



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:35 PM EDT

PDB ID : 6RL5 / pdb_00006rl5
Title : The first crystal structure of the DABA aminotransferase EctB in the ectoine biosynthesis pathway of the model organism *Chromohalobacter salexigens* 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

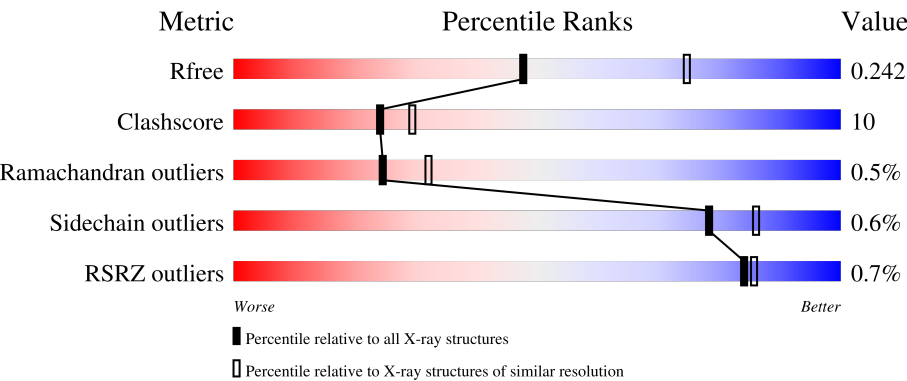
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	78%19%.
1	B	429	76%21%..
1	C	429	% 77%21%.
1	D	429	74%23%.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	429	2% 72% 25%
1	F	429	2% 78% 18%
1	G	429	76% 22%
1	H	429	74% 22%

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

There are 48 discrepancies between the modelled and reference sequences:

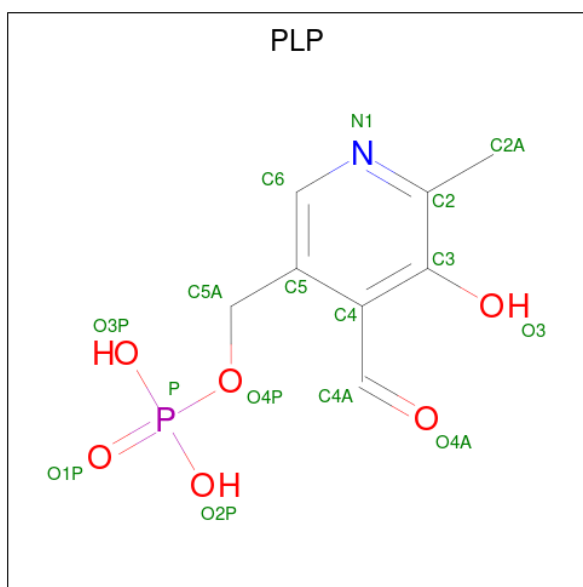
Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP Q9ZEU7
A	425	HIS	-	expression tag	UNP Q9ZEU7
A	426	HIS	-	expression tag	UNP Q9ZEU7
A	427	HIS	-	expression tag	UNP Q9ZEU7
A	428	HIS	-	expression tag	UNP Q9ZEU7
A	429	HIS	-	expression tag	UNP Q9ZEU7
B	424	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

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 (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (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		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

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

Continued on next page...

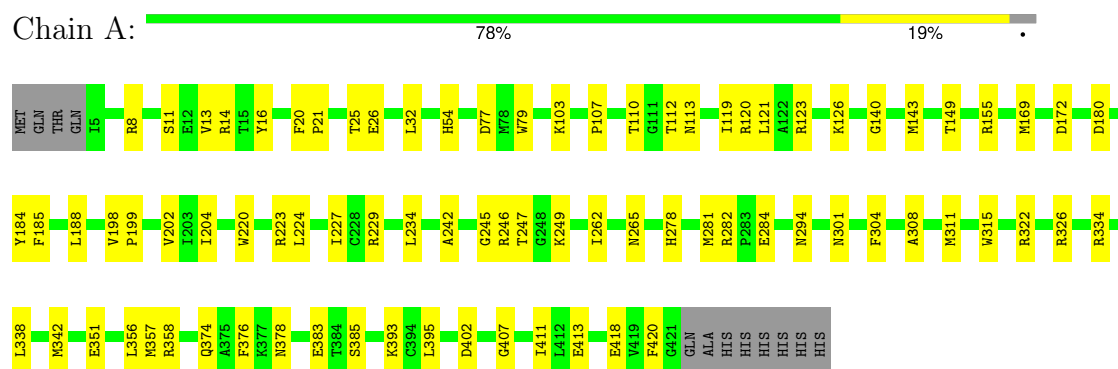
Continued from previous page...

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

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.

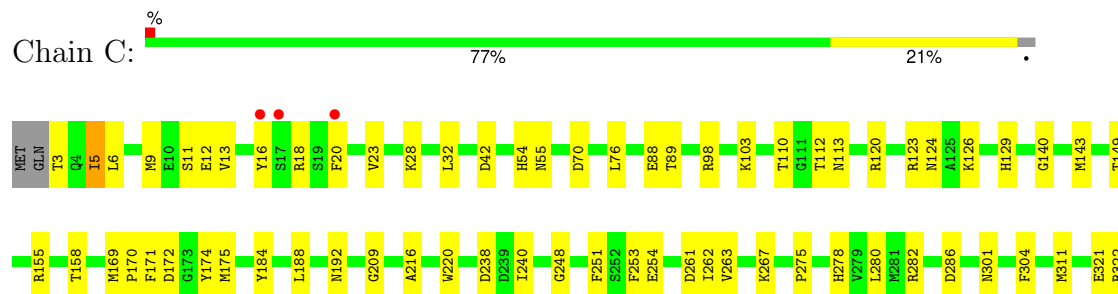
- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

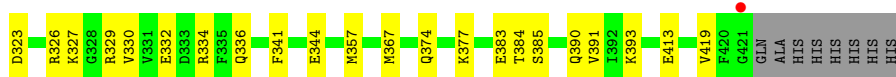


- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase



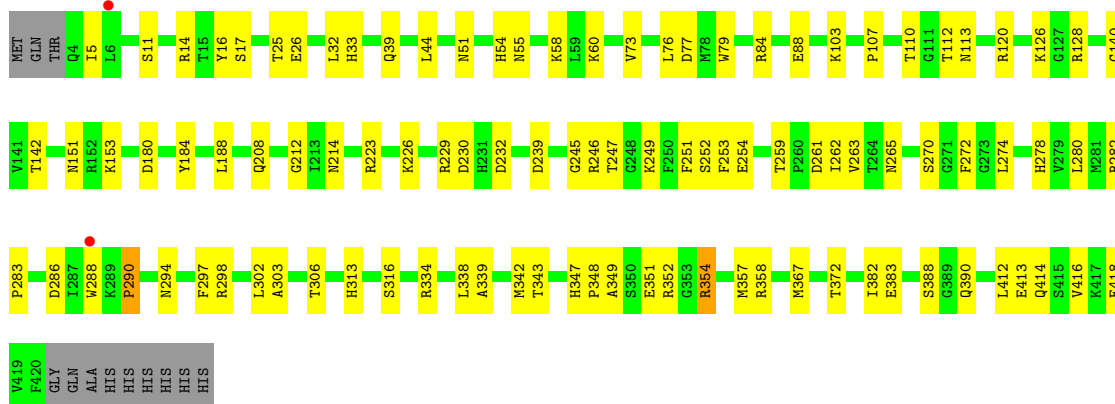
- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase





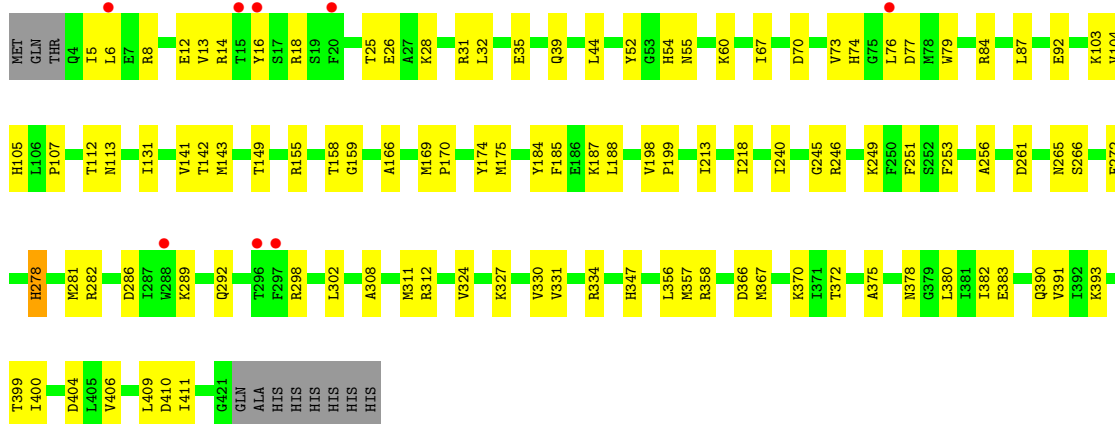
- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

Chain D: 74% 23%



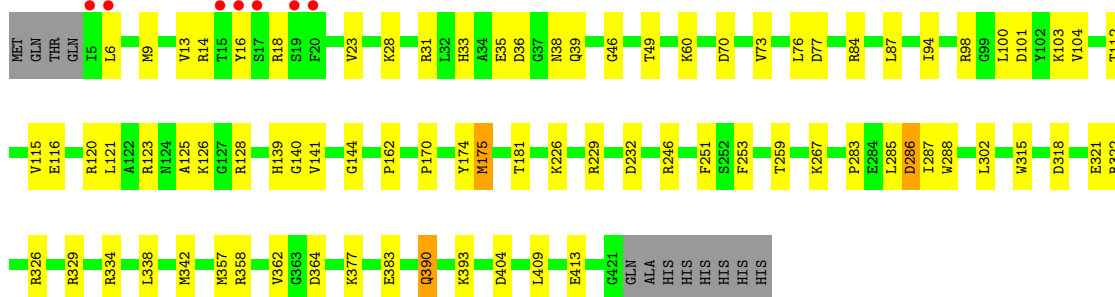
- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

Chain E: 2% 72% 25%



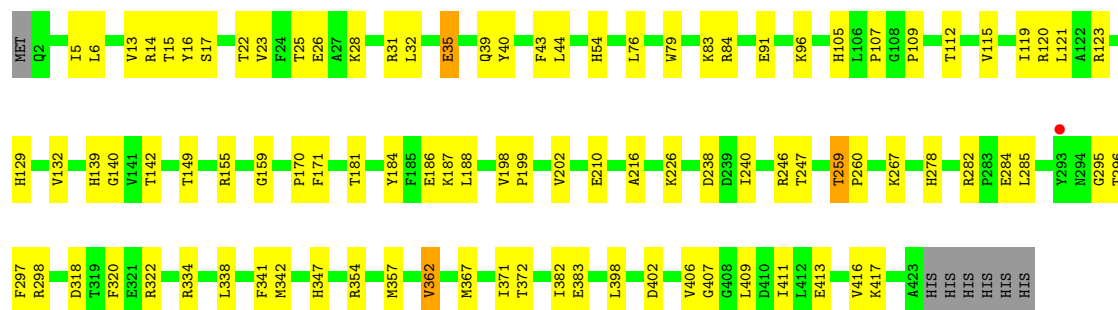
- Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

Chain F: 2% 78% 18%



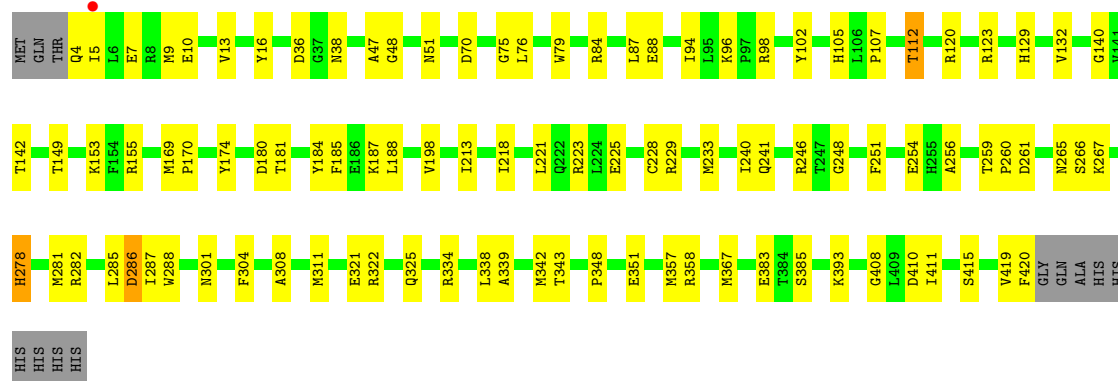
• Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

Chain G:  76% 22% ..



• Molecule 1: Diaminobutyrate--2-oxoglutarate transaminase

Chain H:  74% 22% ..



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)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.185 , 0.243 0.187 , 0.242	Depositor DCC
R_{free} test set	2704 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.42	0/3272	0.62	0/4419
1	B	0.42	0/3288	0.57	0/4441
1	C	0.40	0/3288	0.60	1/4441 (0.0%)
1	D	0.37	0/3277	0.58	0/4426
1	E	0.42	0/3281	0.60	0/4431
1	F	0.43	0/3283	0.62	0/4433
1	G	0.41	0/3311	0.62	0/4472
1	H	0.40	0/3277	0.58	0/4426
All	All	0.41	0/26277	0.60	1/35489 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	ILE	N-CA-C	-6.19	106.77	112.96

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	63	0
1	B	3220	0	3156	67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3220	0	3155	72	0
1	D	3209	0	3145	75	0
1	E	3213	0	3151	82	0
1	F	3215	0	3153	73	0
1	G	3243	0	3176	73	0
1	H	3209	0	3148	77	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	2	0
3	E	50	0	0	6	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	512	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 (512) 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	1.00
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:H:169:MET:HE3	1:H:170:PRO:HD2	1.55	0.88
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:MET:HE3	1:C:170:PRO:HD2	1.71	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:B:175:MET:HE2	1:B:181:THR:HG22	1.74	0.69
1:C:367:MET:HE3	1:C:367:MET:HA	1.73	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:281:MET:HE2	1:H:286:ASP:HA	1.77	0.67
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:3:THR:HG23	1:D:84:ARG:HE	1.61	0.65
1:C:332:GLU:O	1:C:336:GLN:HG3	1.95	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:E:308:ALA:HA	1:E:311:MET:HE3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLU:OE2	1:B:358:ARG:NH1	2.29	0.64
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: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:E:169:MET:HE2	1:E:185:PHE:HA	1.83	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:A:169:MET:HE1	1:A:188:LEU:HD12	1.82	0.61
1:E:13:VAL:HG23	1:F:288:TRP:HB3	1.82	0.61
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:OE1	1:A:284:GLU:N	2.33	0.59
1:B:341:PHE:CZ	1:B:417:LYS:HG2	2.37	0.59
1:B:112:THR:HG21	1:B:142:THR:H	1.68	0.59
1:E:31:ARG:NH2	1:E:404:ASP:OD1	2.35	0.59

Continued on next page...

Continued from previous page...

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:F:175:MET:HE2	1:F:181:THR:HG22	1.83	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: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:A:284:GLU:CD	1:A:284:GLU:H	2.10	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:B:281:MET:HE1	1:B:286:ASP:HA	1.89	0.54
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:F:103:LYS:NZ	1:F:286:ASP:OD2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:112:THR:HG23	1:D:140:GLY:HA3	1.89	0.54
1:E:103:LYS:NZ	1:E:286:ASP:OD2	2.24	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:E:143:MET:HE1	1:E:158:THR:HG22	1.89	0.54
1:H:385:SER:HB3	1:H:393:LYS:HD3	1.89	0.54
1:A:13:VAL:HB	1:B:288:TRP:CB	2.37	0.54
1:A:112:THR:HG22	1:A:140:GLY:CA	2.34	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:G:342:MET:HE1	1:G:362:VAL:HG12	1.91	0.53
1:B:236:ILE:HG12	1:B:262:ILE:HB	1.90	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:E:169:MET:HE1	1:E:188:LEU:HD12	1.91	0.52
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:G:296:THR:OG1	1:H:267:LYS:NZ	2.43	0.52
1:D:229:ARG:HB2	1:D:229:ARG:CZ	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:275:PRO:HG3	1:D:297:PHE:HB3	1.93	0.50
1:C:301:ASN:HA	1:C:304:PHE:CD2	2.46	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:E:347:HIS:CE1	1:E:367:MET:HE2	2.47	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:25:THR:HG22	1:A:26:GLU:N	2.27	0.50
1:A:223:ARG:HD3	3:A:620:HOH:O	2.11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LYS:HB3	1:G:96:LYS:HD3	1.94	0.49
1:D:303:ALA:HA	1:D:306:THR:HG22	1.94	0.49
1:B:213:ILE:O	1:B:215:PRO:HD3	2.11	0.49
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:B:3:THR:O	1:B:7:GLU:HG3	2.11	0.49
1:B:349:ALA:HA	1:B:361:ASP:O	2.13	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:F:126:LYS:NZ	1:F:232:ASP:OD1	2.40	0.49
1:E:143:MET:HE2	1:F:120:ARG:NH2	2.28	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:H:308:ALA:HA	1:H:311:MET:HE3	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:B:121:LEU:HD22	1:B:281:MET:HE3	1.96	0.48
1:G:6:LEU:HD11	1:H:84:ARG:HB2	1.95	0.48
1:H:16:TYR:HE1	1:H:383:GLU:OE2	1.96	0.48
1:C:9:MET:HE1	3:D:616:HOH:O	2.13	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:A:308:ALA:HA	1:A:311:MET:HE3	1.95	0.48
1:B:180:ASP:OD2	1:B:223:ARG:NH1	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLY:HA2	1:A:249:LYS:O	2.14	0.47
1:G:91:GLU:HB2	1:H:9:MET:HE1	1.94	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
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:4:GLN:O	1:B:8:ARG:HD3	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: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: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: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:16:TYR:CE2	1:B:76:LEU:HG	2.50	0.46
1:A:110:THR:OG1	1:A:113:ASN:HB2	2.16	0.46
1:D:126:LYS:HA	1:D:126:LYS:HD3	1.63	0.46
1:C:278:HIS:C	1:C:278:HIS:CD2	2.94	0.46
1:D:414:GLN:NE2	1:D:418:GLU:OE2	2.46	0.46
1:E:60:LYS:NZ	1:F:70:ASP:OD1	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:VAL:HG12	1:E:358:ARG:HD3	1.98	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:A:169:MET:HE2	1:A:185:PHE:HA	1.98	0.45
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
1:B:285:LEU:O	1:B:287:ILE:N	2.49	0.45
1:H:96:LYS:HD3	1:H:96:LYS:HA	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:A:281:MET:HE3	1:A:281:MET:HB2	1.62	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:C:322:ARG:HH12	1:C:329:ARG:HH12	1.63	0.45
1:E:170:PRO:HG3	1:E:175:MET:HE3	1.98	0.45
1:H:301:ASN:HA	1:H:304:PHE:HD2	1.81	0.45
1:H:342:MET:HE3	1:H:367:MET:HE3	1.99	0.45
1:A:278:HIS:CD2	1:A:278:HIS:C	2.94	0.45
1:C:16:TYR:HD1	1:C:20:PHE:HE2	1.65	0.45
1:F:259:THR:O	1:F:259:THR:OG1	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:E:281:MET:HE2	1:E:286:ASP:HA	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:THR:O	1:H:79:TRP:HB2	2.17	0.44
1:G:23:VAL:HG22	1:G:35:GLU:HB2	1.99	0.44
1:G:109:PRO:HD3	1:G:297:PHE:O	2.17	0.44
1:B:316:SER:N	3:B:607:HOH:O	2.49	0.44
1:E:169:MET:HE2	1:E:185:PHE:CA	2.47	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: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:C:143:MET:HE1	1:C:158:THR:CG2	2.48	0.43
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:C:209:GLY:HA2	1:C:357:MET:HE2	2.00	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:D:367:MET:HB2	1:D:367:MET:HE2	1.69	0.43
1:H:240:ILE:HG12	1:H:266:SER:HB3	2.01	0.43
1:E:13:VAL:CG2	1:F:288:TRP:HB3	2.48	0.43
1:E:245:GLY:HA2	1:E:249:LYS:O	2.18	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:6:LEU:HD22	1:D:79:TRP:CD1	2.53	0.43
1:C:184:TYR:CZ	1:C:188:LEU:HD11	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:76:LEU:HD22	1:H:16:TYR:CE2	2.54	0.43
1:G:115:VAL:HG21	1:G:139:HIS:HB3	2.01	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:HD12	1:D:76:LEU:HA	1.82	0.43
1:E:104:VAL:N	1:F:9:MET:O	2.44	0.43
1:E:261:ASP:OD1	1:E:282:ARG:HD2	2.19	0.43
1:F:18:ARG:HH11	1:F:18:ARG:HG2	1.84	0.43
1:F:33:HIS:CD2	1:F:33:HIS:N	2.87	0.43
1:A:11:SER:O	1:A:14:ARG:HD3	2.18	0.42
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:HG2	1:F:18:ARG:NH1	2.34	0.42
1:F:87:LEU:HD23	1:F:87:LEU:HA	1.82	0.42
1:F:251:PHE:HB3	1:F:253:PHE:CE2	2.54	0.42
1:G:367:MET:HE3	1:G:367:MET:HB3	1.88	0.42
1:G:407:GLY:O	1:G:411:ILE:HG13	2.19	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:C:170:PRO:HG3	1:C:175:MET:HE3	2.00	0.42
1:E:174:TYR:O	1:H:187:LYS:NZ	2.44	0.42
1:G:341:PHE:CD1	1:G:341:PHE:C	2.97	0.42
1:H:265:ASN:ND2	1:H:278:HIS:HE1	2.16	0.42
1:A:322:ARG:HG2	1:A:322:ARG:HH11	1.84	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:B:226:LYS:HE2	1:B:230:ASP:OD2	2.18	0.42
1:C:262:ILE:HA	1:C:280:LEU:O	2.19	0.42
1:D:347:HIS:NE2	1:D:367:MET:HE3	2.35	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:F:342:MET:HE1	1:F:362:VAL:HG12	2.01	0.42
1:H:338:LEU:HA	1:H:338:LEU:HD23	1.74	0.42
1:H:385:SER:HA	3:H:631:HOH:O	2.19	0.42
1:C:103:LYS:NZ	1:C:286:ASP:OD2	2.42	0.42
1:C:251:PHE:HB3	1:C:253:PHE:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:H:5:ILE:HG22	2.19	0.42
1:F:116:GLU:CD	1:F:144:GLY:HA3	2.44	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:H:367:MET:HE1	1:H:420:PHE:CZ	2.55	0.42
1:D:229:ARG:HB2	1:D:229:ARG:NH1	2.35	0.42
1:F:6:LEU:HD23	1:F:6:LEU:O	2.20	0.42
1:F:326:ARG:HA	1:F:329:ARG:NH1	2.35	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
1:F:364:ASP:C	1:F:390:GLN:HB2	2.45	0.42
1:A:103:LYS:O	1:A:281:MET:HG2	2.20	0.41
1:A:119:ILE:HG13	1:A:120:ARG:N	2.35	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:5:ILE:HD13	1:H:88:GLU:HG3	2.01	0.41
1:G:32:LEU:HD11	1:G:54:HIS:NE2	2.35	0.41
1:G:278:HIS:CD2	1:G:278:HIS:C	2.98	0.41
1:A:79:TRP:HB3	1:B:6:LEU:HD13	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: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:342:MET:HE1	1:B:360:LEU:HD11	2.01	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: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:A:342:MET:HE3	1:A:420:PHE:CZ	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ASP:OD2	1:F:28:LYS:HE2	2.21	0.41
1:F:76:LEU:HB3	1:F:77:ASP:H	1.56	0.41
1:F:121:LEU:HD13	1:F:288:TRP:NE1	2.36	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:B:86:TYR:OH	1:B:278:HIS:CD2	2.73	0.41
1:B:285:LEU:HD23	1:B:285:LEU:HA	1.95	0.41
1:C:89:THR:HG22	1:C:311:MET:HE3	2.02	0.41
1:C:126:LYS:HA	1:C:126:LYS:HD3	1.92	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
1:D:247:THR:HB	1:D:354:ARG:HG2	2.03	0.41
1:E:13:VAL:HG23	1:F:288:TRP:CG	2.56	0.41
1:E:13:VAL:O	1:E:14:ARG:C	2.64	0.41
1:E:159:GLY:HA3	1:F:123:ARG:HB3	2.03	0.41
1:F:100:LEU:HD23	1:F:100:LEU:HA	1.95	0.41
1:G:259:THR:HA	1:G:260:PRO:HD3	1.90	0.41
1:H:36:ASP:OD1	1:H:38:ASN:HB2	2.21	0.41
1:H:132:VAL:HG21	1:H:185:PHE:CE1	2.55	0.41
1:H:385:SER:CB	1:H:393:LYS:HD3	2.51	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:169:MET:HE3	1:E:170:PRO:HD2	2.03	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:278:HIS:C	1:B:278:HIS:HD1	2.28	0.40
1:B:338:LEU:HD21	1:B:413:GLU:HA	2.03	0.40
1:G:159:GLY:HA3	1:H:123:ARG:HB3	2.02	0.40
1:H:120:ARG:HE	1:H:120:ARG:HB2	1.73	0.40
1:B:31:ARG:HA	1:B:40:TYR:O	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:281:MET:HE2	1:H:286:ASP:CA	2.48	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%)	43	54
1	B	417/429 (97%)	390 (94%)	25 (6%)	2 (0%)	24	32
1	C	417/429 (97%)	390 (94%)	27 (6%)	0	100	100
1	D	415/429 (97%)	382 (92%)	30 (7%)	3 (1%)	18	24
1	E	416/429 (97%)	389 (94%)	26 (6%)	1 (0%)	43	54
1	F	416/429 (97%)	398 (96%)	16 (4%)	2 (0%)	24	32
1	G	420/429 (98%)	397 (94%)	19 (4%)	4 (1%)	12	14
1	H	415/429 (97%)	388 (94%)	25 (6%)	2 (0%)	24	32
All	All	3331/3432 (97%)	3122 (94%)	194 (6%)	15 (0%)	24	32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	331 (100%)	1 (0%)	86	91
1	B	334/343 (97%)	328 (98%)	6 (2%)	51	65
1	C	334/343 (97%)	333 (100%)	1 (0%)	86	91
1	D	333/343 (97%)	331 (99%)	2 (1%)	78	86
1	E	333/343 (97%)	332 (100%)	1 (0%)	86	91
1	F	333/343 (97%)	331 (99%)	2 (1%)	78	86
1	G	336/343 (98%)	335 (100%)	1 (0%)	86	91
1	H	333/343 (97%)	330 (99%)	3 (1%)	70	81
All	All	2668/2744 (97%)	2651 (99%)	17 (1%)	78	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	110	THR
1	B	112	THR
1	B	204	ILE
1	B	249	LYS
1	B	281	MET
1	B	323	ASP
1	C	383	GLU
1	D	259	THR
1	D	354	ARG
1	E	278	HIS
1	F	175	MET
1	F	390	GLN
1	G	259	THR
1	H	112	THR
1	H	259	THR
1	H	278	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	136	ASN
1	B	136	ASN
1	B	278	HIS
1	B	313	HIS
1	B	387	HIS
1	C	241	GLN
1	C	387	HIS
1	C	414	GLN
1	D	74	HIS
1	D	130	ASN
1	D	136	ASN
1	D	192	ASN
1	D	208	GLN
1	D	214	ASN
1	D	231	HIS
1	D	387	HIS
1	E	105	HIS
1	E	136	ASN
1	E	208	GLN
1	E	214	ASN
1	E	265	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	278	HIS
1	E	325	GLN
1	F	61	GLN
1	F	105	HIS
1	G	136	ASN
1	G	208	GLN
1	H	214	ASN
1	H	231	HIS
1	H	241	GLN
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 oligosaccharides 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	F	501	1	15,15,16	2.28	4 (26%)	21,22,23	2.48	7 (33%)
2	PLP	C	501	1	15,15,16	1.25	2 (13%)	21,22,23	1.56	6 (28%)
2	PLP	E	501	-	15,15,16	1.46	2 (13%)	21,22,23	1.23	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	D	501	1	15,15,16	1.13	2 (13%)	21,22,23	1.38	4 (19%)
2	PLP	A	501	1	15,15,16	1.29	2 (13%)	21,22,23	1.93	7 (33%)
2	PLP	B	501	1	15,15,16	1.35	2 (13%)	21,22,23	2.08	6 (28%)
2	PLP	H	501	-	15,15,16	1.28	2 (13%)	21,22,23	1.40	4 (19%)
2	PLP	G	501	1	15,15,16	1.44	2 (13%)	21,22,23	1.65	5 (23%)

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	F	501	1	-	3/6/6/8	0/1/1/1
2	PLP	C	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	A	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	H	501	-	-	5/6/6/8	0/1/1/1
2	PLP	G	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	-5.12	1.35	1.41
2	F	501	PLP	C6-N1	4.44	1.43	1.34
2	F	501	PLP	C2-N1	4.15	1.41	1.33
2	B	501	PLP	C2-N1	3.66	1.40	1.33
2	G	501	PLP	C2-N1	3.56	1.40	1.33
2	A	501	PLP	C2-N1	3.51	1.40	1.33
2	E	501	PLP	C2-N1	3.47	1.40	1.33
2	C	501	PLP	C2-N1	3.29	1.39	1.33
2	H	501	PLP	C2-N1	3.20	1.39	1.33
2	G	501	PLP	C6-N1	2.73	1.40	1.34
2	D	501	PLP	C2-N1	2.66	1.38	1.33
2	B	501	PLP	C6-N1	2.64	1.39	1.34
2	E	501	PLP	C6-N1	2.63	1.39	1.34
2	A	501	PLP	C6-N1	2.60	1.39	1.34
2	H	501	PLP	C6-N1	2.35	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLP	C6-N1	2.29	1.39	1.34
2	D	501	PLP	C6-N1	2.17	1.38	1.34
2	F	501	PLP	C2A-C2	2.02	1.53	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLP	C4A-C4-C5	-5.60	115.17	120.94
2	F	501	PLP	C3-C4-C5	5.60	125.31	118.59
2	F	501	PLP	C4A-C4-C5	-5.40	115.37	120.94
2	F	501	PLP	C5-C6-N1	-5.27	115.25	123.83
2	G	501	PLP	C4A-C4-C3	-4.41	113.17	120.52
2	B	501	PLP	O4P-C5A-C5	4.13	117.11	109.36
2	B	501	PLP	C6-C5-C4	3.79	121.21	118.10
2	C	501	PLP	C2A-C2-C3	-3.57	116.62	120.80
2	H	501	PLP	C6-C5-C4	3.51	120.98	118.10
2	D	501	PLP	C4A-C4-C3	-3.39	114.88	120.52
2	A	501	PLP	C6-C5-C4	3.35	120.85	118.10
2	E	501	PLP	C6-C5-C4	3.22	120.74	118.10
2	A	501	PLP	O4P-C5A-C5	3.15	115.27	109.36
2	A	501	PLP	C4A-C4-C5	-3.14	117.71	120.94
2	A	501	PLP	C5-C6-N1	-3.06	118.85	123.83
2	C	501	PLP	C6-C5-C4	3.04	120.59	118.10
2	A	501	PLP	C5A-C5-C4	-2.98	116.76	122.64
2	G	501	PLP	C6-C5-C4	2.91	120.49	118.10
2	F	501	PLP	C4-C3-C2	-2.83	115.66	119.89
2	H	501	PLP	O3-C3-C2	2.79	123.36	117.58
2	F	501	PLP	O3-C3-C2	2.79	123.36	117.58
2	C	501	PLP	C5-C6-N1	-2.59	119.62	123.83
2	H	501	PLP	C5-C6-N1	-2.58	119.64	123.83
2	E	501	PLP	C4A-C4-C5	-2.56	118.30	120.94
2	G	501	PLP	C5-C6-N1	-2.56	119.67	123.83
2	G	501	PLP	O4P-C5A-C5	2.55	114.13	109.36
2	B	501	PLP	C5-C6-N1	-2.50	119.76	123.83
2	A	501	PLP	C2A-C2-C3	-2.47	117.90	120.80
2	C	501	PLP	C2A-C2-N1	2.45	122.25	117.64
2	B	501	PLP	C4A-C4-C3	-2.44	116.46	120.52
2	H	501	PLP	C4A-C4-C3	-2.40	116.52	120.52
2	F	501	PLP	O3P-P-O4P	2.39	112.91	106.67
2	A	501	PLP	C2A-C2-N1	2.37	122.11	117.64
2	B	501	PLP	C5A-C5-C4	-2.26	118.19	122.64
2	F	501	PLP	C6-C5-C4	2.20	119.90	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	PLP	C5-C6-N1	-2.15	120.33	123.83
2	C	501	PLP	O4P-C5A-C5	2.14	113.36	109.36
2	G	501	PLP	C4A-C4-C5	-2.11	118.77	120.94
2	C	501	PLP	C5A-C5-C4	-2.10	118.50	122.64
2	E	501	PLP	C5-C6-N1	-2.05	120.50	123.83
2	D	501	PLP	O2P-P-O4P	2.05	112.00	106.67
2	D	501	PLP	O4P-C5A-C5	2.04	113.18	109.36

There are no chirality outliers.

All (22) torsion outliers are listed below:

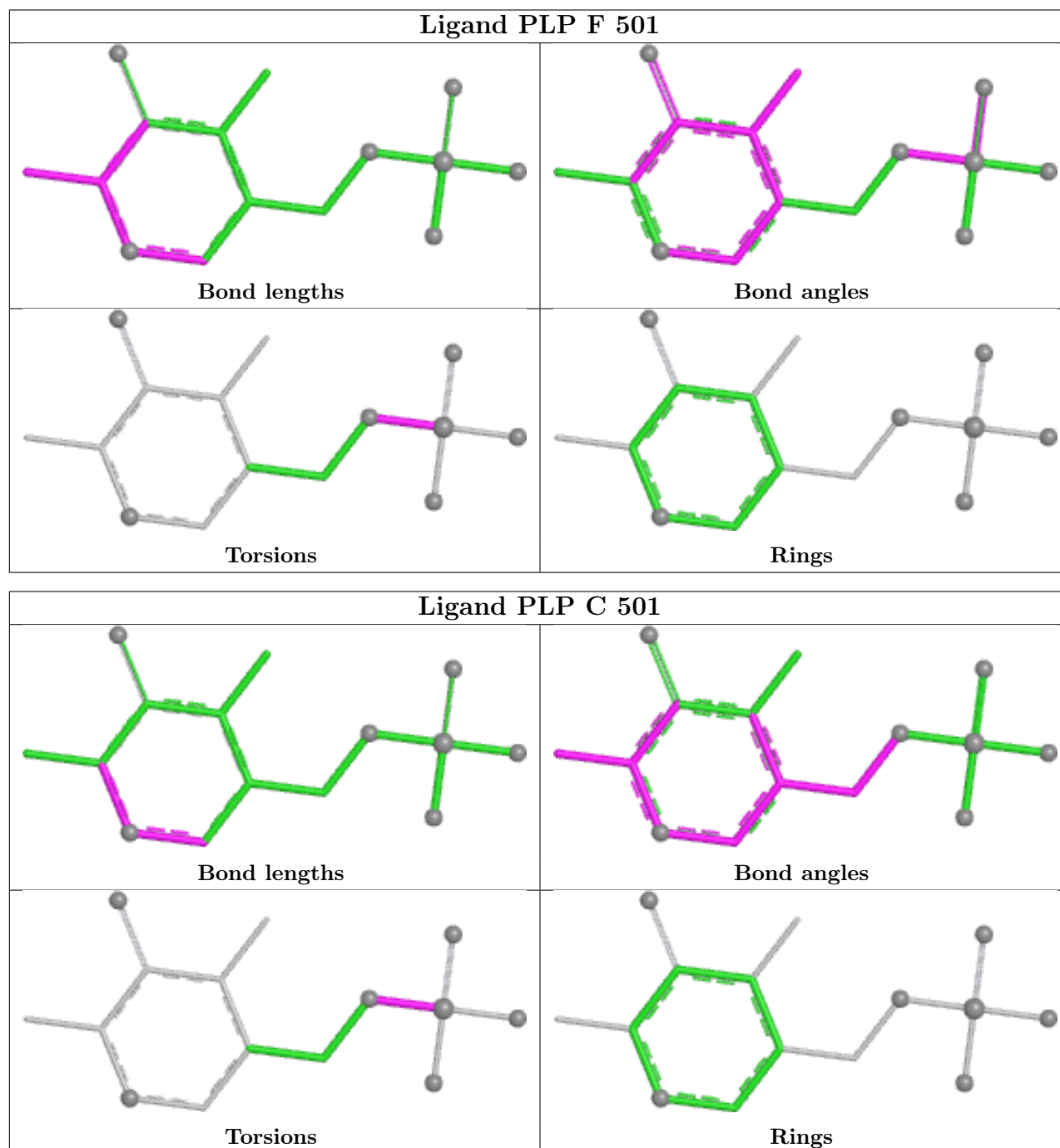
Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C5A-O4P-P-O1P
2	A	501	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C5A-O4P-P-O3P
2	B	501	PLP	C5A-O4P-P-O1P
2	B	501	PLP	C5A-O4P-P-O3P
2	C	501	PLP	C5A-O4P-P-O1P
2	C	501	PLP	C5A-O4P-P-O2P
2	C	501	PLP	C5A-O4P-P-O3P
2	D	501	PLP	C4-C5-C5A-O4P
2	F	501	PLP	C5A-O4P-P-O1P
2	F	501	PLP	C5A-O4P-P-O2P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

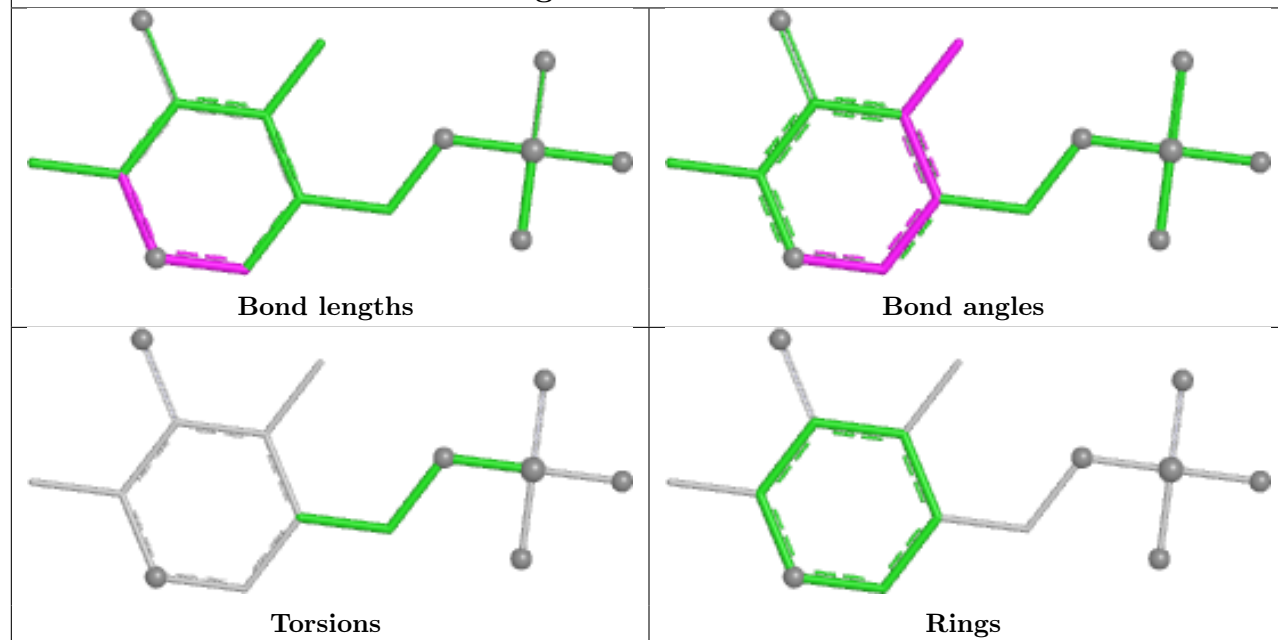
No monomer is involved in short contacts.

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

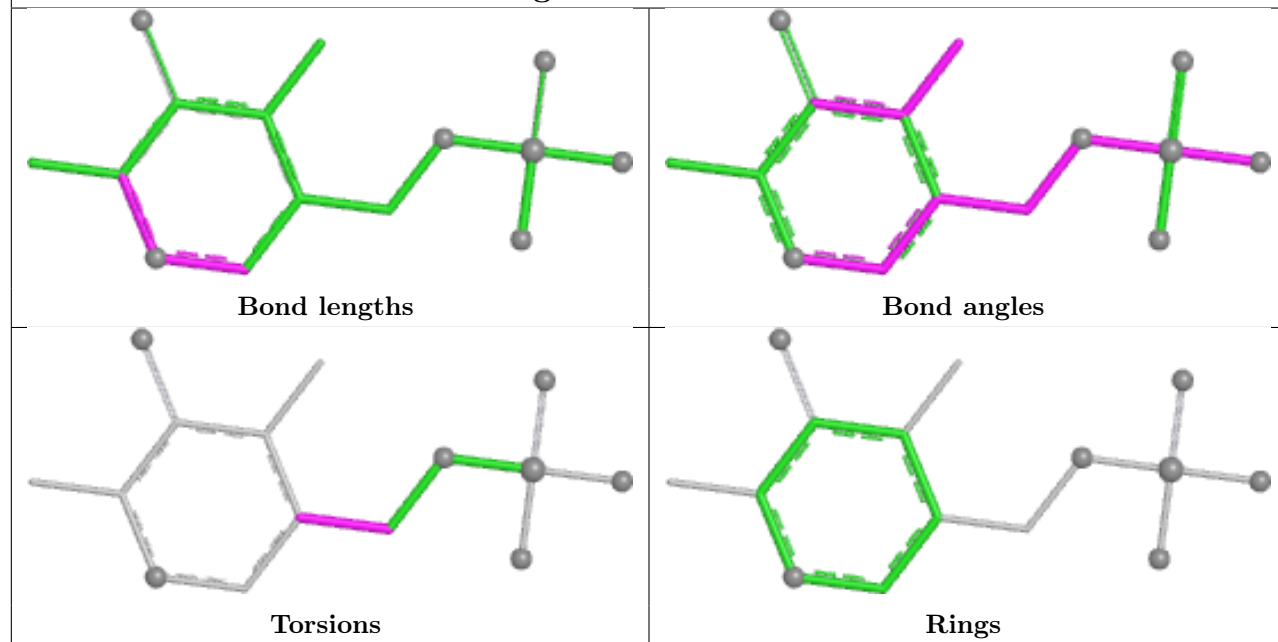
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



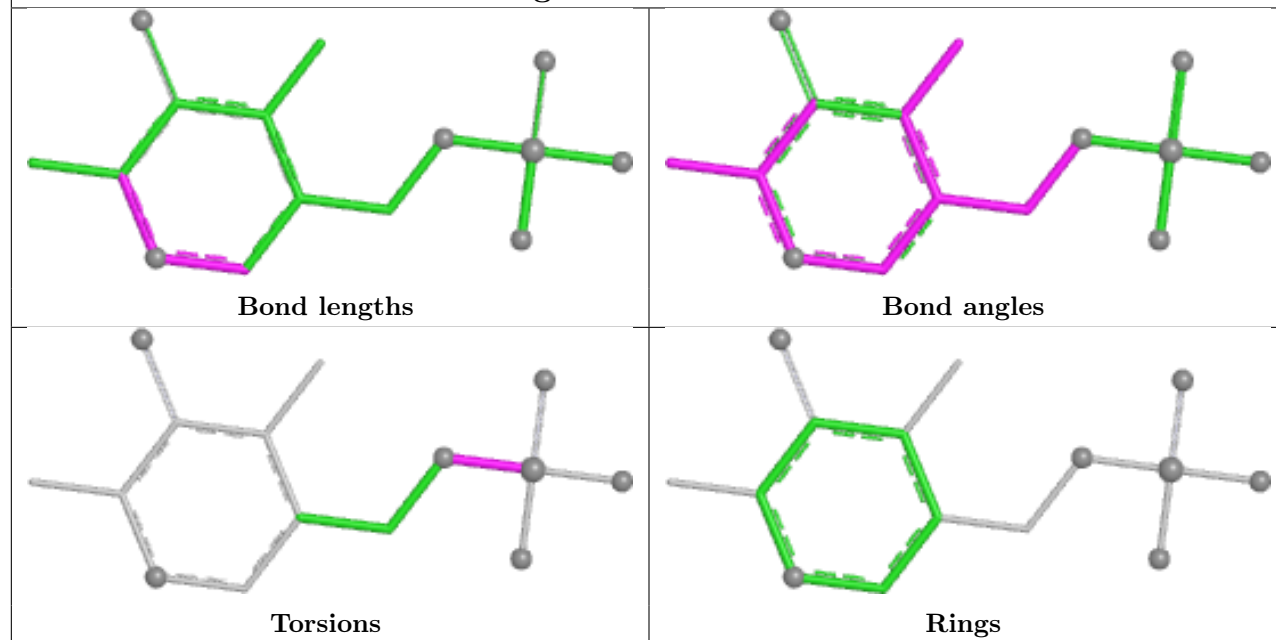
Ligand PLP E 501



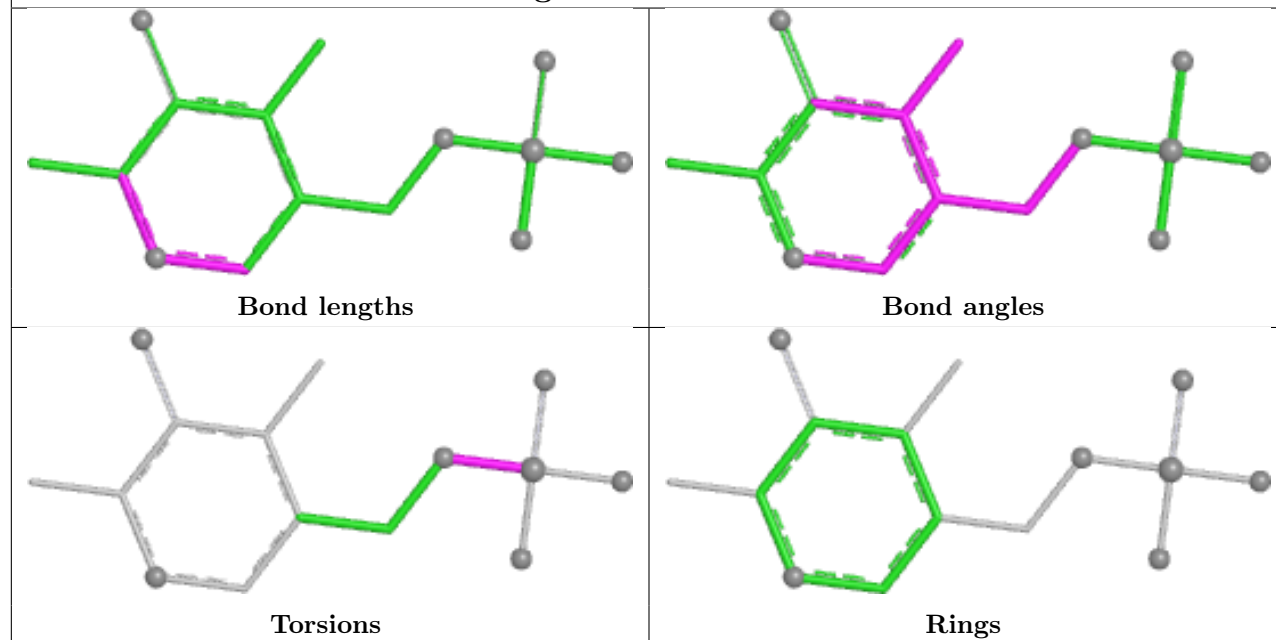
Ligand PLP D 501

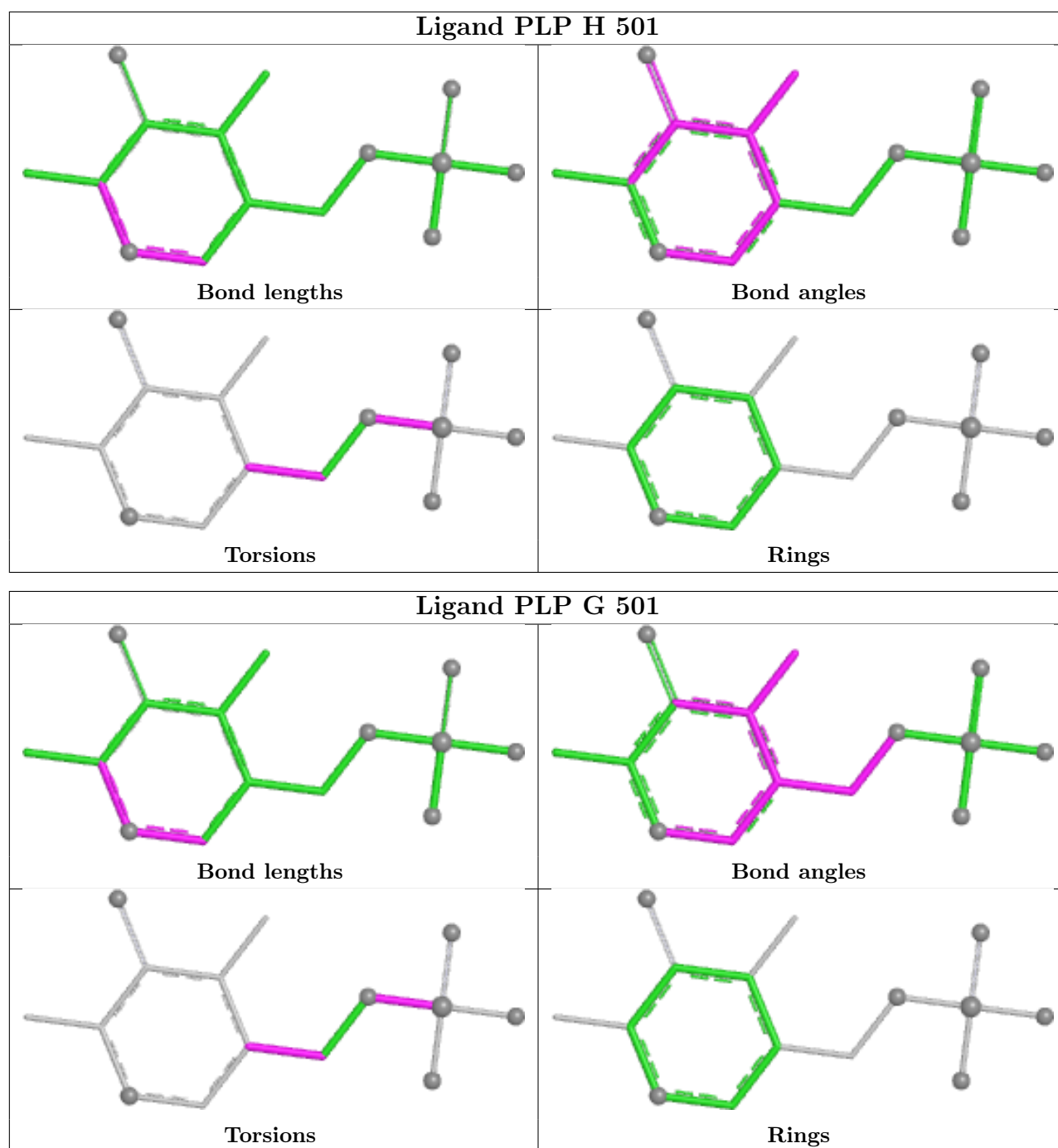


Ligand PLP A 501



Ligand PLP B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.25	0 100 100	46, 58, 84, 106	0
1	B	419/429 (97%)	-0.30	1 (0%) 91 92	42, 56, 84, 97	0
1	C	419/429 (97%)	-0.14	4 (0%) 79 80	48, 66, 97, 112	0
1	D	417/429 (97%)	-0.16	2 (0%) 87 88	46, 64, 98, 114	0
1	E	418/429 (97%)	-0.23	8 (1%) 66 67	42, 58, 94, 109	0
1	F	417/429 (97%)	-0.24	7 (1%) 69 71	30, 55, 92, 112	1 (0%)
1	G	422/429 (98%)	-0.25	1 (0%) 91 92	43, 58, 87, 99	0
1	H	417/429 (97%)	-0.29	1 (0%) 91 92	45, 58, 89, 107	0
All	All	3346/3432 (97%)	-0.23	24 (0%) 84 86	30, 59, 91, 114	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6	LEU	3.1
1	E	296	THR	3.0
1	H	5	ILE	2.8
1	F	5	ILE	2.7
1	C	20	PHE	2.6
1	C	17	SER	2.5
1	C	16	TYR	2.4
1	E	76	LEU	2.4
1	F	17	SER	2.4
1	E	16	TYR	2.4
1	B	6	LEU	2.3
1	E	288	TRP	2.3
1	E	15	THR	2.3
1	F	19	SER	2.3
1	C	421	GLY	2.3
1	F	20	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	16	TYR	2.2
1	D	6	LEU	2.2
1	D	288	TRP	2.2
1	E	6	LEU	2.1
1	E	20	PHE	2.1
1	E	297	PHE	2.1
1	G	293	TYR	2.1
1	F	15	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

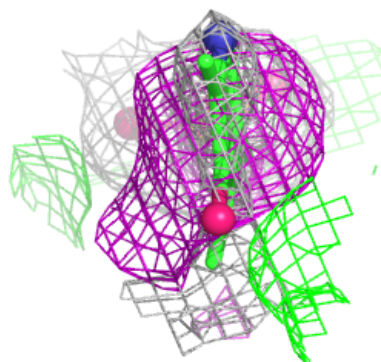
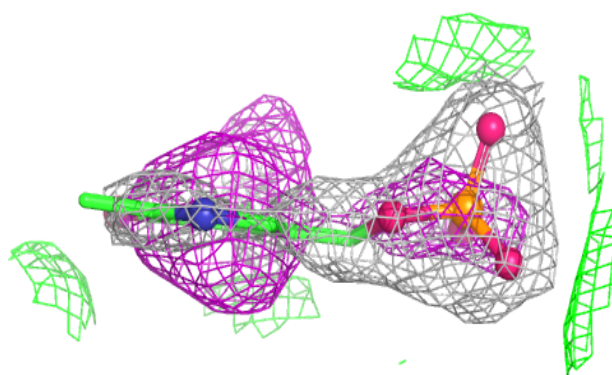
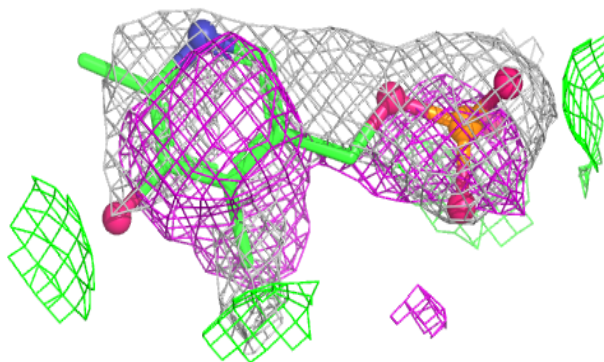
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	F	501	15/16	0.72	0.16	60,70,83,83	0
2	PLP	C	501	15/16	0.83	0.12	68,79,86,95	0
2	PLP	A	501	15/16	0.86	0.10	46,66,73,80	0
2	PLP	E	501	15/16	0.88	0.11	61,66,77,78	0
2	PLP	D	501	15/16	0.89	0.10	62,73,86,87	0
2	PLP	G	501	15/16	0.89	0.09	53,60,68,71	0
2	PLP	H	501	15/16	0.90	0.11	57,66,82,86	0
2	PLP	B	501	15/16	0.92	0.09	56,68,70,72	0

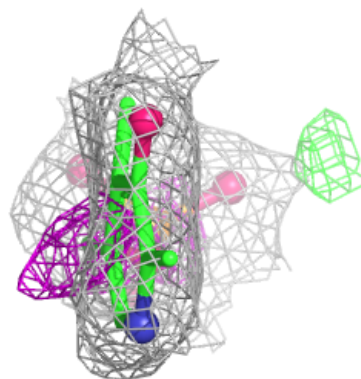
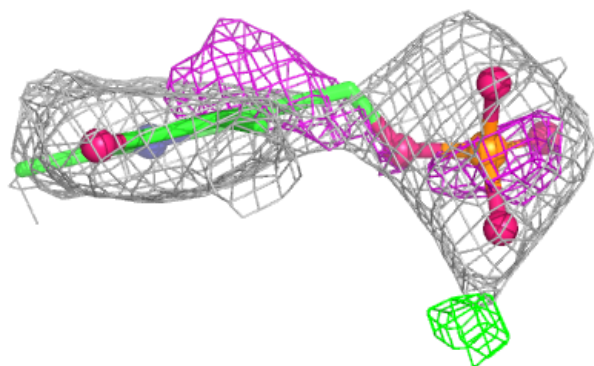
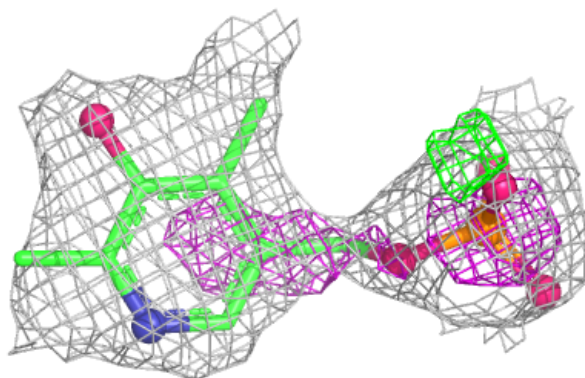
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

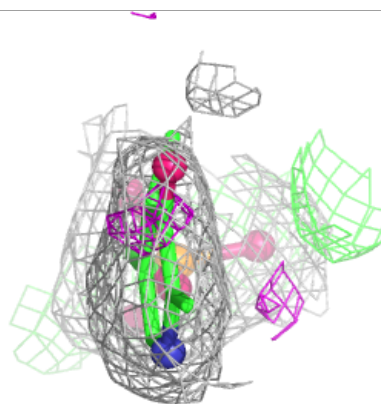
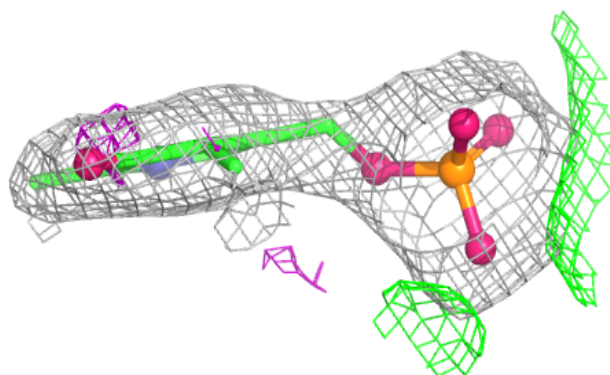
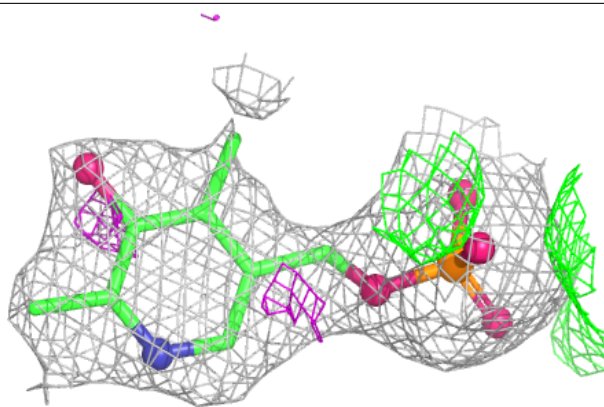
**Electron density around PLP C 501:**

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

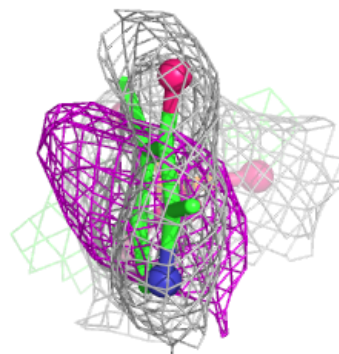
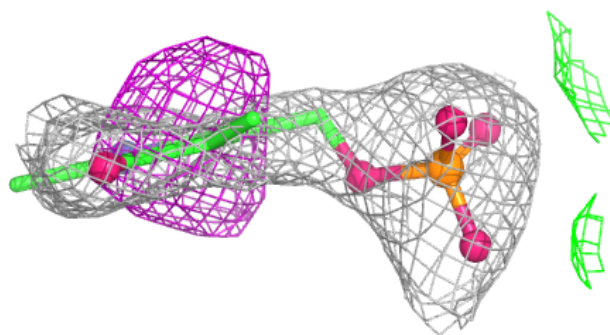
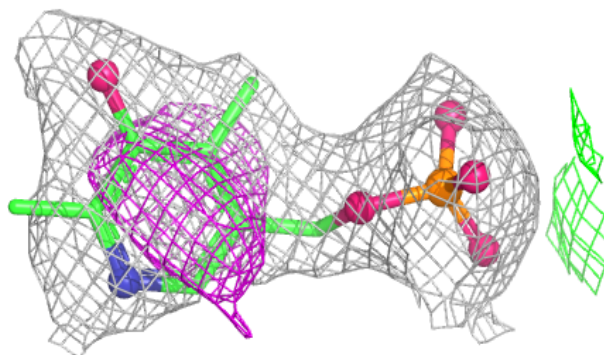


Electron density around PLP A 501:

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

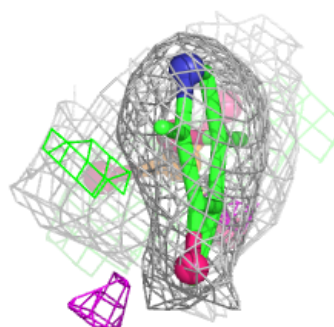
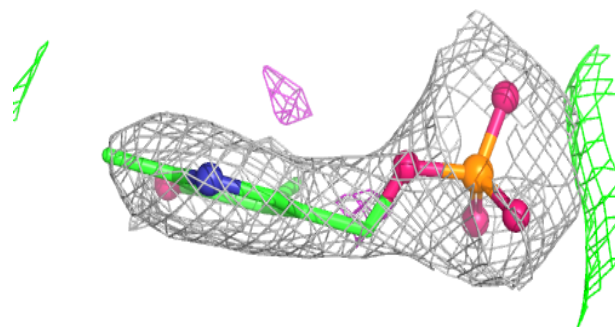
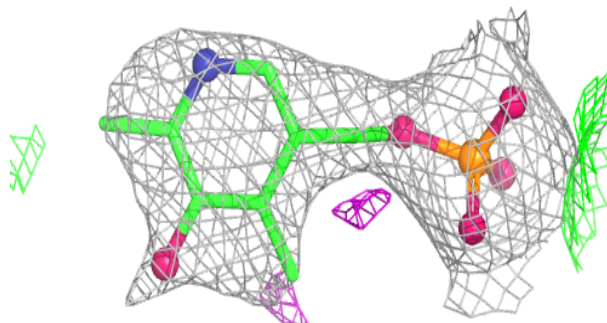
**Electron density around PLP E 501:**

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

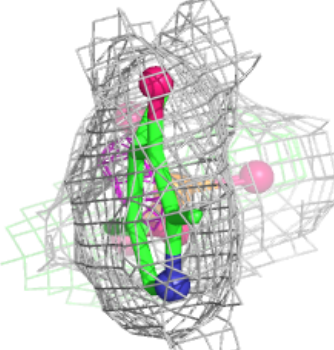
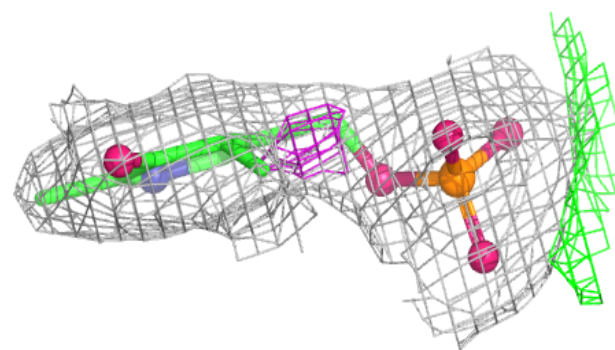
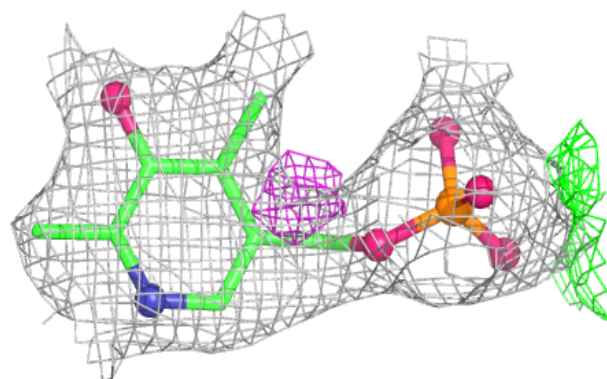


Electron density around PLP D 501:

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

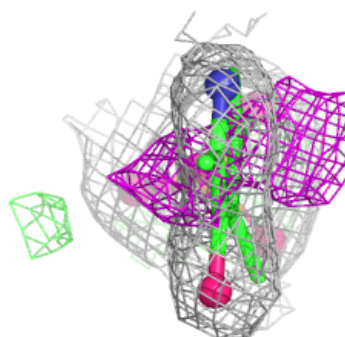
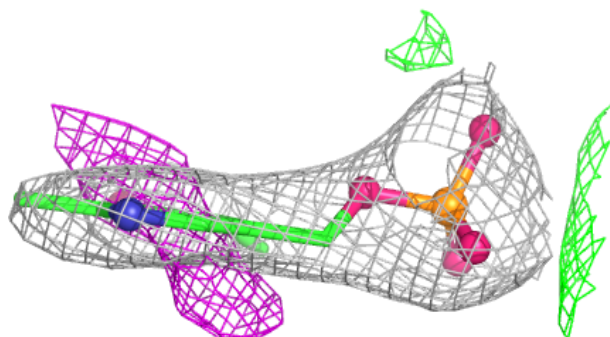
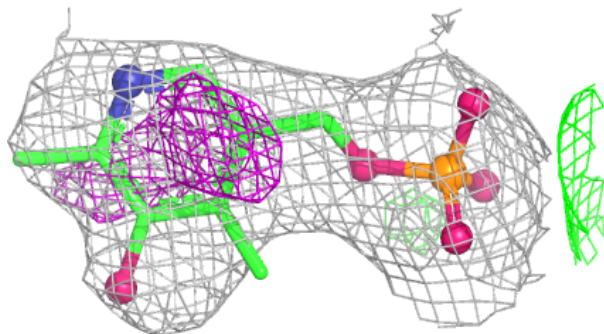
**Electron density around PLP G 501:**

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

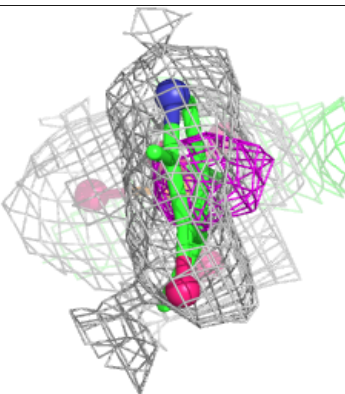
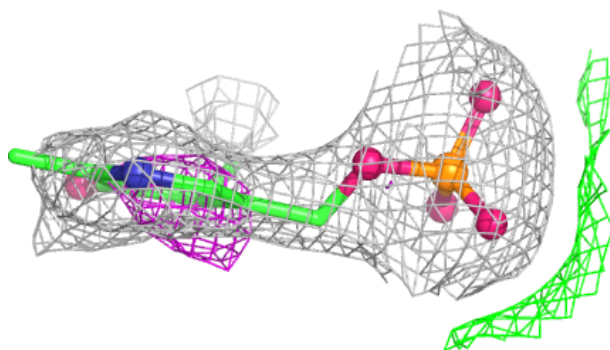
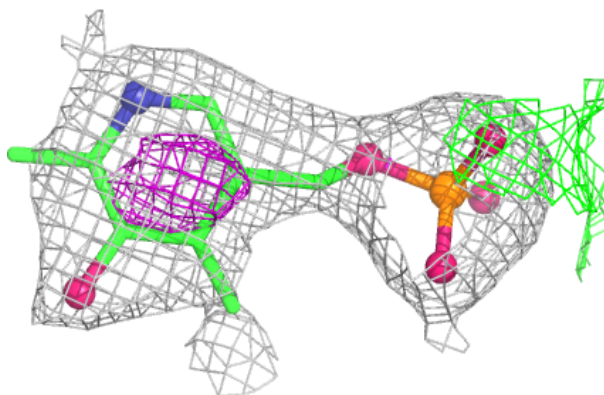


Electron density around PLP H 501:

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

**Electron density around PLP 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.