2	1.99	0.44
1:G:22:THR:O	1:H:79:TRP:HB2	2.17	0.44
1:B:316:SER:N	3:B:607:HOH:O	2.49	0.44
1:A:315:TRP:O	3:A:601:HOH:O	2.21	0.44
1:B:128:ARG:HD2	3:C:628:HOH:O	2.18	0.44
1:C:120:ARG:NH1	3:C:607:HOH:O	2.50	0.44
1:D:245:GLY:HA2	1:D:249:LYS:O	2.18	0.44
1:F:36:ASP:OD1	1:F:38:ASN:ND2	2.51	0.44
1:G:295:GLY:O	1:G:298:ARG:HG3	2.18	0.44
1:G:119:ILE:O	1:G:123:ARG:HG3	2.17	0.44
1:E:226:LYS:NZ	3:E:611:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:VAL:HG12	1:E:410:ASP:OD2	2.18	0.44
1:H:251:PHE:HB2	1:H:254:GLU:HG3	1.99	0.44
1:D:226:LYS:HD2	1:D:229:ARG:NH2	2.32	0.43
1:E:14:ARG:HA	1:F:77:ASP:OD2	2.18	0.43
1:D:270:SER:HB2	1:D:274:LEU:HB2	2.00	0.43
1:A:8:ARG:HH12	1:B:103:LYS:NZ	2.16	0.43
1:B:238:ASP:HA	1:B:264:THR:OG1	2.18	0.43
1:D:334:ARG:HD2	1:D:334:ARG:HA	1.77	0.43
1:E:409:LEU:HD23	1:E:409:LEU:HA	1.85	0.43
1:A:79:TRP:CD1	1:B:6:LEU:HB3	2.53	0.43
1:D:184:TYR:CZ	1:D:188:LEU:HD11	2.53	0.43
1:G:112:THR:HG21	1:G:142:THR:H	1.83	0.43
1:H:149:THR:O	1:H:155:ARG:HD2	2.18	0.43
1:H:184:TYR:CZ	1:H:188:LEU:HD11	2.54	0.43
1:B:289:LYS:O	1:B:292:GLN:HG3	2.18	0.43
1:D:262:ILE:HA	1:D:280:LEU:O	2.18	0.43
1:H:240:ILE:HG12	1:H:266:SER:HB3	2.01	0.43
1:C:209:GLY:HA2	1:C:357:MET:HE1	2.00	0.43
1:E:245:GLY:HA2	1:E:249:LYS:O	2.18	0.43
1:E:13:VAL:CG2	1:F:288:TRP:HB3	2.48	0.43
1:E:52:TYR:HA	1:E:399:THR:HG23	2.01	0.43
1:E:76:LEU:HD13	1:F:16:TYR:CD2	2.53	0.43
1:F:285:LEU:O	1:F:287:ILE:HG22	2.19	0.43
1:F:338:LEU:HD21	1:F:413:GLU:HA	2.00	0.43
1:G:6:LEU:HD22	1:H:79:TRP:CD1	2.54	0.43
1:C:184:TYR:CZ	1:C:188:LEU:HD11	2.53	0.43
1:C:6:LEU:HD22	1:D:79:TRP:CD1	2.53	0.43
1:E:25:THR:OG1	1:E:26:GLU:N	2.50	0.43
1:E:393:LYS:NZ	3:E:612:HOH:O	2.51	0.43
1:G:115:VAL:HG21	1:G:139:HIS:HB3	2.01	0.43
1:G:76:LEU:HD22	1:H:16:TYR:CE2	2.54	0.43
1:H:213:ILE:HD11	1:H:393:LYS:HG2	2.00	0.43
1:A:242:ALA:O	1:A:247:THR:HG23	2.19	0.43
1:B:269:LEU:HD23	1:B:276:PHE:CD2	2.54	0.43
1:D:16:TYR:CE1	1:D:383:GLU:HG3	2.54	0.43
1:D:76:LEU:HA	1:D:76:LEU:HD12	1.82	0.43
1:E:261:ASP:OD1	1:E:282:ARG:HD2	2.19	0.43
1:F:18:ARG:HG2	1:F:18:ARG:HH11	1.84	0.43
1:F:33:HIS:N	1:F:33:HIS:CD2	2.87	0.43
1:E:104:VAL:N	1:F:9:MET:O	2.44	0.43
1:A:11:SER:O	1:A:14:ARG:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:SER:HB3	1:C:13:VAL:HG12	2.01	0.42
1:D:246:ARG:HG3	1:D:357:MET:HB2	2.01	0.42
1:F:18:ARG:NH1	1:F:18:ARG:HG2	2.34	0.42
1:F:251:PHE:HB3	1:F:253:PHE:CE2	2.54	0.42
1:F:87:LEU:HA	1:F:87:LEU:HD23	1.82	0.42
1:G:407:GLY:O	1:G:411:ILE:HG13	2.19	0.42
1:A:121:LEU:HD21	1:A:281:MET:HE3	2.01	0.42
1:A:169:MET:HE1	1:A:188:LEU:HD12	2.01	0.42
1:B:109:PRO:HG3	1:B:297:PHE:HB2	2.01	0.42
1:C:16:TYR:HB2	1:D:77:ASP:CB	2.43	0.42
1:E:174:TYR:O	1:H:187:LYS:NZ	2.44	0.42
1:H:265:ASN:ND2	1:H:278:HIS:HE1	2.16	0.42
1:A:322:ARG:HH11	1:A:322:ARG:HG2	1.84	0.42
1:B:226:LYS:HE2	1:B:230:ASP:OD2	2.18	0.42
1:B:77:ASP:HB2	1:B:298:ARG:NH2	2.31	0.42
1:B:91:GLU:OE2	1:F:377:LYS:NZ	2.32	0.42
1:C:262:ILE:HA	1:C:280:LEU:O	2.19	0.42
1:G:15:THR:HG23	1:G:16:TYR:N	2.33	0.42
1:H:48:GLY:HA3	1:H:241:GLN:HE22	1.82	0.42
1:H:75:GLY:O	1:H:76:LEU:HB2	2.20	0.42
1:H:338:LEU:HD23	1:H:338:LEU:HA	1.74	0.42
1:H:385:SER:HA	3:H:631:HOH:O	2.19	0.42
1:A:8:ARG:HH12	1:B:103:LYS:HZ2	1.66	0.42
1:C:251:PHE:HB3	1:C:253:PHE:CE2	2.54	0.42
1:C:103:LYS:NZ	1:C:286:ASP:OD2	2.42	0.42
1:D:76:LEU:HD12	1:D:298:ARG:HH12	1.83	0.42
1:E:141:VAL:HG22	3:E:644:HOH:O	2.19	0.42
1:H:5:ILE:HG22	1:H:5:ILE:O	2.19	0.42
1:F:383:GLU:O	1:F:393:LYS:HG2	2.20	0.42
1:H:221:LEU:HD23	1:H:221:LEU:HA	1.85	0.42
1:C:322:ARG:HH22	1:C:329:ARG:NH1	2.18	0.42
1:C:322:ARG:NH1	1:C:329:ARG:HH22	2.18	0.42
1:D:263:VAL:HB	1:D:280:LEU:HB2	2.01	0.42
1:D:229:ARG:NH1	1:D:229:ARG:HB2	2.35	0.42
1:F:326:ARG:HA	1:F:329:ARG:NH1	2.35	0.42
1:F:6:LEU:O	1:F:6:LEU:HD23	2.20	0.42
1:G:13:VAL:HG11	1:H:105:HIS:CE1	2.55	0.42
1:H:322:ARG:HA	1:H:325:GLN:HG3	2.02	0.42
1:A:16:TYR:HE2	1:B:298:ARG:HH22	1.68	0.42
1:C:6:LEU:HD11	1:D:84:ARG:HB2	2.02	0.42
1:F:334:ARG:HG3	1:F:409:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HG13	1:A:120:ARG:N	2.35	0.41
1:A:103:LYS:O	1:A:281:MET:HG2	2.20	0.41
1:C:76:LEU:HD13	1:D:16:TYR:CE2	2.55	0.41
1:F:226:LYS:HE3	1:F:229:ARG:HH22	1.84	0.41
1:G:32:LEU:HD11	1:G:54:HIS:NE2	2.35	0.41
1:G:5:ILE:HD13	1:H:88:GLU:HG3	2.01	0.41
1:A:223:ARG:O	1:A:227:ILE:HG13	2.19	0.41
1:B:335:PHE:HB3	1:B:351:GLU:HG3	2.02	0.41
1:A:79:TRP:HB3	1:B:6:LEU:HD13	2.01	0.41
1:C:123:ARG:HG2	1:C:129:HIS:HA	2.02	0.41
1:F:246:ARG:HG3	1:F:357:MET:HB2	2.02	0.41
1:G:186:GLU:OE1	1:G:226:LYS:NZ	2.53	0.41
1:B:143:MET:HE2	1:B:161:ILE:HB	2.02	0.41
1:D:251:PHE:HB3	1:D:253:PHE:CE2	2.55	0.41
1:F:31:ARG:HH11	1:F:39:GLN:HE21	1.68	0.41
1:H:228:CYS:HB3	1:H:233:MET:O	2.19	0.41
1:B:175:MET:HE3	1:B:175:MET:HB2	1.90	0.41
1:A:281:MET:HE3	1:A:281:MET:HB2	1.70	0.41
1:B:389:GLY:N	1:B:390:GLN:OE1	2.53	0.41
1:G:79:TRP:CZ2	1:H:7:GLU:HB3	2.55	0.41
1:C:384:THR:O	1:C:393:LYS:HE2	2.20	0.41
1:D:338:LEU:O	1:D:342:MET:HG3	2.21	0.41
1:E:70:ASP:OD2	1:F:28:LYS:HE2	2.21	0.41
1:F:121:LEU:HD13	1:F:288:TRP:NE1	2.36	0.41
1:F:76:LEU:HB3	1:F:77:ASP:H	1.56	0.41
1:G:13:VAL:HB	1:H:288:TRP:CB	2.51	0.41
1:C:32:LEU:HD11	1:C:54:HIS:NE2	2.36	0.41
1:E:187:LYS:HD3	1:H:174:TYR:CE2	2.56	0.41
1:A:202:VAL:HG11	1:A:224:LEU:HD11	2.02	0.41
1:B:301:ASN:HA	1:B:304:PHE:CD2	2.56	0.41
1:G:121:LEU:HD11	1:G:285:LEU:O	2.20	0.41
1:G:282:ARG:O	1:G:285:LEU:HB2	2.21	0.41
1:C:126:LYS:HA	1:C:126:LYS:HD3	1.92	0.41
1:D:247:THR:HB	1:D:354:ARG:HG2	2.03	0.41
1:G:259:THR:HA	1:G:260:PRO:HD3	1.90	0.41
1:H:385:SER:CB	1:H:393:LYS:HD3	2.51	0.41
1:B:86:TYR:OH	1:B:278:HIS:CD2	2.73	0.41
1:B:285:LEU:HA	1:B:285:LEU:HD23	1.95	0.41
1:C:171:PHE:CZ	1:C:216:ALA:HB2	2.56	0.41
1:C:341:PHE:O	1:C:344:GLU:HG2	2.21	0.41
1:D:58:LYS:HG3	1:D:313:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:GLY:HA3	1:F:123:ARG:HB3	2.03	0.41
1:F:100:LEU:HA	1:F:100:LEU:HD23	1.95	0.41
1:E:13:VAL:HG23	1:F:288:TRP:CG	2.56	0.41
1:H:132:VAL:HG21	1:H:185:PHE:CE1	2.55	0.41
1:H:36:ASP:OD1	1:H:38:ASN:HB2	2.21	0.41
1:A:121:LEU:HD23	1:A:262:ILE:HD13	2.02	0.41
1:D:208:GLN:HB2	1:D:214:ASN:HB2	2.01	0.41
1:A:198:VAL:HA	1:A:199:PRO:HD3	1.84	0.40
1:D:239:ASP:OD1	1:D:252:SER:OG	2.38	0.40
1:E:312:ARG:NH2	3:E:613:HOH:O	2.54	0.40
1:G:14:ARG:HD2	1:G:17:SER:HB2	2.04	0.40
1:H:248:GLY:O	1:H:321:GLU:HG3	2.20	0.40
1:B:338:LEU:HD21	1:B:413:GLU:HA	2.03	0.40
1:H:120:ARG:HB2	1:H:120:ARG:HE	1.73	0.40
1:G:159:GLY:HA3	1:H:123:ARG:HB3	2.02	0.40
1:A:281:MET:HE1	1:A:286:ASP:HA	2.02	0.40
1:B:31:ARG:HA	1:B:40:TYR:O	2.22	0.40
1:C:278:HIS:C	1:C:278:HIS:CD2	2.94	0.40
1:E:44:LEU:HD13	1:E:383:GLU:HB3	2.02	0.40
1:G:198:VAL:HA	1:G:199:PRO:HD3	1.95	0.40
1:H:87:LEU:HD23	1:H:87:LEU:HA	1.82	0.40
1:A:378:ASN:HB3	1:A:411:ILE:HG23	2.02	0.40
1:B:320:PHE:O	1:B:324:VAL:HG23	2.21	0.40
1:C:88:GLU:CG	1:D:5:ILE:HD12	2.52	0.40
1:F:115:VAL:HG21	1:F:139:HIS:HB3	2.02	0.40
1:G:320:PHE:HZ	1:G:398:LEU:HB2	1.87	0.40
1:E:327:LYS:HA	1:E:330:VAL:HG12	2.03	0.40
1:G:84:ARG:HH11	1:H:4:GLN:N	2.19	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	415/429 (97%)	388 (94%)	26 (6%)	1 (0%)	47	57
1	B	417/429 (97%)	390 (94%)	25 (6%)	2 (0%)	29	34
1	C	417/429 (97%)	390 (94%)	27 (6%)	0	100	100
1	D	415/429 (97%)	382 (92%)	30 (7%)	3 (1%)	22	25
1	E	416/429 (97%)	389 (94%)	26 (6%)	1 (0%)	47	57
1	F	416/429 (97%)	398 (96%)	16 (4%)	2 (0%)	29	34
1	G	420/429 (98%)	397 (94%)	19 (4%)	4 (1%)	15	16
1	H	415/429 (97%)	388 (94%)	25 (6%)	2 (0%)	29	34
All	All	3331/3432 (97%)	3122 (94%)	194 (6%)	15 (0%)	29	34

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	LYS
1	G	35	GLU
1	H	286	ASP
1	B	266	SER
1	D	286	ASP
1	F	286	ASP
1	D	107	PRO
1	D	290	PRO
1	G	267	LYS
1	G	362	VAL
1	F	267	LYS
1	H	107	PRO
1	A	107	PRO
1	E	107	PRO
1	G	107	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/343 (97%)	326 (98%)	6 (2%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	334/343 (97%)	324 (97%)	10 (3%)	41	52
1	C	334/343 (97%)	326 (98%)	8 (2%)	49	61
1	D	333/343 (97%)	325 (98%)	8 (2%)	49	61
1	E	333/343 (97%)	323 (97%)	10 (3%)	41	52
1	F	333/343 (97%)	327 (98%)	6 (2%)	59	71
1	G	336/343 (98%)	330 (98%)	6 (2%)	59	71
1	H	333/343 (97%)	324 (97%)	9 (3%)	44	57
All	All	2668/2744 (97%)	2605 (98%)	63 (2%)	49	61

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	58	LYS
1	A	113	ASN
1	A	143	MET
1	A	278	HIS
1	A	289	LYS
1	B	96	LYS
1	B	110	THR
1	B	112	THR
1	B	113	ASN
1	B	204	ILE
1	B	239	ASP
1	B	249	LYS
1	B	278	HIS
1	B	281	MET
1	B	323	ASP
1	C	14	ARG
1	C	77	ASP
1	C	239	ASP
1	C	278	HIS
1	C	318	ASP
1	C	337	LYS
1	C	383	GLU
1	C	394	CYS
1	D	38	ASN
1	D	77	ASP
1	D	239	ASP
1	D	259	THR

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Mol	Chain	Res	Type
1	D	278	HIS
1	D	354	ARG
1	D	358	ARG
1	D	369	ASP
1	E	8	ARG
1	E	14	ARG
1	E	239	ASP
1	E	278	HIS
1	E	288	TRP
1	E	312	ARG
1	E	333	ASP
1	E	334	ARG
1	E	394	CYS
1	E	402	ASP
1	F	36	ASP
1	F	77	ASP
1	F	175	MET
1	F	278	HIS
1	F	281	MET
1	F	390	GLN
1	G	77	ASP
1	G	136	ASN
1	G	229	ARG
1	G	259	THR
1	G	278	HIS
1	G	322	ARG
1	H	105	HIS
1	H	112	THR
1	H	128	ARG
1	H	153	LYS
1	H	229	ARG
1	H	259	THR
1	H	278	HIS
1	H	344	GLU
1	H	367	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	GLN
1	B	278	HIS
1	B	387	HIS

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Mol	Chain	Res	Type
1	D	192	ASN
1	E	105	HIS
1	E	265	ASN
1	E	278	HIS
1	H	265	ASN
1	H	278	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	A	501	1	15,15,16	1.23	2 (13%)	20,22,23	1.84	6 (30%)
2	PLP	H	501	-	15,15,16	1.25	2 (13%)	20,22,23	1.41	4 (20%)
2	PLP	C	501	1	15,15,16	1.19	2 (13%)	20,22,23	1.50	5 (25%)
2	PLP	B	501	1	15,15,16	1.30	2 (13%)	20,22,23	2.05	5 (25%)
2	PLP	E	501	-	15,15,16	1.42	2 (13%)	20,22,23	1.21	2 (10%)
2	PLP	D	501	1	15,15,16	1.09	2 (13%)	20,22,23	1.39	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	G	501	1	15,15,16	1.39	3 (20%)	20,22,23	1.66	5 (25%)
2	PLP	F	501	1	15,15,16	2.23	3 (20%)	20,22,23	2.58	7 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	501	1	-	3/6/6/8	0/1/1/1
2	PLP	H	501	-	-	5/6/6/8	0/1/1/1
2	PLP	C	501	1	-	3/6/6/8	0/1/1/1
2	PLP	B	501	1	-	3/6/6/8	0/1/1/1
2	PLP	E	501	-	-	0/6/6/8	0/1/1/1
2	PLP	D	501	1	-	2/6/6/8	0/1/1/1
2	PLP	G	501	1	-	3/6/6/8	0/1/1/1
2	PLP	F	501	1	-	3/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	PLP	C3-C2	-5.24	1.35	1.40
2	F	501	PLP	C6-N1	4.29	1.43	1.34
2	F	501	PLP	C2-N1	3.92	1.41	1.33
2	B	501	PLP	C2-N1	3.45	1.40	1.33
2	G	501	PLP	C2-N1	3.36	1.40	1.33
2	A	501	PLP	C2-N1	3.31	1.40	1.33
2	E	501	PLP	C2-N1	3.27	1.40	1.33
2	C	501	PLP	C2-N1	3.11	1.39	1.33
2	H	501	PLP	C2-N1	3.02	1.39	1.33
2	G	501	PLP	C6-N1	2.64	1.40	1.34
2	B	501	PLP	C6-N1	2.54	1.39	1.34
2	E	501	PLP	C6-N1	2.54	1.39	1.34
2	D	501	PLP	C2-N1	2.51	1.38	1.33
2	A	501	PLP	C6-N1	2.50	1.39	1.34
2	H	501	PLP	C6-N1	2.26	1.39	1.34
2	C	501	PLP	C6-N1	2.21	1.39	1.34
2	D	501	PLP	C6-N1	2.09	1.38	1.34
2	G	501	PLP	C5-C4	2.07	1.42	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	PLP	C3-C4-C5	6.08	125.31	118.74
2	B	501	PLP	C4A-C4-C5	-5.60	115.17	120.94
2	F	501	PLP	C4A-C4-C5	-5.40	115.37	120.94
2	F	501	PLP	C5-C6-N1	-5.15	115.25	123.82
2	G	501	PLP	C4A-C4-C3	-4.32	113.17	120.50
2	B	501	PLP	O4P-C5A-C5	4.07	117.11	109.35
2	B	501	PLP	C6-C5-C4	3.87	121.21	118.16
2	H	501	PLP	C6-C5-C4	3.58	120.98	118.16
2	C	501	PLP	C2A-C2-C3	-3.45	116.62	120.89
2	A	501	PLP	C6-C5-C4	3.41	120.85	118.16
2	D	501	PLP	C4A-C4-C3	-3.32	114.88	120.50
2	E	501	PLP	C6-C5-C4	3.28	120.74	118.16
2	A	501	PLP	C4A-C4-C5	-3.13	117.71	120.94
2	A	501	PLP	O4P-C5A-C5	3.10	115.27	109.35
2	C	501	PLP	C6-C5-C4	3.09	120.59	118.16
2	F	501	PLP	C4-C3-C2	-2.99	115.66	120.07
2	A	501	PLP	C5-C6-N1	-2.98	118.85	123.82
2	G	501	PLP	C6-C5-C4	2.96	120.49	118.16
2	H	501	PLP	O3-C3-C2	2.69	123.36	117.49
2	F	501	PLP	O3-C3-C2	2.69	123.36	117.49
2	E	501	PLP	C4A-C4-C5	-2.56	118.30	120.94
2	C	501	PLP	C5-C6-N1	-2.52	119.62	123.82
2	H	501	PLP	C5-C6-N1	-2.51	119.64	123.82
2	G	501	PLP	O4P-C5A-C5	2.51	114.13	109.35
2	G	501	PLP	C5-C6-N1	-2.49	119.67	123.82
2	B	501	PLP	C5-C6-N1	-2.44	119.76	123.82
2	A	501	PLP	C2A-C2-C3	-2.42	117.90	120.89
2	B	501	PLP	C4A-C4-C3	-2.38	116.46	120.50
2	H	501	PLP	C4A-C4-C3	-2.35	116.52	120.50
2	C	501	PLP	C2A-C2-N1	2.35	122.25	117.67
2	F	501	PLP	O3P-P-O4P	2.32	112.91	106.73
2	A	501	PLP	C2A-C2-N1	2.28	122.11	117.67
2	F	501	PLP	C6-C5-C4	2.21	119.90	118.16
2	G	501	PLP	C4A-C4-C5	-2.11	118.77	120.94
2	C	501	PLP	O4P-C5A-C5	2.10	113.36	109.35
2	D	501	PLP	C5-C6-N1	-2.09	120.33	123.82
2	D	501	PLP	O4P-C5A-C5	2.01	113.18	109.35
2	D	501	PLP	C6-C5-C4	2.00	119.73	118.16

There are no chirality outliers.

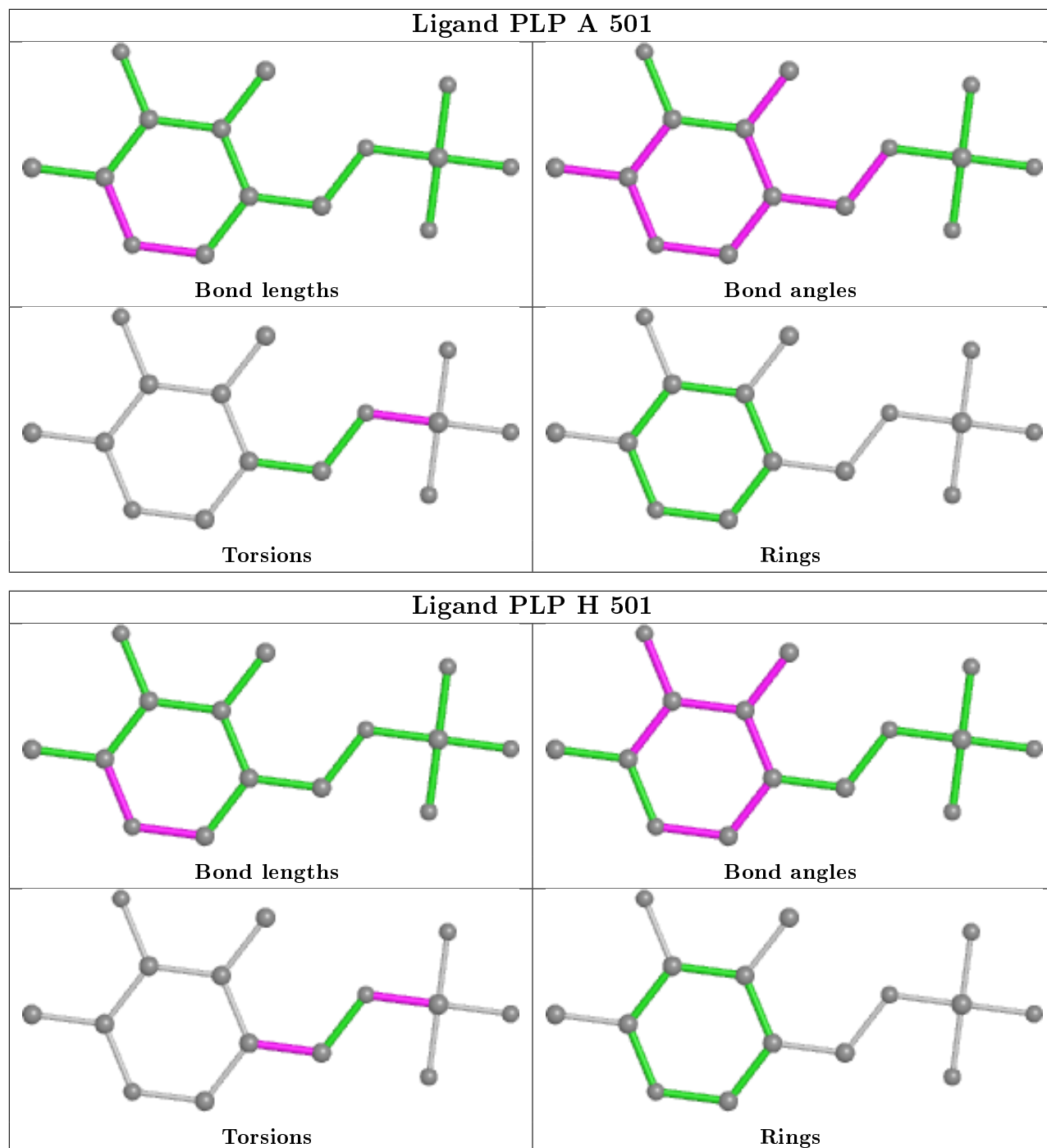
All (22) torsion outliers are listed below:

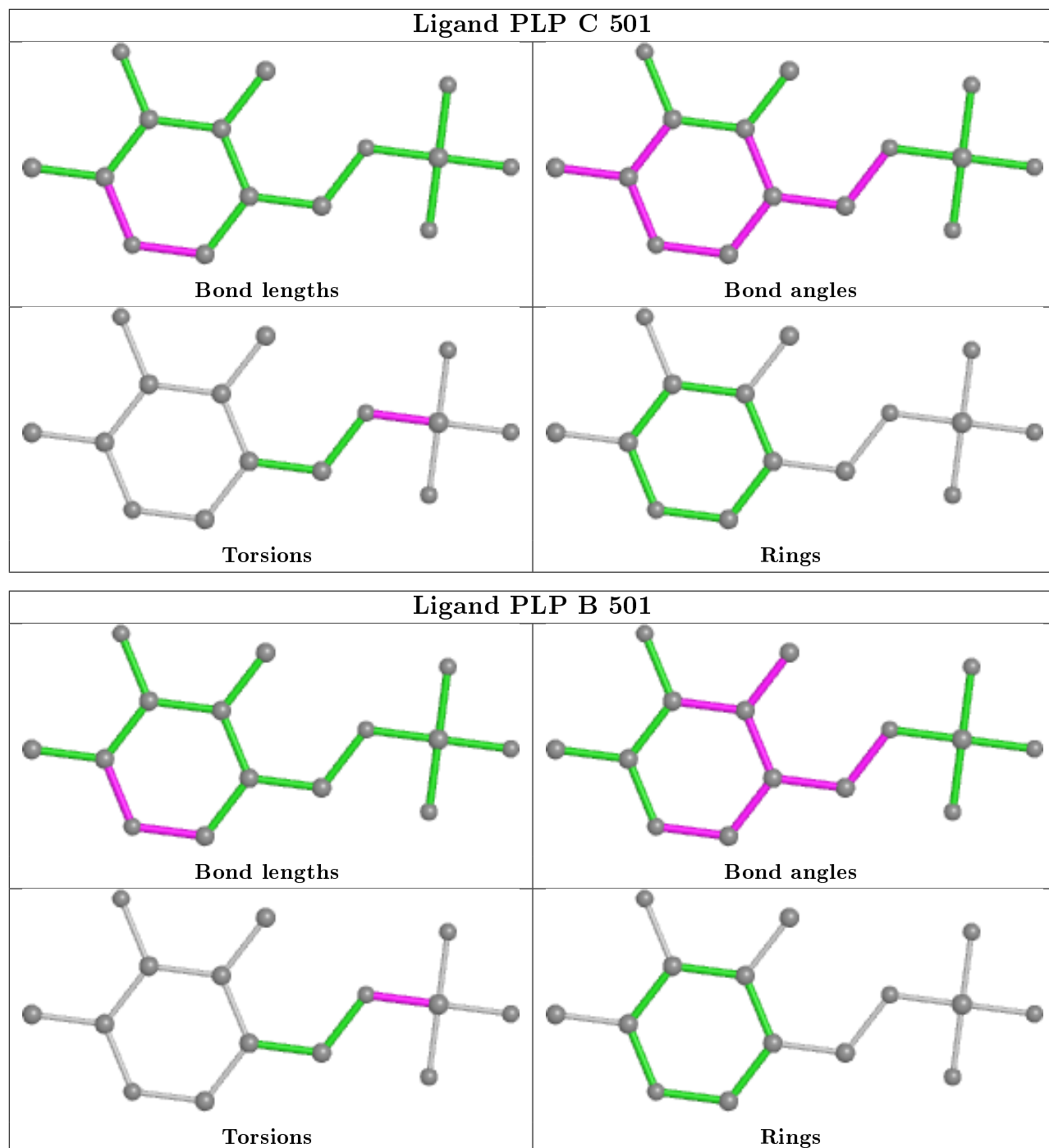
Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C5A-O4P-P-O1P
2	A	501	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C5A-O4P-P-O3P
2	H	501	PLP	C4-C5-C5A-O4P
2	H	501	PLP	C6-C5-C5A-O4P
2	H	501	PLP	C5A-O4P-P-O2P
2	H	501	PLP	C5A-O4P-P-O3P
2	C	501	PLP	C5A-O4P-P-O1P
2	C	501	PLP	C5A-O4P-P-O2P
2	C	501	PLP	C5A-O4P-P-O3P
2	B	501	PLP	C5A-O4P-P-O1P
2	B	501	PLP	C5A-O4P-P-O3P
2	D	501	PLP	C4-C5-C5A-O4P
2	G	501	PLP	C4-C5-C5A-O4P
2	F	501	PLP	C5A-O4P-P-O1P
2	F	501	PLP	C5A-O4P-P-O2P
2	F	501	PLP	C5A-O4P-P-O3P
2	D	501	PLP	C6-C5-C5A-O4P
2	H	501	PLP	C5A-O4P-P-O1P
2	G	501	PLP	C5A-O4P-P-O1P
2	B	501	PLP	C5A-O4P-P-O2P
2	G	501	PLP	C5A-O4P-P-O3P

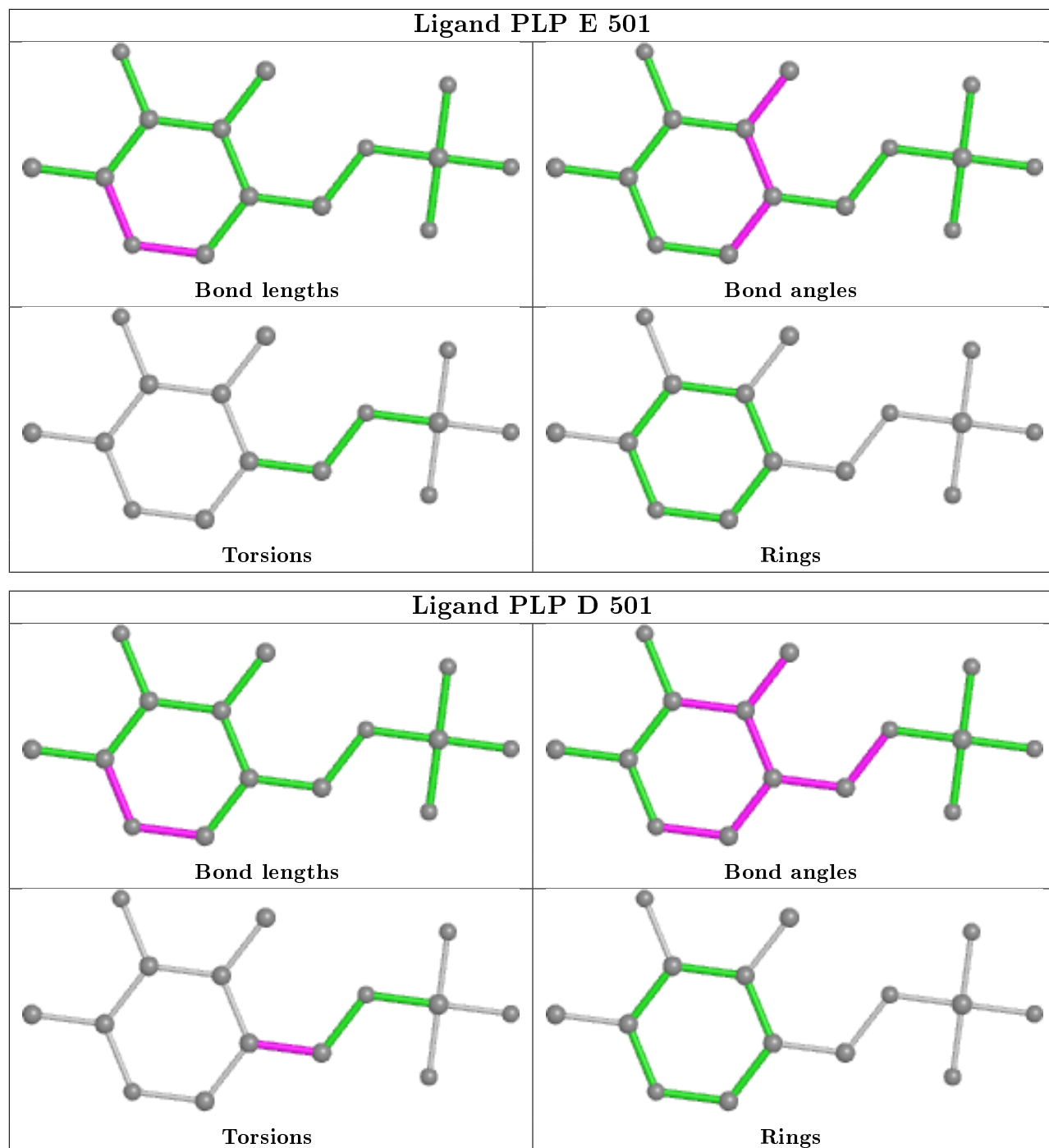
There are no ring outliers.

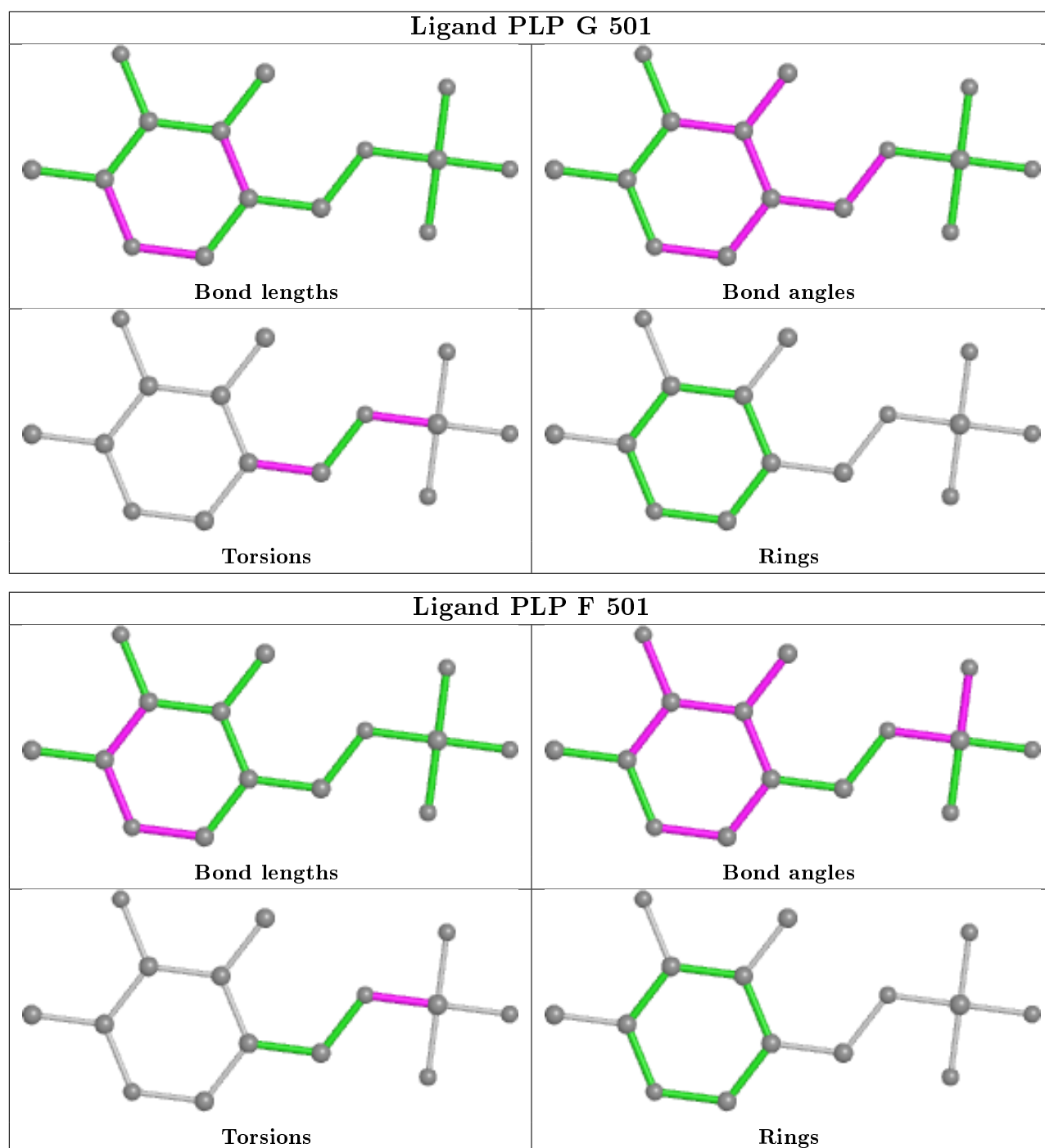
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/429 (97%)	0.03	10 (2%) 59 54	46, 58, 84, 106	0
1	B	419/429 (97%)	0.00	13 (3%) 49 45	42, 56, 84, 97	0
1	C	419/429 (97%)	0.17	22 (5%) 26 23	48, 66, 97, 112	0
1	D	417/429 (97%)	0.17	21 (5%) 28 26	46, 64, 98, 114	0
1	E	418/429 (97%)	0.10	19 (4%) 33 30	42, 58, 94, 109	0
1	F	417/429 (97%)	0.18	31 (7%) 14 11	42, 55, 92, 112	0
1	G	422/429 (98%)	0.07	15 (3%) 42 39	43, 58, 87, 99	0
1	H	417/429 (97%)	0.05	18 (4%) 35 32	45, 58, 89, 107	0
All	All	3346/3432 (97%)	0.10	149 (4%) 33 30	42, 59, 91, 114	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	LEU	8.7
1	A	178	GLY	6.6
1	D	8	ARG	5.8
1	F	17	SER	5.7
1	E	16	TYR	5.6
1	D	19	SER	5.6
1	D	18	ARG	5.3
1	F	8	ARG	5.2
1	E	6	LEU	5.0
1	F	9	MET	5.0
1	H	5	ILE	4.9
1	F	5	ILE	4.9
1	E	15	THR	4.5
1	E	17	SER	4.3
1	F	20	PHE	4.2
1	F	19	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	ILE	4.0
1	E	9	MET	4.0
1	E	5	ILE	3.9
1	D	5	ILE	3.9
1	F	6	LEU	3.8
1	C	20	PHE	3.8
1	E	20	PHE	3.8
1	F	15	THR	3.8
1	G	5	ILE	3.7
1	D	16	TYR	3.7
1	E	21	PRO	3.6
1	F	112	THR	3.6
1	H	8	ARG	3.6
1	D	9	MET	3.6
1	D	7	GLU	3.4
1	G	163	THR	3.4
1	C	17	SER	3.4
1	H	419	VAL	3.4
1	E	8	ARG	3.4
1	C	4	GLN	3.3
1	H	420	PHE	3.3
1	B	347	HIS	3.3
1	G	290	PRO	3.2
1	A	11	SER	3.1
1	E	79	TRP	3.1
1	F	145	ALA	3.1
1	B	420	PHE	3.1
1	G	2	GLN	3.1
1	D	12	GLU	3.1
1	H	364	ASP	3.0
1	H	365	GLY	3.0
1	D	20	PHE	3.0
1	F	21	PRO	3.0
1	A	19	SER	2.9
1	F	115	VAL	2.9
1	G	420	PHE	2.9
1	C	16	TYR	2.8
1	B	179	VAL	2.8
1	F	10	GLU	2.8
1	C	143	MET	2.8
1	F	420	PHE	2.8
1	F	16	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	166	ALA	2.8
1	E	7	GLU	2.7
1	D	112	THR	2.7
1	F	11	SER	2.7
1	F	147	ALA	2.7
1	A	14	ARG	2.7
1	C	19	SER	2.6
1	C	5	ILE	2.6
1	D	346	GLY	2.6
1	H	347	HIS	2.6
1	F	166	ALA	2.6
1	A	20	PHE	2.6
1	F	119	ILE	2.6
1	F	165	GLY	2.6
1	D	143	MET	2.6
1	C	165	GLY	2.6
1	D	11	SER	2.5
1	H	18	ARG	2.5
1	C	145	ALA	2.5
1	B	163	THR	2.5
1	F	146	LEU	2.5
1	B	110	THR	2.5
1	G	165	GLY	2.5
1	B	178	GLY	2.5
1	D	146	LEU	2.4
1	F	18	ARG	2.4
1	H	17	SER	2.4
1	C	166	ALA	2.4
1	C	79	TRP	2.4
1	C	290	PRO	2.4
1	D	420	PHE	2.4
1	B	341	PHE	2.4
1	H	417	LYS	2.4
1	C	146	LEU	2.4
1	D	144	GLY	2.4
1	E	161	ILE	2.4
1	G	9	MET	2.4
1	C	142	THR	2.3
1	C	148	THR	2.3
1	H	290	PRO	2.3
1	D	161	ILE	2.3
1	A	16	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	114	ALA	2.3
1	F	111	GLY	2.3
1	G	147	ALA	2.3
1	D	142	THR	2.3
1	E	142	THR	2.3
1	F	144	GLY	2.3
1	B	146	LEU	2.3
1	H	388	SER	2.3
1	G	229	ARG	2.3
1	H	387	HIS	2.3
1	F	7	GLU	2.3
1	E	141	VAL	2.3
1	E	112	THR	2.3
1	C	9	MET	2.2
1	C	3	THR	2.2
1	F	14	ARG	2.2
1	F	117	ALA	2.2
1	E	147	ALA	2.2
1	A	8	ARG	2.2
1	C	177	GLU	2.2
1	C	318	ASP	2.2
1	E	163	THR	2.2
1	G	7	GLU	2.2
1	D	4	GLN	2.1
1	A	15	THR	2.1
1	E	113	ASN	2.1
1	B	165	GLY	2.1
1	G	423	ALA	2.1
1	H	348	PRO	2.1
1	G	8	ARG	2.1
1	B	141	VAL	2.1
1	C	114	ALA	2.1
1	B	79	TRP	2.1
1	F	12	GLU	2.1
1	C	149	THR	2.1
1	D	10	GLU	2.1
1	F	110	THR	2.1
1	F	148	THR	2.1
1	G	162	PRO	2.1
1	B	143	MET	2.1
1	H	342	MET	2.1
1	B	145	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	289	LYS	2.1
1	H	367	MET	2.0
1	C	131	ILE	2.0
1	A	177	GLU	2.0
1	G	11	SER	2.0
1	H	363	GLY	2.0
1	H	16	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 carbohydrates in this entry.

6.4 Ligands [i](#)

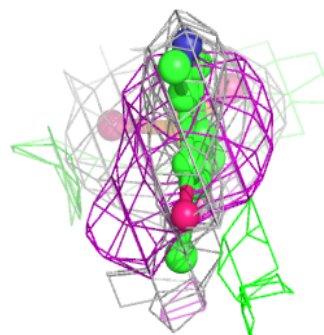
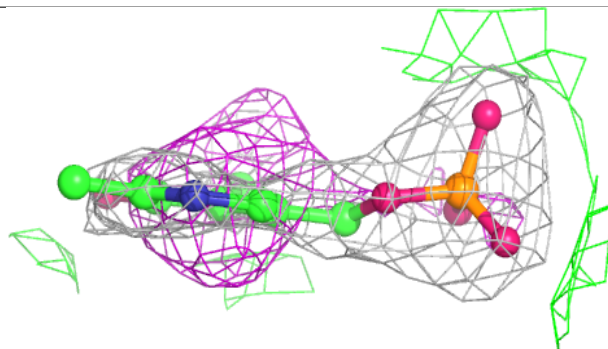
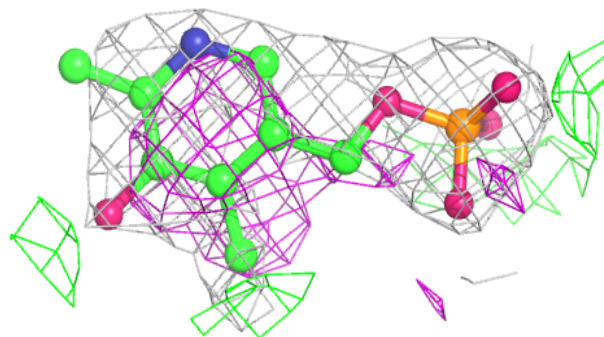
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	F	501	15/16	0.86	0.24	60,70,83,83	0
2	PLP	C	501	15/16	0.91	0.18	68,79,86,95	0
2	PLP	E	501	15/16	0.92	0.17	61,66,77,78	0
2	PLP	H	501	15/16	0.94	0.17	57,66,82,86	0
2	PLP	D	501	15/16	0.94	0.15	62,73,86,87	0
2	PLP	G	501	15/16	0.94	0.13	53,60,68,71	0
2	PLP	A	501	15/16	0.94	0.14	46,66,73,80	0
2	PLP	B	501	15/16	0.95	0.16	56,68,70,72	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.

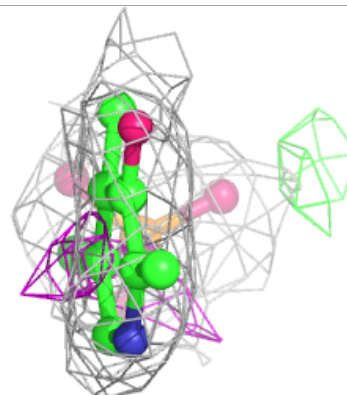
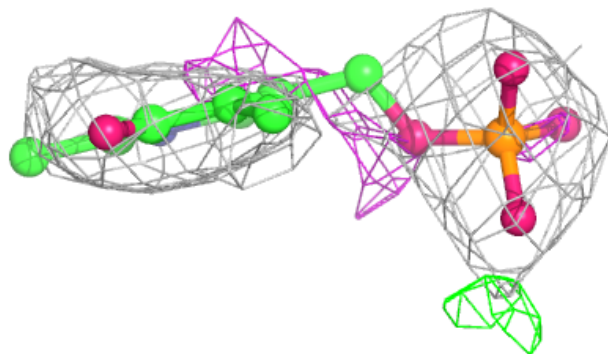
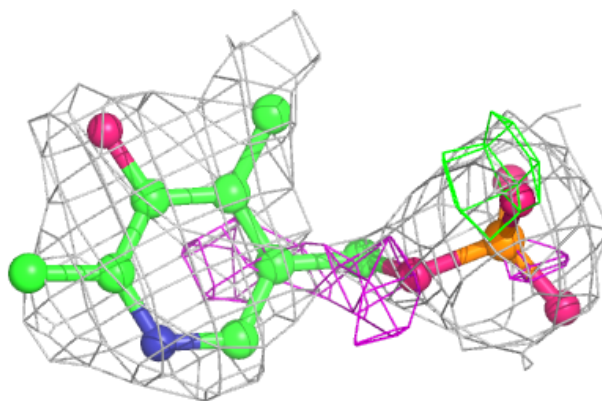
Electron density around PLP F 501:

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



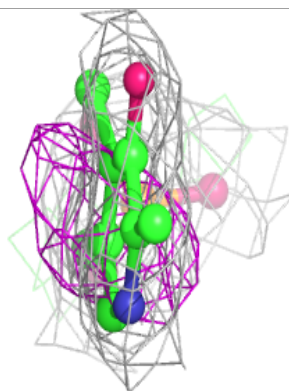
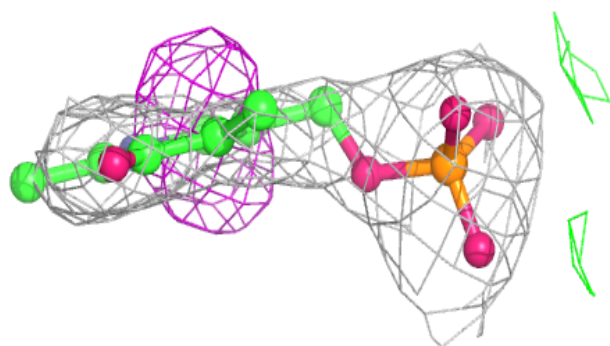
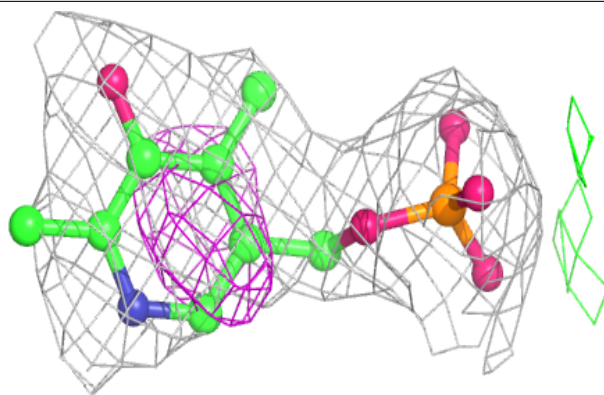
Electron density around PLP C 501:

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

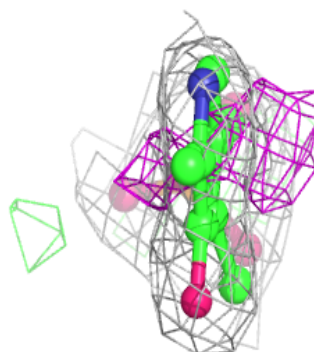
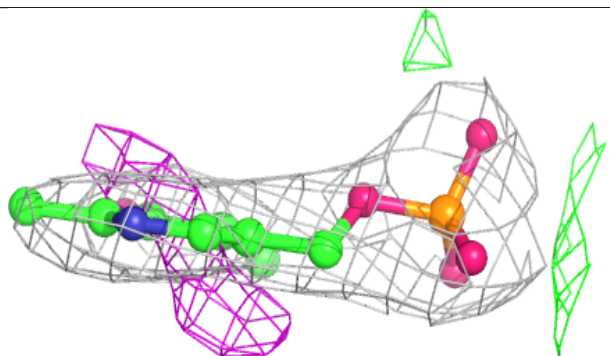
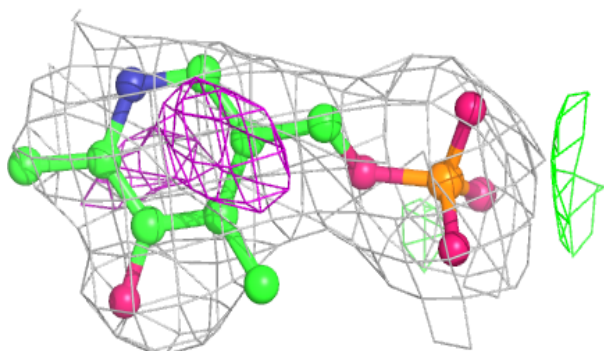


Electron density around PLP E 501:

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

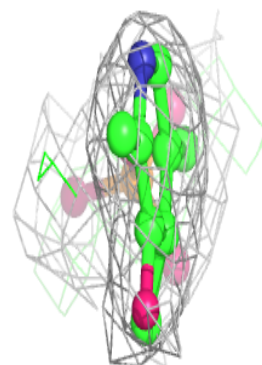
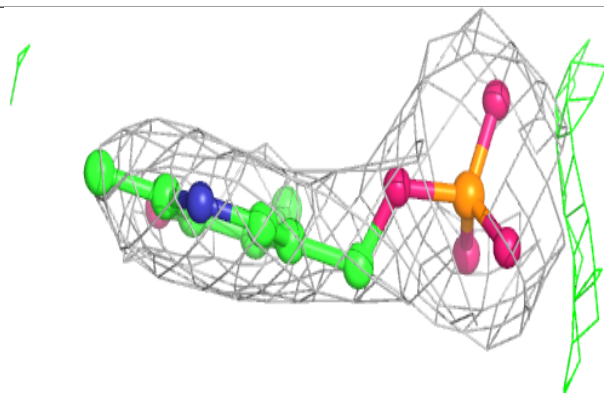
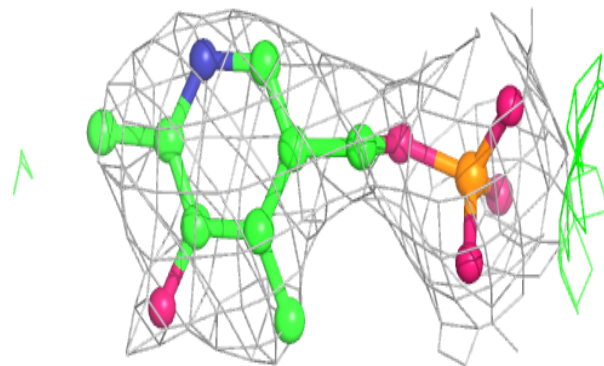
**Electron density around PLP H 501:**

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

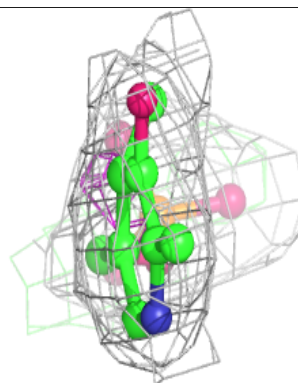
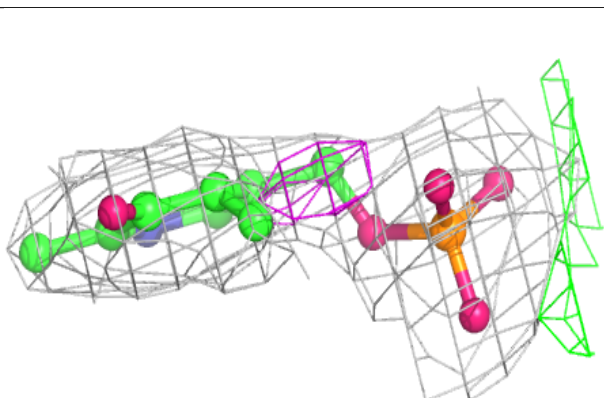
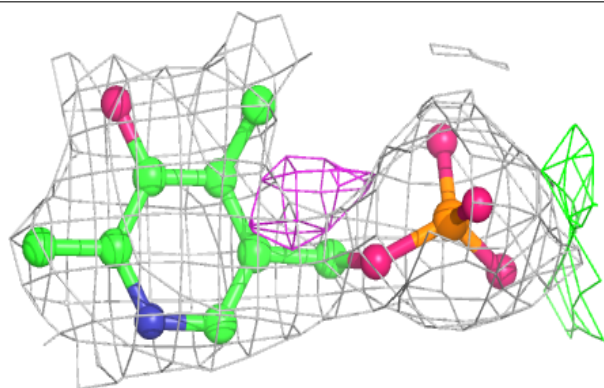


Electron density around PLP D 501:

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

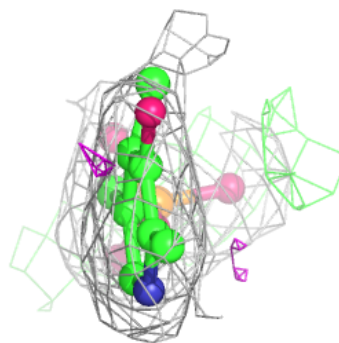
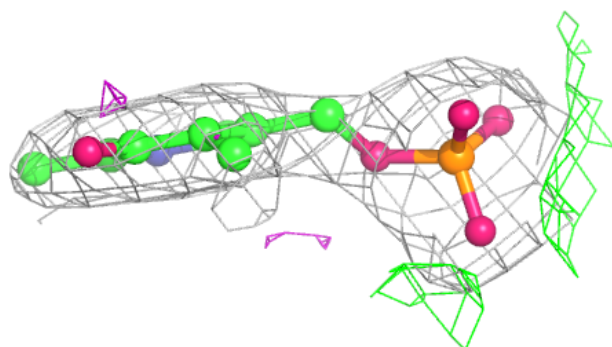
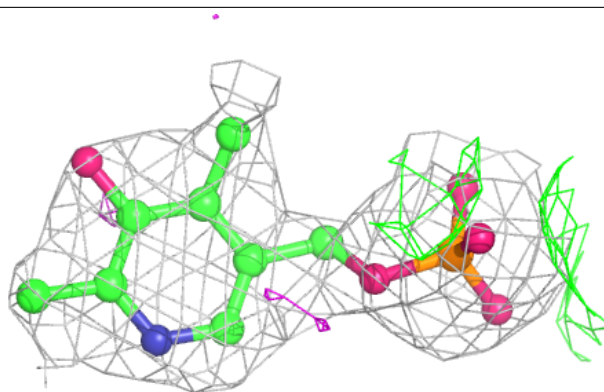
**Electron density around PLP G 501:**

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

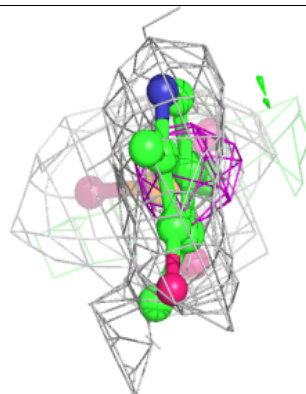
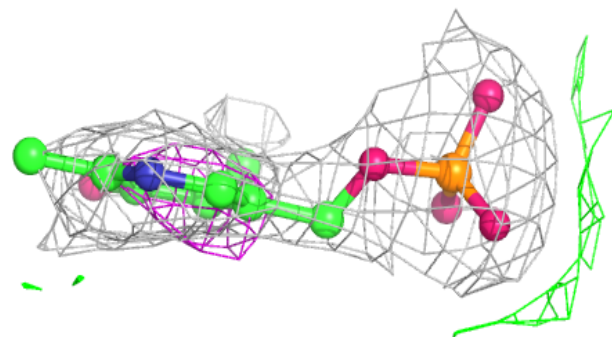
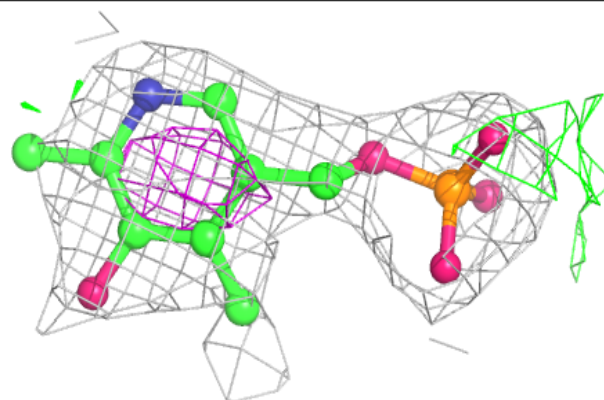


Electron density around PLP A 501:

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

**Electron density around PLP B 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

There are no such residues in this entry.