Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 03:45 PM JST

PDB ID	:	7CWZ
Title	:	Crystal structure of a tyrosine decarboxylase from Enterococcus faecalis K392A mutant in complex with the cofactor PLP and L-dopa
Authors	:	Yu, X.; Gong, M.; Huang, J.; Liu, W.; Chen, C.; Guo, R.
Deposited on	:	2020-09-01
Resolution	:	2.97 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:

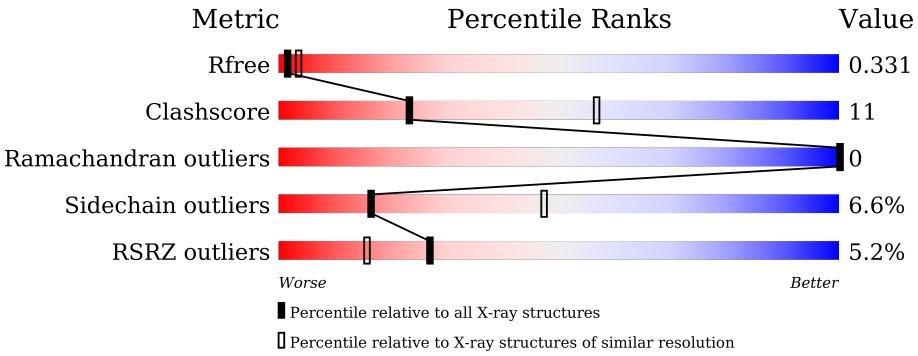
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	620	5% 73% 22%
1	B	620	5% 72% 23%
1	C	620	5% 71% 23% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LDP	A	703	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14274 atoms, of which 51 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 Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4711	3008	780	902	21			
1	B	601	Total	C	N	O	S	0	0	0
			4748	3032	786	909	21			
1	C	592	Total	C	N	O	S	0	0	0
			4628	2957	766	886	19			

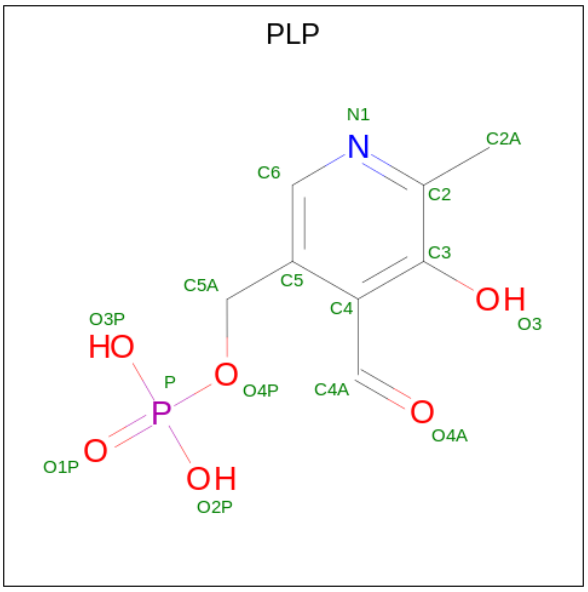
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LYS	GLU	conflict	UNP Q8KXD2
A	392	ALA	LYS	engineered mutation	UNP Q8KXD2
B	62	LYS	GLU	conflict	UNP Q8KXD2
B	392	ALA	LYS	engineered mutation	UNP Q8KXD2
C	62	LYS	GLU	conflict	UNP Q8KXD2
C	392	ALA	LYS	engineered mutation	UNP Q8KXD2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

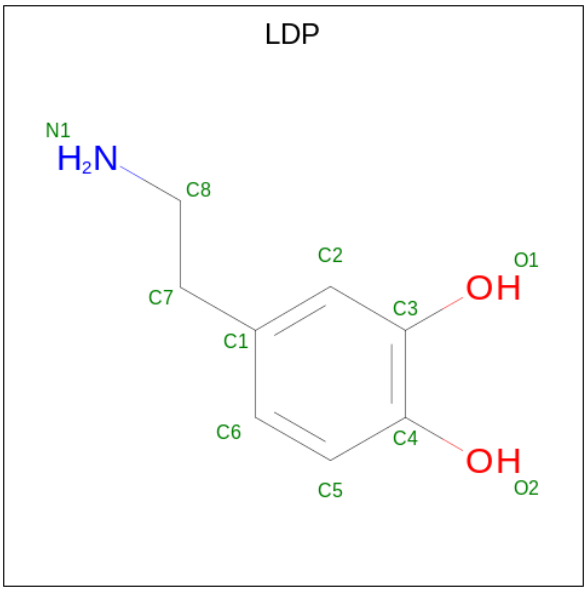
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			23	8	8	1	5	1		
3	B	1	Total	C	H	N	O	P	0	0
			23	8	8	1	5	1		
3	C	1	Total	C	H	N	O	P	0	0
			23	8	8	1	5	1		

- Molecule 4 is L-DOPAMINE (three-letter code: LDP) (formula: $C_8H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			20	8	9	1	2		
4	B	1	Total	C	H	N	O	0	0
			20	8	9	1	2		
4	C	1	Total	C	H	N	O	0	0
			20	8	9	1	2		

- Molecule 5 is water.

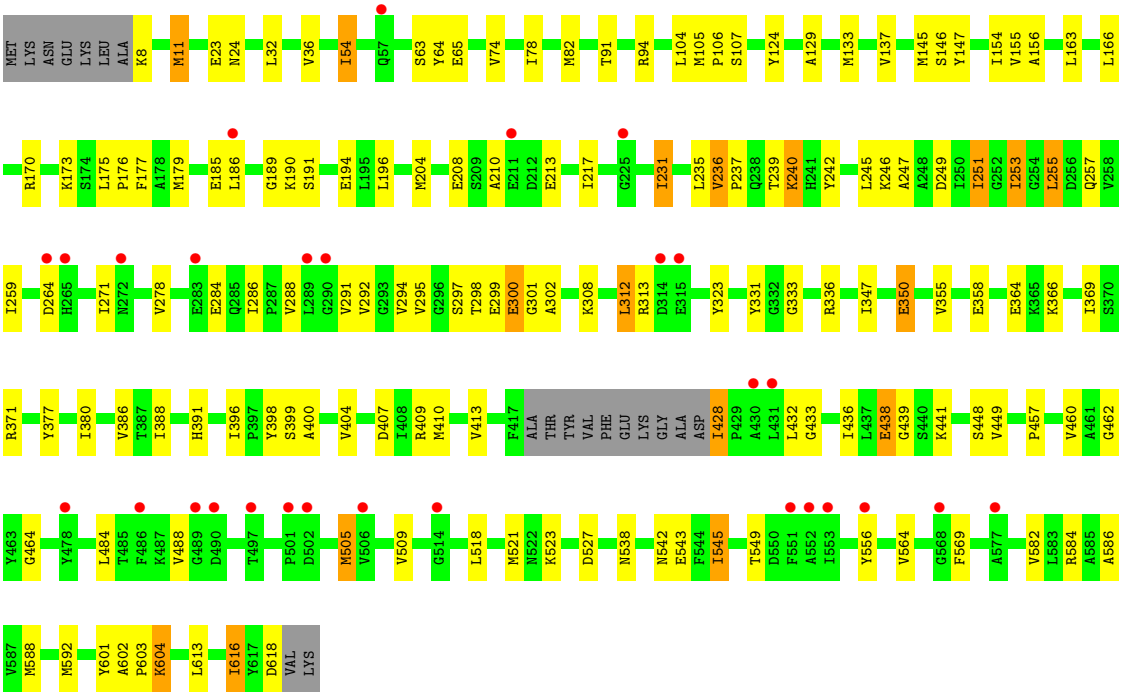
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	18	Total	O	0	0
			18	18		
5	C	21	Total	O	0	0
			21	21		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

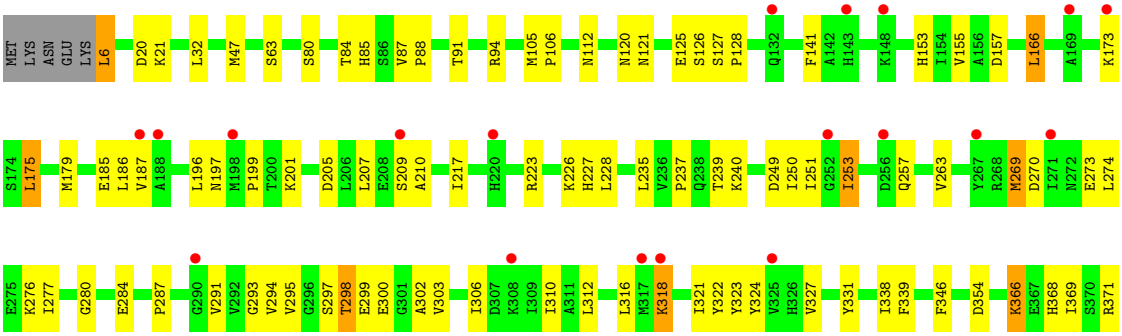
• Molecule 1: Decarboxylase

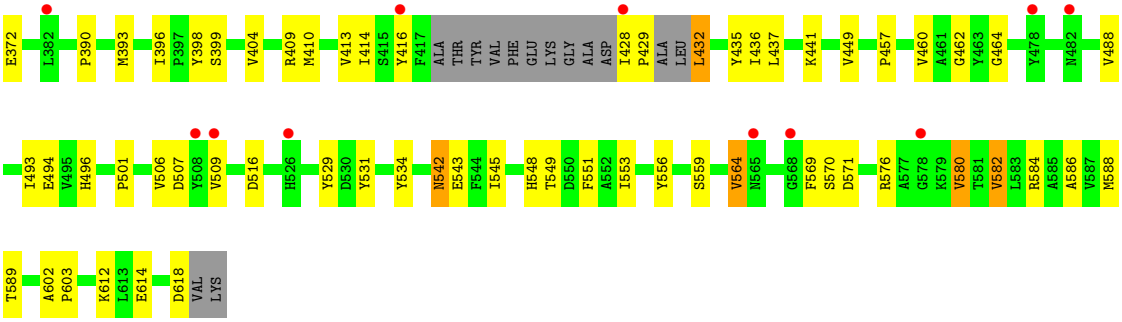
Chain A:



• Molecule 1: Decarboxylase

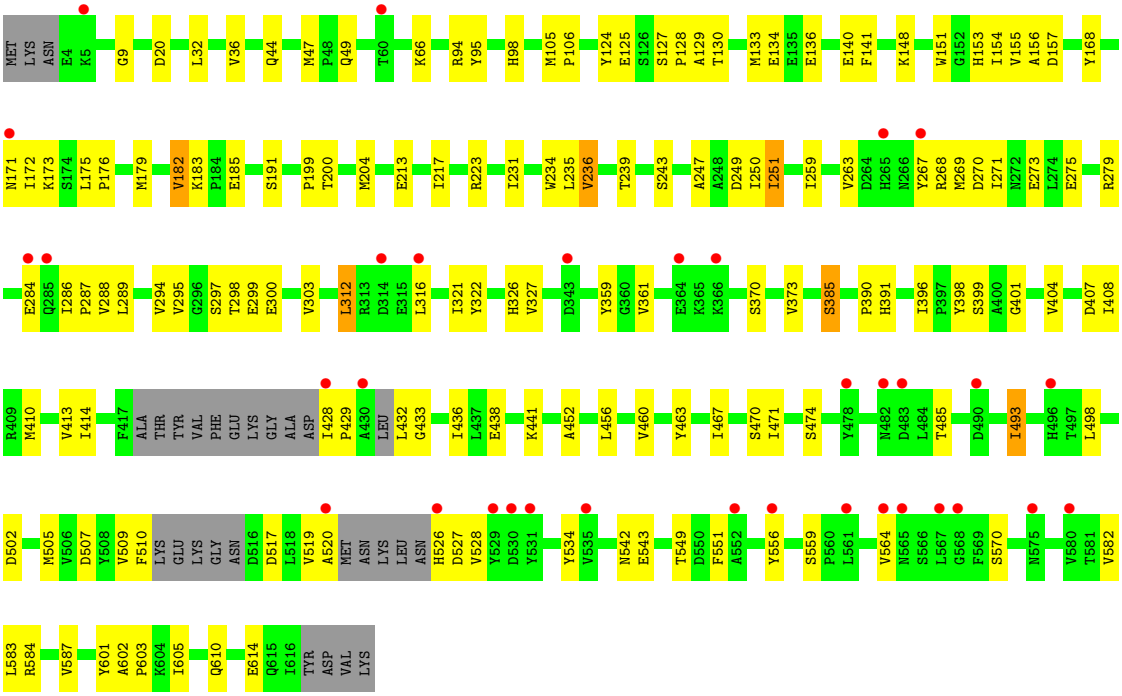
Chain B:





• Molecule 1: Decarboxylase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	133.31Å 133.31Å 390.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.85 – 2.97 24.85 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.1 (24.85-2.97) 98.1 (24.85-2.97)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.99Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.243 , 0.293 0.254 , 0.331	Depositor DCC
R_{free} test set	640 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14274	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.46	0/4829	0.70	0/6564
1	B	0.49	0/4864	0.72	0/6602
1	C	0.44	0/4742	0.65	0/6447
All	All	0.47	0/14435	0.69	0/19613

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4711	0	4465	113	0
1	B	4748	0	4547	91	0
1	C	4628	0	4377	124	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	8	7	0	0
3	B	15	8	7	1	0
3	C	15	8	7	1	0
4	A	11	9	9	0	0
4	B	11	9	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	11	9	10	0	0
5	A	17	0	0	0	0
5	B	18	0	0	0	0
5	C	21	0	0	0	0
All	All	14223	51	13439	313	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 11.

All (313) 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:C:199:PRO:HA	1:C:322:TYR:CE2	1.95	1.00
1:A:333:GLY:HA3	1:A:388:ILE:HG13	1.51	0.93
1:C:151:TRP:HB2	1:C:408:ILE:HG13	1.53	0.91
1:A:295:VAL:HG21	1:A:380:ILE:HD11	1.54	0.90
1:B:297:SER:HB3	1:B:302:ALA:H	1.36	0.90
1:B:564:VAL:HG13	1:B:569:PHE:HB2	1.55	0.88
1:A:235:LEU:HB2	1:A:291:VAL:HG12	1.55	0.86
1:A:410:MET:O	1:A:413:VAL:HG22	1.78	0.84
1:C:199:PRO:HA	1:C:322:TYR:CD2	2.14	0.83
1:C:235:LEU:HD23	1:C:288:VAL:HG13	1.61	0.82
1:A:166:LEU:HD22	1:A:251:ILE:HG21	1.60	0.82
1:C:172:ILE:HA	1:C:175:LEU:HD23	1.61	0.82
1:B:85:HIS:HB3	1:C:128:PRO:HB2	1.63	0.80
1:B:80:SER:O	1:B:84:THR:HG23	1.83	0.79
1:A:433:GLY:HA2	1:A:436:ILE:HG12	1.64	0.79
1:C:239:THR:HG23	1:C:263:VAL:HG11	1.63	0.77
1:C:407:ASP:HB3	1:C:410:MET:HG3	1.66	0.77
1:B:270:ASP:HB3	1:B:273:GLU:HB2	1.66	0.77
1:C:551:PHE:HD1	1:C:556:TYR:CE2	2.02	0.76
1:A:407:ASP:HB3	1:A:410:MET:HG3	1.67	0.75
1:A:231:ILE:HD11	1:A:253:ILE:HD11	1.67	0.75
1:C:433:GLY:HA2	1:C:436:ILE:HD11	1.69	0.74
1:A:190:LYS:HD2	1:A:190:LYS:N	2.03	0.72
1:C:239:THR:HG22	1:C:556:TYR:HE1	1.54	0.72
1:C:299:GLU:HG2	1:C:549:THR:CB	2.19	0.72
1:C:299:GLU:HA	1:C:584:ARG:HD2	1.73	0.71
1:A:364:GLU:HG2	1:A:366:LYS:HG3	1.73	0.70
1:C:551:PHE:CD1	1:C:556:TYR:CE2	2.80	0.70
1:A:237:PRO:HG2	1:A:294:VAL:HG23	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:HG22	1:B:556:TYR:HE1	1.58	0.69
1:C:295:VAL:HG13	1:C:303:VAL:HG13	1.75	0.69
1:A:284:GLU:HB3	1:A:286:ILE:HD12	1.74	0.69
1:C:326:HIS:ND1	1:C:385:SER:HB3	2.07	0.69
1:A:237:PRO:HD3	1:A:292:VAL:CG2	2.22	0.68
1:A:213:GLU:O	1:A:217:ILE:HG13	1.94	0.68
1:C:270:ASP:HB3	1:C:273:GLU:HB2	1.74	0.67
1:B:494:GLU:HG3	1:B:496:HIS:NE2	2.09	0.67
1:B:488:VAL:CG2	1:B:493:ILE:HD13	2.24	0.67
1:C:204:MET:HE3	1:C:204:MET:HA	1.76	0.66
1:B:235:LEU:HB2	1:B:291:VAL:HG22	1.79	0.65
1:C:129:ALA:O	1:C:133:MET:HG3	1.97	0.64
1:C:173:LYS:O	1:C:176:PRO:HD2	1.98	0.63
1:A:32:LEU:O	1:A:36:VAL:HG23	1.98	0.63
1:A:236:VAL:HA	1:A:292:VAL:HG22	1.79	0.63
1:C:299:GLU:HG2	1:C:549:THR:OG1	1.99	0.63
1:C:127:SER:HB2	1:C:130:THR:OG1	1.99	0.63
1:A:407:ASP:O	1:A:410:MET:HG3	1.98	0.63
1:C:141:PHE:HB3	1:C:404:VAL:HG22	1.81	0.63
1:B:295:VAL:HG13	1:B:303:VAL:HG13	1.81	0.62
1:C:267:TYR:OH	1:C:498:LEU:HD11	1.99	0.62
1:A:396:ILE:HD13	1:A:449:VAL:HG22	1.80	0.62
1:A:189:GLY:C	1:A:190:LYS:HD2	2.21	0.62
1:B:94:ARG:NH1	1:B:543:GLU:HB3	2.15	0.62
1:C:98:HIS:CD2	1:C:584:ARG:HH21	2.18	0.61
1:A:284:GLU:HB3	1:A:286:ILE:CD1	2.29	0.61
1:C:300:GLU:N	1:C:300:GLU:OE1	2.33	0.61
1:C:493:ILE:HD11	1:C:510:PHE:HB3	1.82	0.61
1:A:104:LEU:HB3	1:A:106:PRO:HD2	1.83	0.61
1:A:386:VAL:HB	1:A:404:VAL:CG1	2.30	0.61
1:C:298:THR:O	1:C:584:ARG:NH1	2.34	0.61
1:B:602:ALA:HB3	1:B:603:PRO:HD3	1.83	0.60
1:C:153:HIS:CE1	1:C:436:ILE:HG22	2.36	0.60
1:A:407:ASP:HB3	1:A:410:MET:CG	2.30	0.60
1:B:457:PRO:HD2	1:B:462:GLY:HA3	1.83	0.60
1:C:98:HIS:HD2	1:C:584:ARG:HH21	1.47	0.60
1:C:124:TYR:CD2	1:C:428:ILE:HD11	2.36	0.60
1:A:163:LEU:HD13	1:A:247:ALA:HA	1.84	0.59
1:B:413:VAL:HG23	1:B:414:ILE:HG23	1.83	0.59
1:B:488:VAL:HG23	1:B:493:ILE:HD13	1.84	0.59
1:B:551:PHE:HB2	1:B:580:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASP:HB3	1:A:616:ILE:HG21	1.84	0.59
1:C:361:VAL:HG21	1:C:460:VAL:CG2	2.32	0.59
1:B:460:VAL:HA	1:B:464:GLY:HA3	1.83	0.59
1:A:564:VAL:HG13	1:A:569:PHE:HB2	1.83	0.59
1:B:250:ILE:O	1:C:251:ILE:HA	2.04	0.58
1:B:186:LEU:HD11	1:B:210:ALA:HB2	1.84	0.58
1:C:151:TRP:CB	1:C:408:ILE:HG13	2.31	0.58
1:A:237:PRO:HD3	1:A:292:VAL:HG22	1.85	0.57
1:C:299:GLU:HG2	1:C:549:THR:HB	1.86	0.57
1:A:24:ASN:N	1:A:24:ASN:HD22	2.01	0.57
1:A:24:ASN:N	1:A:24:ASN:ND2	2.51	0.57
1:A:240:LYS:HE2	1:A:245:LEU:HD21	1.85	0.57
1:A:204:MET:HB2	1:A:409:ARG:NH2	2.20	0.56
1:C:429:PRO:HB2	1:C:432:LEU:N	2.21	0.56
1:A:154:ILE:O	1:A:441:LYS:HE2	2.06	0.56
1:C:316:LEU:HB3	1:C:321:ILE:HB	1.88	0.55
1:C:520:ALA:HA	1:C:526:HIS:HD2	1.71	0.55
1:C:433:GLY:HA2	1:C:436:ILE:CD1	2.37	0.55
1:A:208:GLU:HG3	1:A:409:ARG:HD2	1.89	0.55
1:B:153:HIS:CE1	1:B:155:VAL:HG22	2.42	0.55
1:B:410:MET:O	1:B:413:VAL:HG22	2.06	0.54
1:C:303:VAL:HG23	1:C:502:ASP:HB3	1.89	0.54
1:A:129:ALA:O	1:A:133:MET:HG3	2.06	0.54
1:B:157:ASP:HB2	3:B:702:PLP:O3P	2.07	0.54
1:C:610:GLN:O	1:C:614:GLU:HG2	2.08	0.54
1:A:278:VAL:HG13	1:A:288:VAL:HG21	1.88	0.54
1:B:396:ILE:HD13	1:B:449:VAL:HG22	1.90	0.54
1:C:297:SER:OG	1:C:300:GLU:HG2	2.07	0.54
1:C:173:LYS:HD2	1:C:289:LEU:HA	1.89	0.53
1:C:520:ALA:HA	1:C:526:HIS:CD2	2.43	0.53
1:C:410:MET:O	1:C:413:VAL:HG22	2.08	0.53
1:C:601:TYR:O	1:C:605:ILE:HG12	2.08	0.53
1:C:9:GLY:HA2	1:C:359:TYR:O	2.08	0.53
1:C:200:THR:N	1:C:322:TYR:CE2	2.75	0.53
1:A:237:PRO:HD3	1:A:292:VAL:HG23	1.91	0.53
1:A:391:HIS:ND1	1:A:400:ALA:O	2.42	0.53
1:C:94:ARG:NH1	1:C:543:GLU:HB3	2.24	0.53
1:A:239:THR:HG22	1:A:556:TYR:CE2	2.44	0.53
1:B:91:THR:HG21	1:B:94:ARG:HB2	1.90	0.52
1:C:470:SER:HB2	1:C:587:VAL:O	2.08	0.52
1:B:253:ILE:HG13	1:B:253:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HB2	1:A:323:TYR:CE1	2.44	0.52
1:A:592:MET:HE1	1:A:601:TYR:HB2	1.91	0.51
1:C:134:GLU:OE2	1:C:441:LYS:NZ	2.43	0.51
1:A:186:LEU:HD11	1:A:210:ALA:HB2	1.91	0.51
1:B:239:THR:HG23	1:B:263:VAL:HG11	1.92	0.51
1:A:297:SER:HB2	1:A:302:ALA:H	1.76	0.51
1:B:105:MET:N	1:B:106:PRO:HD2	2.26	0.51
1:B:94:ARG:HH12	1:B:543:GLU:HB3	1.74	0.50
1:C:124:TYR:CE2	1:C:428:ILE:HD11	2.45	0.50
1:C:200:THR:N	1:C:322:TYR:HE2	2.09	0.50
1:A:299:GLU:HA	1:A:584:ARG:HD2	1.93	0.50
1:A:191:SER:OG	1:A:194:GLU:HG3	2.12	0.50
1:C:200:THR:H	1:C:322:TYR:HE2	1.59	0.50
1:A:457:PRO:HD2	1:A:462:GLY:HA3	1.93	0.50
1:A:91:THR:HG23	1:A:94:ARG:H	1.77	0.50
1:A:147:TYR:HE2	1:A:404:VAL:HG22	1.77	0.50
1:A:133:MET:O	1:A:137:VAL:HG23	2.12	0.49
1:A:23:GLU:C	1:A:24:ASN:HD22	2.15	0.49
1:A:488:VAL:HG21	1:A:613:LEU:HB3	1.93	0.49
1:B:196:LEU:HD13	1:B:287:PRO:HG2	1.94	0.49
1:A:301:GLY:HA3	1:A:505:MET:HB3	1.94	0.49
1:A:235:LEU:CB	1:A:291:VAL:HG12	2.35	0.49
1:B:141:PHE:HB3	1:B:404:VAL:HG22	1.95	0.49
1:A:331:TYR:OH	1:A:586:ALA:HB1	2.13	0.49
1:C:127:SER:N	1:C:128:PRO:HD3	2.28	0.49
1:C:173:LYS:HE3	1:C:288:VAL:O	2.13	0.49
1:C:361:VAL:HG21	1:C:460:VAL:HG23	1.94	0.49
1:A:336:ARG:HB2	1:A:377:TYR:HD2	1.78	0.49
1:A:391:HIS:HA	1:A:396:ILE:O	2.12	0.49
1:A:177:PHE:CZ	1:A:196:LEU:HD11	2.48	0.49
1:B:127:SER:N	1:B:128:PRO:HD3	2.28	0.49
1:B:493:ILE:N	1:B:493:ILE:HD12	2.27	0.49
1:A:190:LYS:N	1:A:190:LYS:CD	2.75	0.48
1:B:237:PRO:O	1:B:240:LYS:HB3	2.13	0.48
1:B:249:ASP:OD2	1:C:223:ARG:HG2	2.13	0.48
1:C:95:TYR:OH	1:C:98:HIS:HB2	2.13	0.48
1:C:32:LEU:O	1:C:36:VAL:HG23	2.13	0.48
1:C:370:SER:OG	1:C:373:VAL:HG22	2.14	0.48
1:B:85:HIS:HB2	1:C:129:ALA:HB2	1.94	0.48
1:C:171:ASN:O	1:C:175:LEU:HD22	2.14	0.48
1:C:243:SER:O	1:C:247:ALA:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:H	1:A:350:GLU:HG3	1.34	0.48
1:C:98:HIS:HD2	1:C:584:ARG:NH2	2.11	0.48
1:C:105:MET:N	1:C:106:PRO:HD2	2.29	0.48
1:B:125:GLU:HG2	1:C:534:TYR:HE1	1.79	0.48
1:C:235:LEU:CD1	1:C:259:ILE:HB	2.44	0.48
1:B:179:MET:HG2	1:B:217:ILE:HD13	1.95	0.47
1:C:271:ILE:HG22	1:C:312:LEU:HD13	1.95	0.47
1:C:157:ASP:HB2	3:C:701:PLP:O2P	2.14	0.47
1:C:391:HIS:HA	1:C:396:ILE:O	2.14	0.47
1:A:146:SER:HB2	1:A:336:ARG:NH2	2.30	0.47
1:A:179:MET:HG2	1:A:217:ILE:HG21	1.95	0.47
1:B:390:PRO:HB3	1:B:396:ILE:HD12	1.95	0.47
1:C:509:VAL:CG1	1:C:582:VAL:HG12	2.45	0.47
1:B:251:ILE:HD12	1:C:250:ILE:HG23	1.97	0.47
1:B:306:ILE:HD12	1:B:327:VAL:HG22	1.97	0.47
1:A:170:ARG:HD3	1:A:251:ILE:HG13	1.95	0.47
1:A:601:TYR:HA	1:A:604:LYS:HD2	1.96	0.47
1:B:121:ASN:HA	1:B:127:SER:OG	2.15	0.47
1:A:602:ALA:N	1:A:603:PRO:HD2	2.29	0.47
1:C:213:GLU:O	1:C:217:ILE:HG13	2.15	0.47
1:B:393:MET:SD	1:B:588:MET:HG2	2.55	0.47
1:C:171:ASN:O	1:C:175:LEU:CD2	2.63	0.47
1:C:526:HIS:HB2	1:C:528:VAL:HG23	1.96	0.47
1:C:614:GLU:O	1:C:614:GLU:HG3	2.15	0.47
1:A:336:ARG:HB2	1:A:377:TYR:CD2	2.50	0.47
1:B:205:ASP:HA	1:B:409:ARG:HH12	1.80	0.47
1:C:551:PHE:CE2	1:C:582:VAL:HG21	2.50	0.47
1:A:146:SER:OG	1:A:336:ARG:NH2	2.48	0.46
1:C:295:VAL:HG23	1:C:327:VAL:HG13	1.97	0.46
1:C:467:ILE:O	1:C:471:ILE:HG13	2.15	0.46
1:B:175:LEU:HD13	1:B:175:LEU:HA	1.78	0.46
1:B:273:GLU:O	1:B:277:ILE:HG12	2.15	0.46
1:C:303:VAL:HB	1:C:373:VAL:HG12	1.97	0.46
1:C:551:PHE:HD1	1:C:556:TYR:HE2	1.57	0.46
1:B:488:VAL:HG13	1:B:614:GLU:HG2	1.98	0.46
1:A:155:VAL:CG1	1:A:156:ALA:N	2.79	0.46
1:A:331:TYR:HE1	1:A:588:MET:CE	2.29	0.46
1:A:347:ILE:HD13	1:A:355:VAL:HG11	1.98	0.46
1:A:235:LEU:HD23	1:A:259:ILE:HB	1.97	0.46
1:A:391:HIS:CD2	1:A:398:TYR:CE1	3.03	0.46
1:A:124:TYR:CD1	1:A:428:ILE:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:CE2	1:A:404:VAL:HG22	2.50	0.46
1:A:333:GLY:C	1:A:388:ILE:HD11	2.37	0.46
1:A:54:ILE:H	1:A:54:ILE:HG12	1.63	0.45
1:A:185:GLU:OE2	1:A:185:GLU:N	2.37	0.45
1:B:339:PHE:CZ	1:B:369:ILE:HG21	2.52	0.45
1:A:146:SER:CB	1:A:336:ARG:NH2	2.80	0.45
1:B:318:LYS:HE2	1:B:318:LYS:HB3	1.82	0.45
1:B:428:ILE:HA	1:B:429:PRO:HD2	1.82	0.45
1:A:391:HIS:CD2	1:A:398:TYR:HE1	2.34	0.45
1:C:154:ILE:O	1:C:441:LYS:NZ	2.44	0.45
1:C:20:ASP:OD1	1:C:20:ASP:N	2.50	0.45
1:A:11:MET:HE2	1:A:11:MET:HB2	1.72	0.45
1:C:498:LEU:HD13	1:C:582:VAL:HG11	1.98	0.45
1:A:91:THR:HG21	1:A:94:ARG:HB2	1.97	0.45
1:C:433:GLY:HA2	1:C:436:ILE:CG1	2.47	0.45
1:B:251:ILE:HA	1:C:250:ILE:O	2.17	0.45
1:B:269:MET:HE1	1:B:274:LEU:HD22	1.99	0.45
1:C:300:GLU:HA	1:C:507:ASP:OD2	2.16	0.45
1:A:163:LEU:CD1	1:A:247:ALA:HA	2.48	0.44
1:B:120:ASN:HB3	1:B:126:SER:OG	2.17	0.44
1:B:293:GLY:HA3	1:B:306:ILE:CD1	2.48	0.44
1:B:299:GLU:HA	1:B:584:ARG:HD2	1.99	0.44
1:A:235:LEU:CD2	1:A:259:ILE:HB	2.48	0.44
1:B:21:LYS:HD3	1:C:44:GLN:HA	2.00	0.44
1:A:355:VAL:HA	1:A:358:GLU:HG2	1.98	0.44
1:C:432:LEU:O	1:C:436:ILE:HG12	2.18	0.44
1:A:297:SER:HB2	1:A:300:GLU:HG2	1.99	0.44
1:A:175:LEU:O	1:A:179:MET:HG3	2.17	0.44
1:C:148:LYS:HD3	1:C:148:LYS:HA	1.79	0.44
1:C:200:THR:O	1:C:204:MET:HG2	2.18	0.44
1:C:168:TYR:CZ	1:C:414:ILE:HD11	2.53	0.44
1:A:204:MET:HB2	1:A:409:ARG:HH21	1.83	0.43
1:B:20:ASP:OD1	1:B:20:ASP:N	2.51	0.43
1:A:249:ASP:HB2	1:A:255:LEU:HD12	1.99	0.43
1:C:474:SER:HA	1:C:587:VAL:HG21	1.99	0.43
1:C:47:MET:SD	1:C:49:GLN:NE2	2.91	0.43
1:B:157:ASP:OD2	1:C:438:GLU:HB2	2.18	0.43
1:B:580:VAL:HG22	1:B:582:VAL:HG12	1.99	0.43
1:A:155:VAL:HG12	1:A:156:ALA:N	2.33	0.43
1:A:484:LEU:HD12	1:A:484:LEU:HA	1.87	0.43
1:A:542:ASN:HB3	1:A:545:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:PRO:HD2	1:B:462:GLY:CA	2.47	0.43
1:B:501:PRO:HG3	1:B:506:VAL:HG22	2.01	0.43
1:C:294:VAL:CG1	1:C:297:SER:HA	2.49	0.43
1:A:173:LYS:O	1:A:176:PRO:HD2	2.18	0.43
1:A:336:ARG:NH1	1:A:377:TYR:O	2.50	0.43
1:A:347:ILE:CD1	1:A:355:VAL:HG11	2.48	0.43
1:B:509:VAL:HG12	1:B:582:VAL:HA	2.01	0.43
1:C:275:GLU:HG3	1:C:312:LEU:HD21	2.00	0.43
1:C:507:ASP:HA	1:C:583:LEU:O	2.18	0.43
1:A:107:SER:HB3	1:A:448:SER:HB2	2.01	0.43
1:A:509:VAL:HG12	1:A:582:VAL:HA	2.01	0.43
1:C:298:THR:O	1:C:505:MET:HE1	2.18	0.43
1:A:242:TYR:HD1	1:A:246:LYS:HD3	1.84	0.43
1:B:398:TYR:HA	1:B:399:SER:HA	1.76	0.43
1:C:173:LYS:HD3	1:C:231:ILE:O	2.19	0.42
1:B:416:TYR:OH	1:C:249:ASP:HB2	2.19	0.42
1:B:531:TYR:HB3	1:B:612:LYS:HG2	2.01	0.42
1:C:153:HIS:CE1	1:C:155:VAL:HG22	2.54	0.42
1:C:234:TRP:CD1	1:C:236:VAL:HG13	2.53	0.42
1:C:390:PRO:HD2	1:C:401:GLY:HA2	2.00	0.42
1:C:398:TYR:HA	1:C:399:SER:HA	1.76	0.42
1:A:251:ILE:HD12	1:A:251:ILE:HA	1.74	0.42
1:B:542:ASN:HB3	1:B:545:ILE:HD11	2.01	0.42
1:C:182:VAL:O	1:C:183:LYS:C	2.58	0.42
1:C:390:PRO:HD2	1:C:401:GLY:CA	2.50	0.42
1:B:432:LEU:HD23	1:B:436:ILE:HD13	2.00	0.42
1:A:74:VAL:O	1:A:78:ILE:HG13	2.20	0.42
1:A:145:MET:CE	1:A:388:ILE:HD12	2.49	0.42
1:B:166:LEU:HD22	1:B:251:ILE:HG21	2.00	0.42
1:B:429:PRO:HB3	1:B:435:TYR:HE2	1.84	0.42
1:B:534:TYR:CE1	1:C:125:GLU:HG3	2.54	0.42
1:C:452:ALA:HB1	1:C:463:TYR:OH	2.19	0.42
1:A:364:GLU:OE1	1:A:366:LYS:HD2	2.19	0.42
1:B:237:PRO:HG2	1:B:294:VAL:HG23	2.01	0.42
1:C:153:HIS:NE2	1:C:436:ILE:HG22	2.35	0.42
1:A:602:ALA:HB3	1:A:603:PRO:CD	2.48	0.42
1:B:6:LEU:N	1:C:66:LYS:HZ1	2.17	0.42
1:B:331:TYR:OH	1:B:586:ALA:HB1	2.20	0.42
1:C:127:SER:HB2	1:C:130:THR:HG1	1.82	0.42
1:C:299:GLU:HB3	1:C:549:THR:HG21	2.01	0.42
1:C:141:PHE:HB3	1:C:404:VAL:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ILE:HA	1:C:287:PRO:HD3	1.92	0.42
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.83	0.42
1:C:136:GLU:O	1:C:140:GLU:HG3	2.20	0.42
1:A:78:ILE:O	1:A:82:MET:HG2	2.19	0.41
1:A:518:LEU:HD23	1:A:518:LEU:O	2.20	0.41
1:B:316:LEU:HB3	1:B:321:ILE:HB	2.02	0.41
1:B:488:VAL:HG21	1:B:493:ILE:HD13	1.98	0.41
1:B:549:THR:HG23	1:B:582:VAL:HG22	2.03	0.41
1:A:237:PRO:HG2	1:A:294:VAL:CG2	2.46	0.41
1:B:298:THR:HB	1:B:299:GLU:H	1.61	0.41
1:B:280:GLY:O	1:B:284:GLU:HG2	2.21	0.41
1:C:155:VAL:HG12	1:C:156:ALA:N	2.36	0.41
1:A:170:ARG:HG3	1:A:253:ILE:HD11	2.03	0.41
1:A:398:TYR:HA	1:A:399:SER:HA	1.79	0.41
1:B:207:LEU:HD12	1:B:207:LEU:HA	1.76	0.41
1:A:438:GLU:HB2	1:A:439:GLY:H	1.78	0.41
1:B:6:LEU:HA	1:B:6:LEU:HD13	1.81	0.41
1:B:366:LYS:HG2	1:B:368:HIS:NE2	2.36	0.41
1:C:602:ALA:N	1:C:603:PRO:HD2	2.36	0.41
1:B:529:TYR:HE1	1:C:125:GLU:OE1	2.04	0.40
1:A:235:LEU:O	1:A:291:VAL:HA	2.22	0.40
1:A:460:VAL:HA	1:A:464:GLY:HA3	2.03	0.40
1:B:312:LEU:HG	1:B:316:LEU:HD13	2.03	0.40
1:A:105:MET:N	1:A:106:PRO:CD	2.83	0.40
1:A:271:ILE:HG13	1:A:308:LYS:HE3	2.03	0.40
1:A:505:MET:HE2	1:A:505:MET:HB2	1.59	0.40
1:B:47:MET:CE	1:C:543:GLU:HA	2.52	0.40
1:B:87:VAL:HA	1:B:88:PRO:HD3	1.88	0.40
1:B:253:ILE:HD12	1:B:257:GLN:HB2	2.03	0.40
1:B:534:TYR:HE1	1:C:125:GLU:HG3	1.85	0.40
1:A:333:GLY:HA3	1:A:388:ILE:CG1	2.34	0.40
1:B:32:LEU:HD11	1:B:112:ASN:OD1	2.21	0.40
1:B:300:GLU:HA	1:B:507:ASP:OD2	2.21	0.40
1:B:339:PHE:HZ	1:B:369:ILE:HG21	1.86	0.40
1:C:294:VAL:HG11	1:C:297:SER:HA	2.02	0.40
1:C:556:TYR:HB3	1:C:559:SER:OG	2.22	0.40
1:B:199:PRO:HA	1:B:322:TYR:CE2	2.57	0.40
1:B:441:LYS:HE3	1:B:441:LYS:HB2	1.85	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	597/620 (96%)	560 (94%)	37 (6%)	0	100	100
1	B	595/620 (96%)	552 (93%)	43 (7%)	0	100	100
1	C	582/620 (94%)	546 (94%)	36 (6%)	0	100	100
All	All	1774/1860 (95%)	1658 (94%)	116 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	489/524 (93%)	456 (93%)	33 (7%)	16	47
1	B	499/524 (95%)	456 (91%)	43 (9%)	10	35
1	C	479/524 (91%)	458 (96%)	21 (4%)	28	63
All	All	1467/1572 (93%)	1370 (93%)	97 (7%)	16	47

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	11	MET
1	A	54	ILE
1	A	63	SER
1	A	64	TYR

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Mol	Chain	Res	Type
1	A	65	GLU
1	A	231	ILE
1	A	236	VAL
1	A	240	LYS
1	A	251	ILE
1	A	253	ILE
1	A	255	LEU
1	A	257	GLN
1	A	264	ASP
1	A	298	THR
1	A	300	GLU
1	A	312	LEU
1	A	350	GLU
1	A	369	ILE
1	A	371	ARG
1	A	428	ILE
1	A	432	LEU
1	A	438	GLU
1	A	505	MET
1	A	521	MET
1	A	523	LYS
1	A	538	ASN
1	A	543	GLU
1	A	545	ILE
1	A	549	THR
1	A	604	LYS
1	A	616	ILE
1	A	618	ASP
1	B	6	LEU
1	B	63	SER
1	B	166	LEU
1	B	173	LYS
1	B	175	LEU
1	B	185	GLU
1	B	187	VAL
1	B	197	ASN
1	B	201	LYS
1	B	209	SER
1	B	223	ARG
1	B	226	LYS
1	B	227	HIS
1	B	228	LEU

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Mol	Chain	Res	Type
1	B	253	ILE
1	B	269	MET
1	B	276	LYS
1	B	298	THR
1	B	310	ILE
1	B	318	LYS
1	B	323	TYR
1	B	324	TYR
1	B	338	ILE
1	B	346	PHE
1	B	354	ASP
1	B	366	LYS
1	B	371	ARG
1	B	372	GLU
1	B	432	LEU
1	B	437	LEU
1	B	516	ASP
1	B	542	ASN
1	B	548	HIS
1	B	553	ILE
1	B	559	SER
1	B	564	VAL
1	B	570	SER
1	B	571	ASP
1	B	576	ARG
1	B	580	VAL
1	B	582	VAL
1	B	589	THR
1	B	618	ASP
1	C	179	MET
1	C	182	VAL
1	C	185	GLU
1	C	191	SER
1	C	236	VAL
1	C	251	ILE
1	C	268	ARG
1	C	269	MET
1	C	279	ARG
1	C	284	GLU
1	C	312	LEU
1	C	385	SER
1	C	456	LEU

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Mol	Chain	Res	Type
1	C	485	THR
1	C	493	ILE
1	C	517	ASP
1	C	519	VAL
1	C	527	ASP
1	C	542	ASN
1	C	564	VAL
1	C	570	SER

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	44	GLN
1	B	112	ASN
1	B	171	ASN
1	C	98	HIS
1	C	100	ASN
1	C	229	GLN
1	C	526	HIS
1	C	565	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PLP	A	702	4	15,15,16	1.09	0	20,22,23	1.24	2 (10%)
4	LDP	A	703	3	10,11,11	0.98	1 (10%)	13,14,14	0.90	0
4	LDP	C	702	3	10,11,11	1.03	2 (20%)	13,14,14	1.51	2 (15%)
4	LDP	B	703	3	10,11,11	1.02	2 (20%)	13,14,14	1.68	3 (23%)
3	PLP	C	701	4	15,15,16	1.16	0	20,22,23	0.94	0
3	PLP	B	702	4	15,15,16	1.17	0	20,22,23	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	702	4	-	1/6/6/8	0/1/1/1
4	LDP	A	703	3	-	2/3/3/3	0/1/1/1
4	LDP	C	702	3	-	0/3/3/3	0/1/1/1
4	LDP	B	703	3	-	0/3/3/3	0/1/1/1
3	PLP	C	701	4	-	3/6/6/8	0/1/1/1
3	PLP	B	702	4	-	3/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	LDP	O1-C3	2.22	1.40	1.36
4	C	702	LDP	O2-C4	2.10	1.40	1.36
4	B	703	LDP	O2-C4	2.08	1.40	1.36
4	C	702	LDP	O1-C3	2.07	1.40	1.36
4	B	703	LDP	O1-C3	2.01	1.40	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	703	LDP	C7-C1-C2	3.65	126.52	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	PLP	C4A-C4-C5	3.39	124.43	120.94
4	B	703	LDP	C7-C1-C6	-3.35	112.75	121.23
4	C	702	LDP	C7-C1-C2	3.27	125.91	120.54
4	C	702	LDP	C7-C1-C6	-2.96	113.74	121.23
3	B	702	PLP	C4A-C4-C5	2.46	123.46	120.94
4	B	703	LDP	C3-C2-C1	-2.32	118.37	120.83
3	A	702	PLP	O3-C3-C2	2.19	122.27	117.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	PLP	C5A-O4P-P-O1P
3	B	702	PLP	C5A-O4P-P-O2P
3	B	702	PLP	C5A-O4P-P-O3P
3	C	701	PLP	C5A-O4P-P-O1P
3	C	701	PLP	C5A-O4P-P-O2P
3	C	701	PLP	C5A-O4P-P-O3P
3	A	702	PLP	C5A-O4P-P-O1P
4	A	703	LDP	C6-C1-C7-C8
4	A	703	LDP	C2-C1-C7-C8

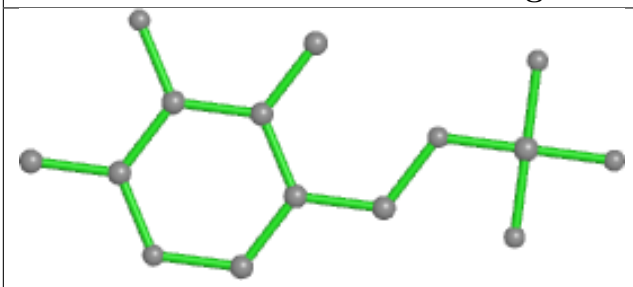
There are no ring outliers.

2 monomers are involved in 2 short contacts:

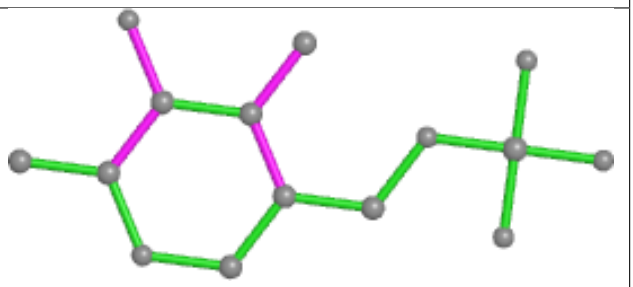
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	PLP	1	0
3	B	702	PLP	1	0

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

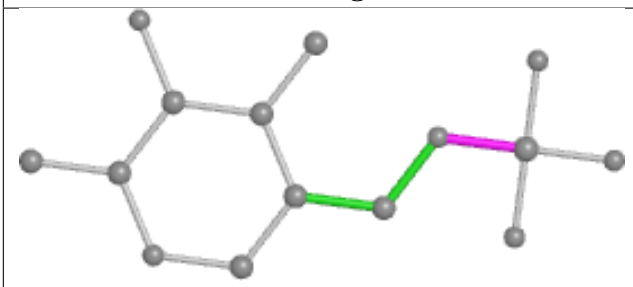
Ligand PLP A 702



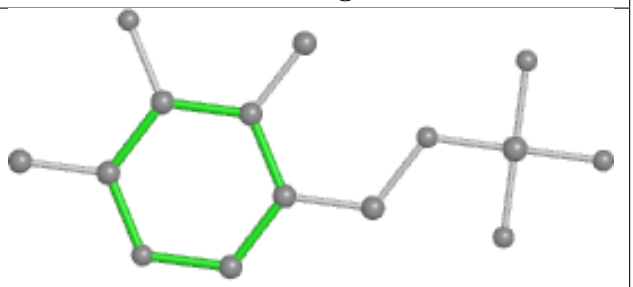
Bond lengths



Bond angles

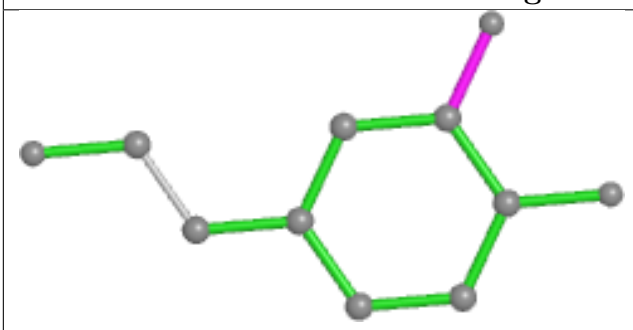


Torsions

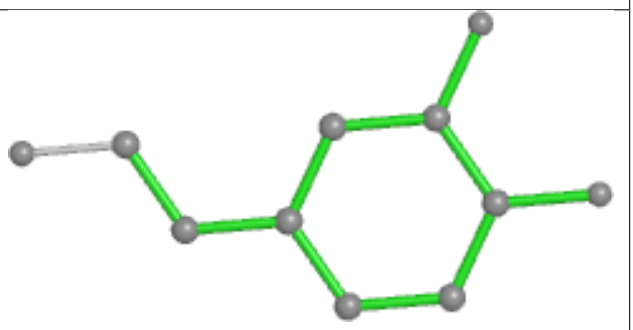


Rings

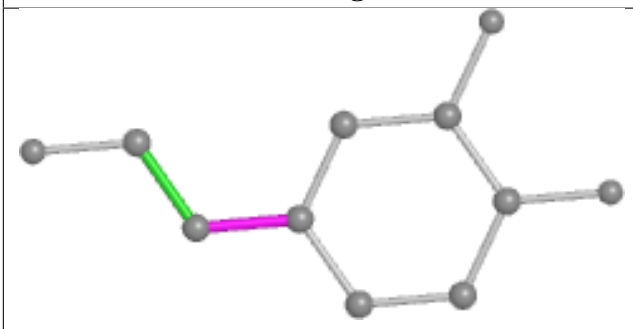
Ligand LDP A 703



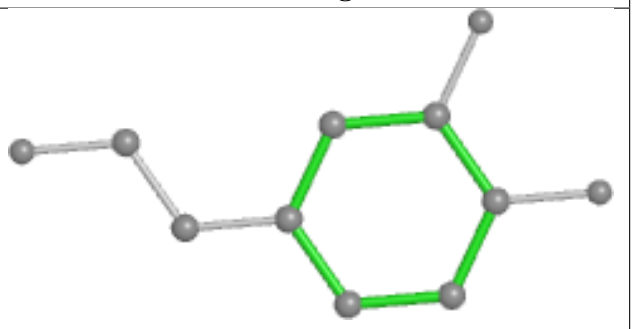
Bond lengths



Bond angles

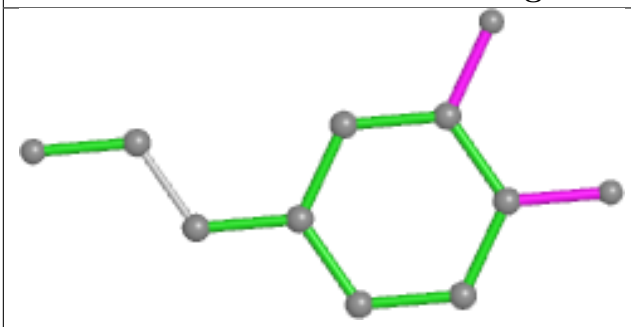


Torsions

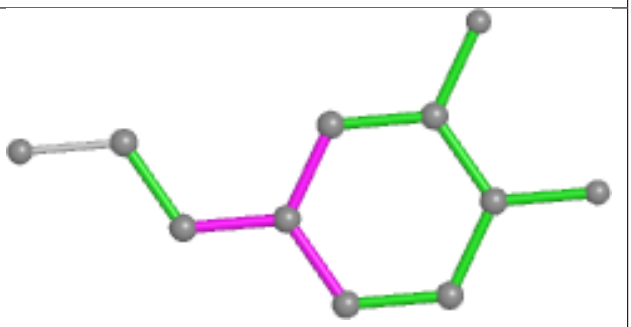


Rings

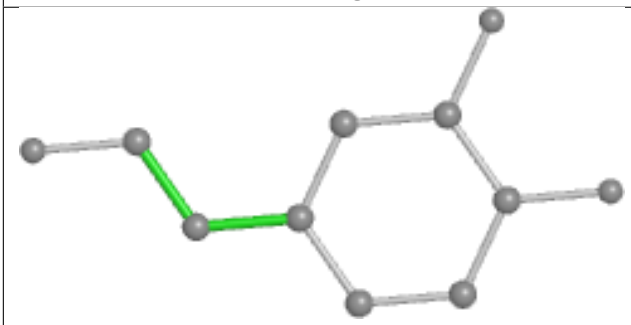
Ligand LDP C 702



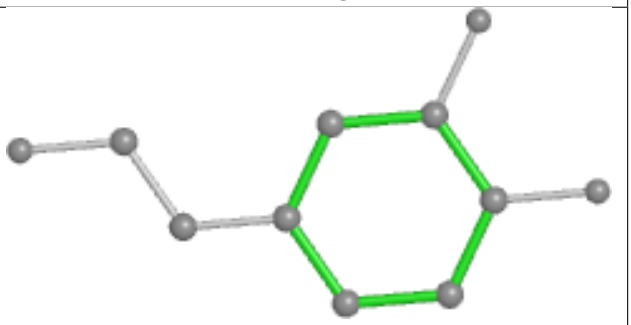
Bond lengths



Bond angles

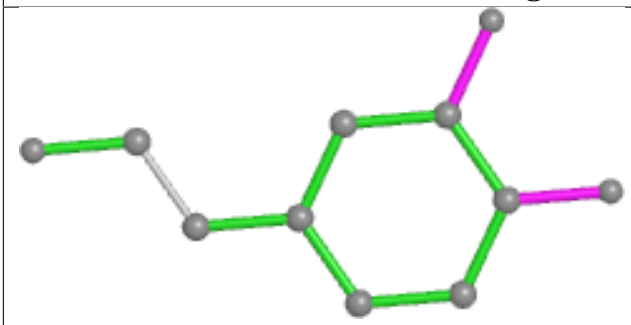


Torsions

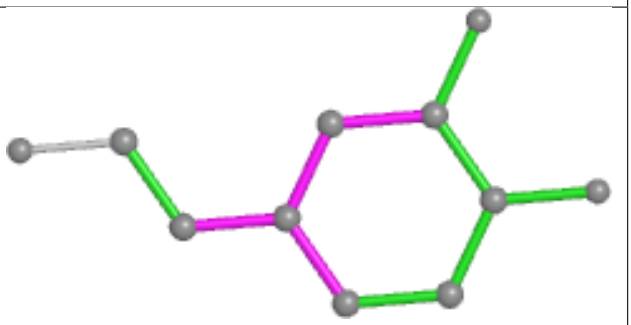


Rings

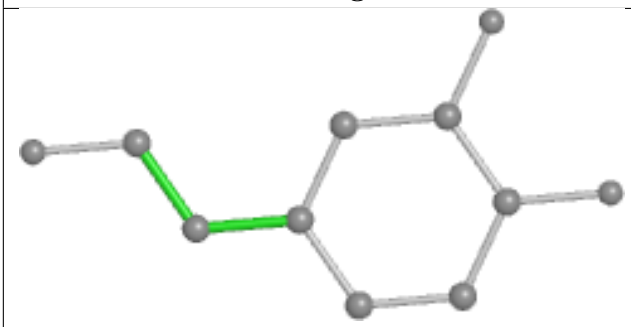
Ligand LDP B 703



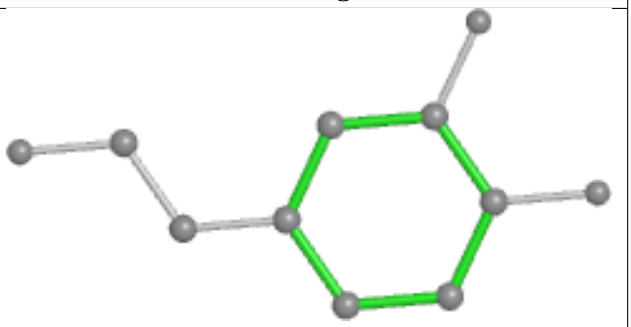
Bond lengths



Bond angles

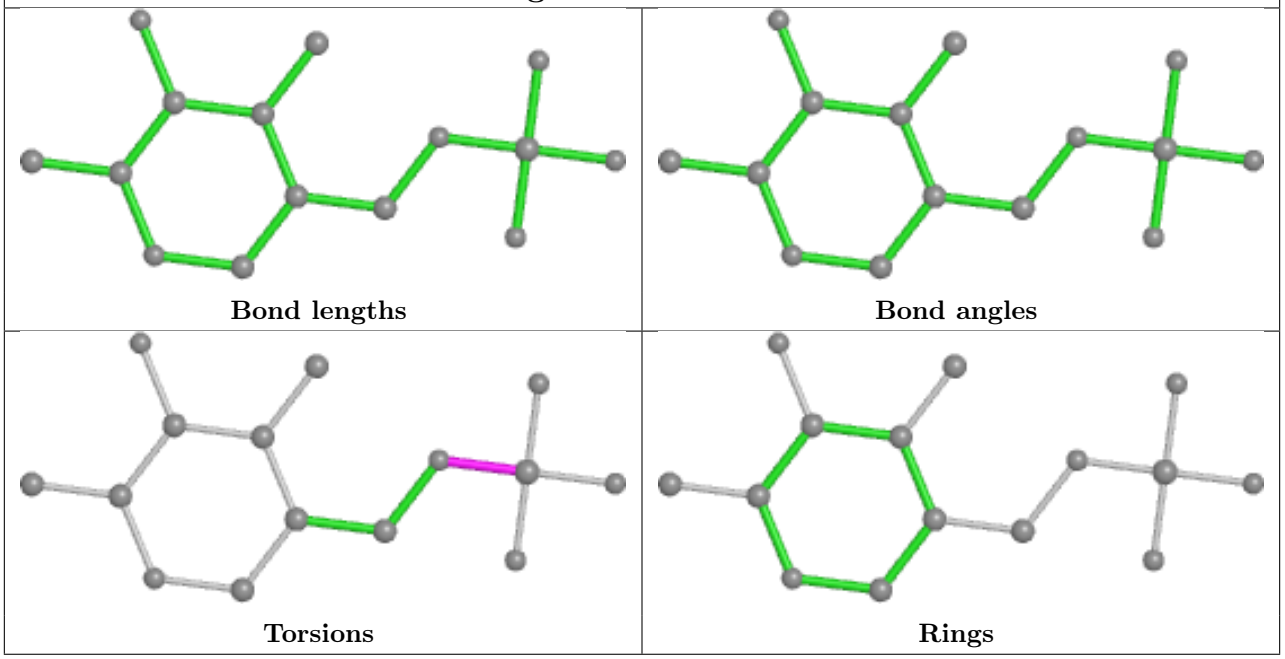


Torsions

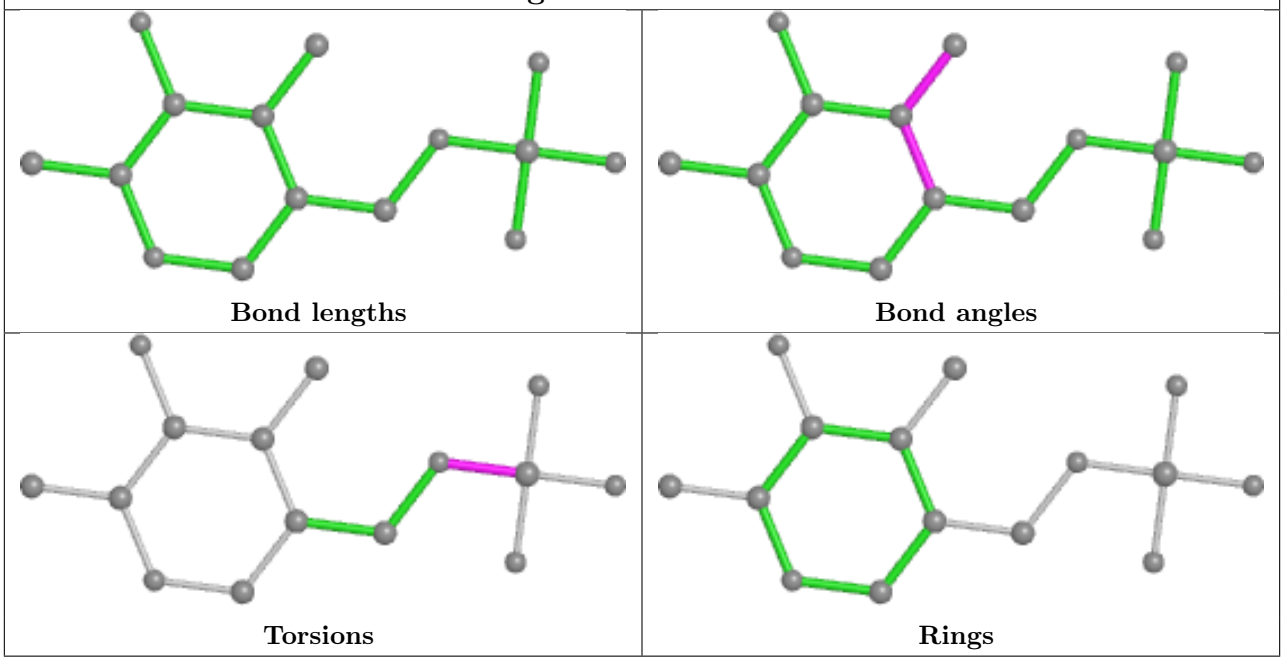


Rings

Ligand PLP C 701



Ligand PLP B 702



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	601/620 (96%)	0.34	29 (4%)	30	18	28, 49, 74, 89	0
1	B	601/620 (96%)	0.31	30 (4%)	28	17	27, 53, 77, 95	0
1	C	592/620 (95%)	0.27	34 (5%)	23	13	26, 51, 83, 100	0
All	All	1794/1860 (96%)	0.31	93 (5%)	27	16	26, 51, 79, 100	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	552	ALA	4.9
1	B	568	GLY	4.8
1	A	265	HIS	4.5
1	C	496	HIS	4.4
1	C	428	ILE	4.3
1	C	561	LEU	4.0
1	C	565	ASN	3.9
1	C	430	ALA	3.7
1	A	568	GLY	3.7
1	C	520	ALA	3.6
1	C	580	VAL	3.6
1	A	478	TYR	3.5
1	A	489	GLY	3.4
1	A	211	GLU	3.3
1	C	483	ASP	3.3
1	B	509	VAL	3.3
1	A	553	ILE	3.2
1	C	265	HIS	3.2
1	A	314	ASP	3.2
1	A	431	LEU	3.2
1	B	482	ASN	3.1
1	C	364	GLU	3.0
1	C	526	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	564	VAL	3.0
1	A	486	PHE	3.0
1	B	169	ALA	2.9
1	B	428	ILE	2.9
1	B	416	TYR	2.9
1	B	290	GLY	2.9
1	B	325	VAL	2.9
1	A	577	ALA	2.8
1	C	575	ASN	2.8
1	C	5	LYS	2.8
1	A	490	ASP	2.7
1	C	314	ASP	2.7
1	B	526	HIS	2.7
1	B	209	SER	2.7
1	A	501	PRO	2.7
1	A	430	ALA	2.7
1	B	148	LYS	2.7
1	C	568	GLY	2.7
1	A	556	TYR	2.6
1	C	529	TYR	2.6
1	B	252	GLY	2.5
1	B	478	TYR	2.5
1	C	531	TYR	2.5
1	C	60	THR	2.5
1	B	308	LYS	2.5
1	B	508	TYR	2.5
1	A	497	THR	2.5
1	A	186	LEU	2.5
1	A	290	GLY	2.4
1	C	530	ASP	2.4
1	B	317	MET	2.4
1	A	264	ASP	2.4
1	B	220	HIS	2.4
1	B	187	VAL	2.4
1	C	552	ALA	2.4
1	C	267	TYR	2.4
1	C	343	ASP	2.3
1	B	188	ALA	2.3
1	C	284	GLU	2.3
1	B	198	MET	2.3
1	A	272	ASN	2.3
1	A	502	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	285	GLN	2.3
1	B	565	ASN	2.2
1	C	490	ASP	2.2
1	C	316	LEU	2.2
1	B	382	LEU	2.2
1	B	267	TYR	2.2
1	A	315	GLU	2.2
1	C	482	ASN	2.2
1	B	143	HIS	2.2
1	A	514	GLY	2.1
1	B	318	LYS	2.1
1	A	283	GLU	2.1
1	A	506	VAL	2.1
1	B	132	GLN	2.1
1	C	535	VAL	2.1
1	B	256	ASP	2.1
1	C	366	LYS	2.1
1	C	478	TYR	2.1
1	C	556	TYR	2.1
1	B	271	ILE	2.0
1	A	551	PHE	2.0
1	A	57	GLN	2.0
1	A	289	LEU	2.0
1	C	171	ASN	2.0
1	C	567	LEU	2.0
1	A	225	GLY	2.0
1	B	578	GLY	2.0
1	B	173	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

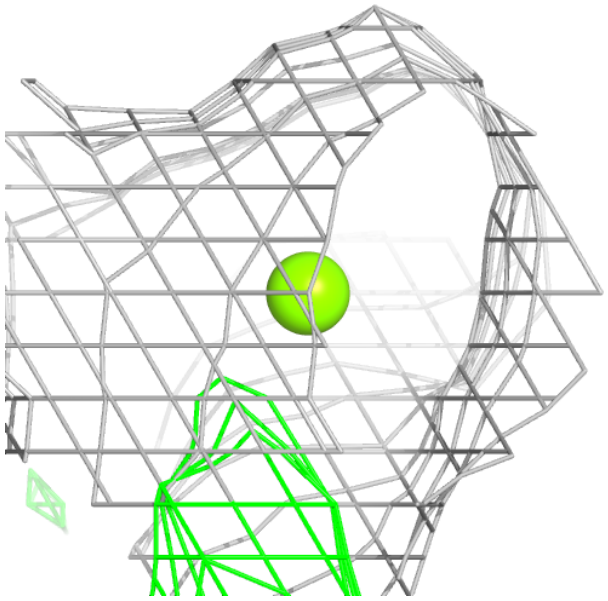
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

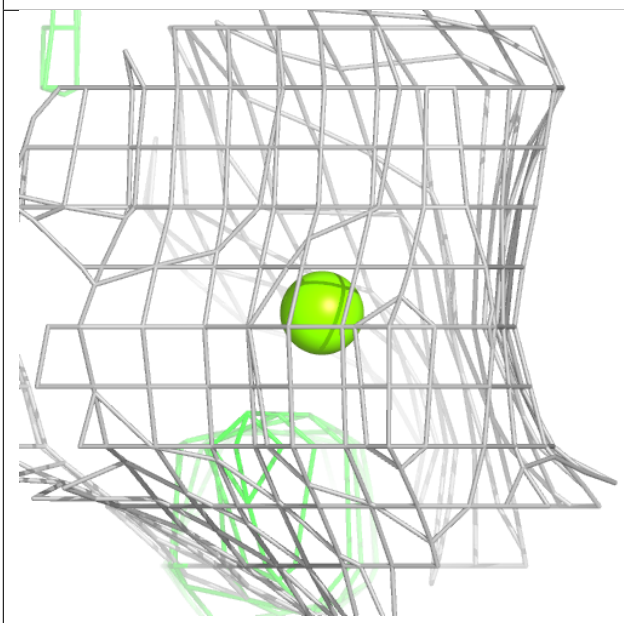
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	701	1/1	0.69	0.29	87,87,87,87	0
2	MG	B	701	1/1	0.74	0.37	58,58,58,58	0
4	LDP	A	703	11/11	0.77	0.52	52,60,72,72	0
4	LDP	B	703	11/11	0.85	0.51	44,52,62,62	0
4	LDP	C	702	11/11	0.85	0.40	45,54,67,67	0
3	PLP	B	702	15/16	0.88	0.22	46,54,65,67	0
3	PLP	A	702	15/16	0.90	0.23	45,53,63,65	0
3	PLP	C	701	15/16	0.94	0.23	44,53,64,67	0

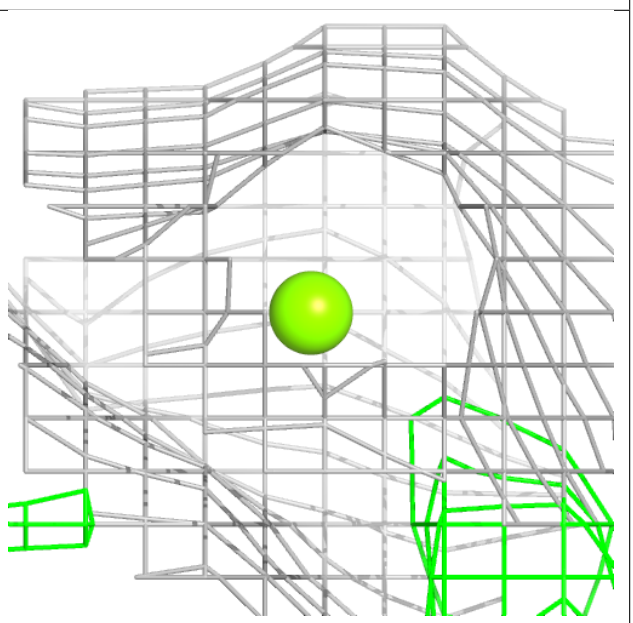
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG A 701:

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

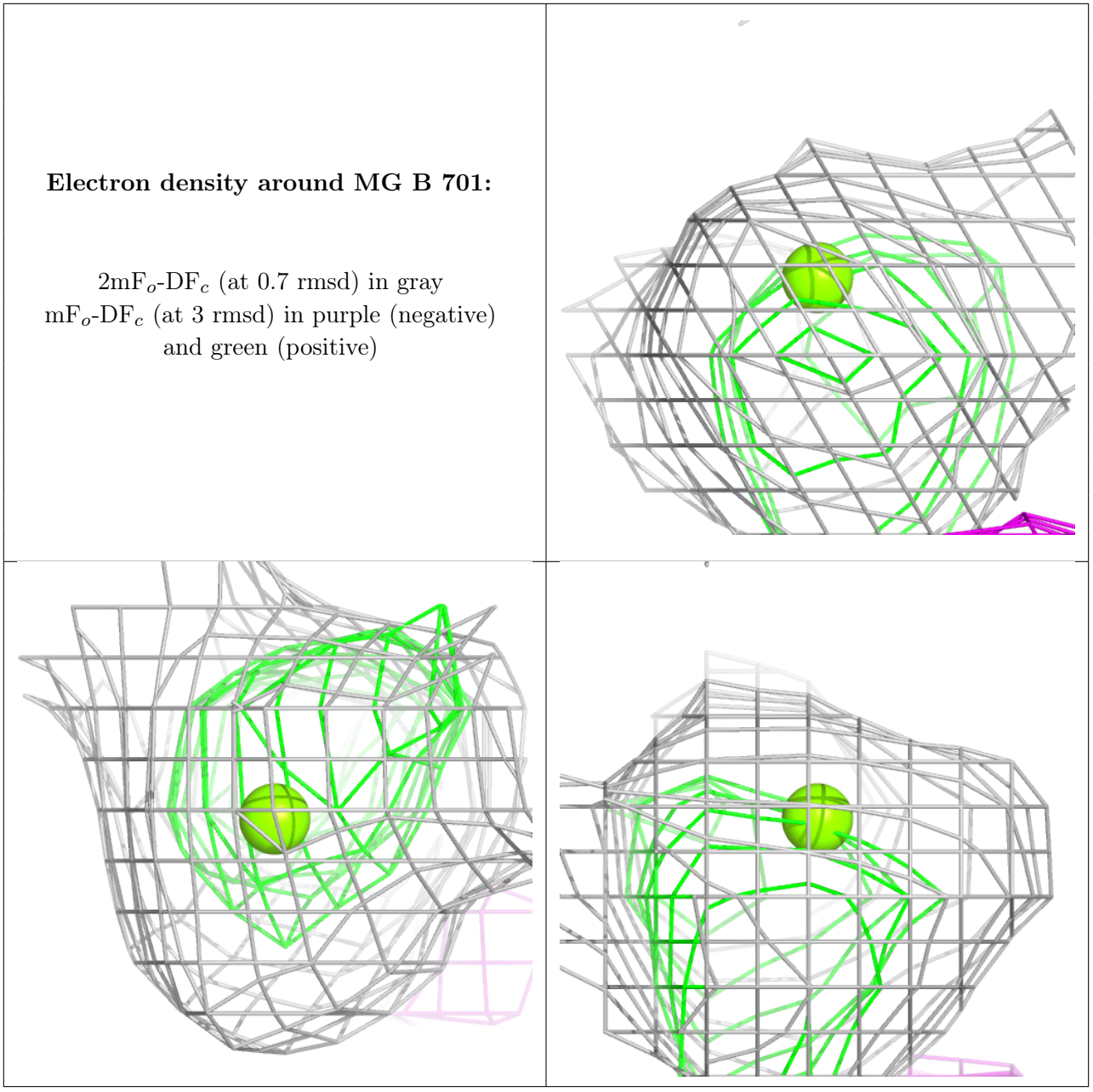






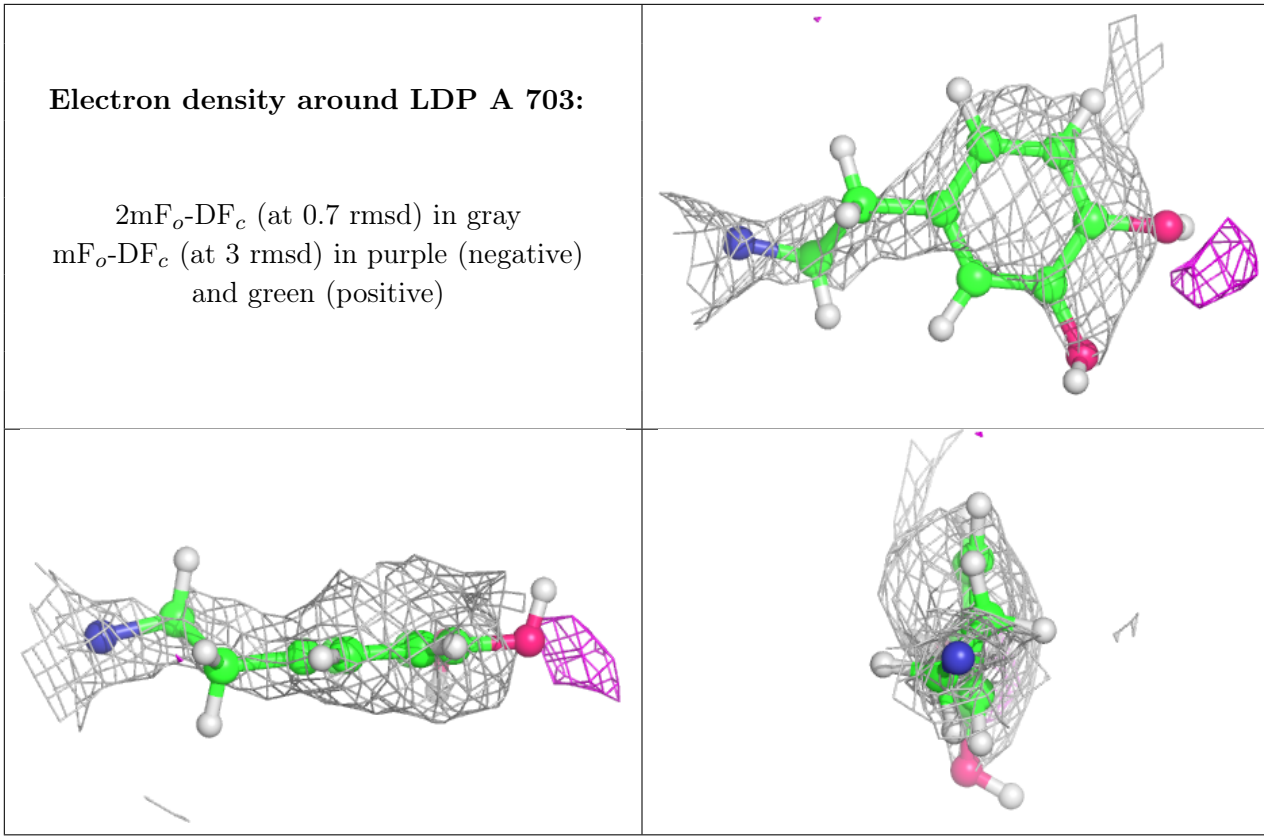
Electron density around MG B 701:

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



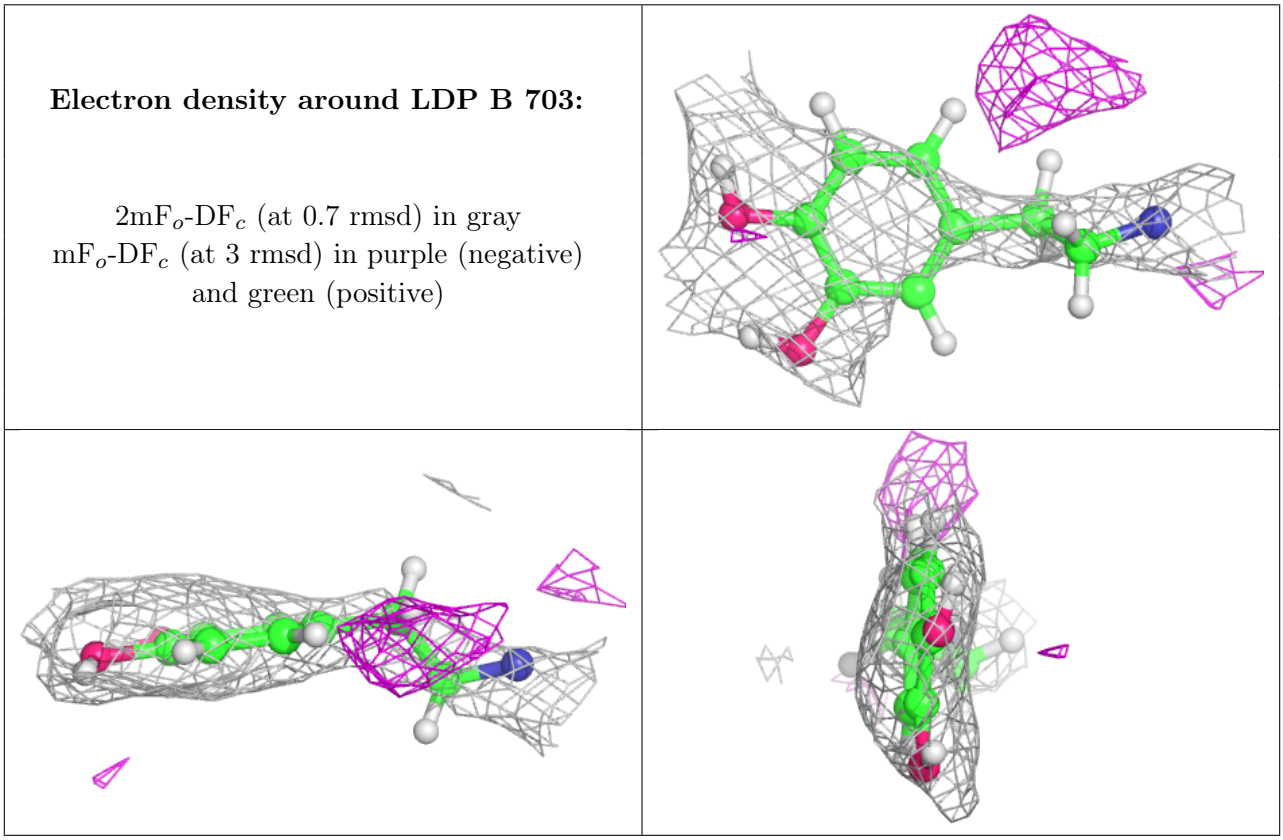
Electron density around LDP A 703:

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



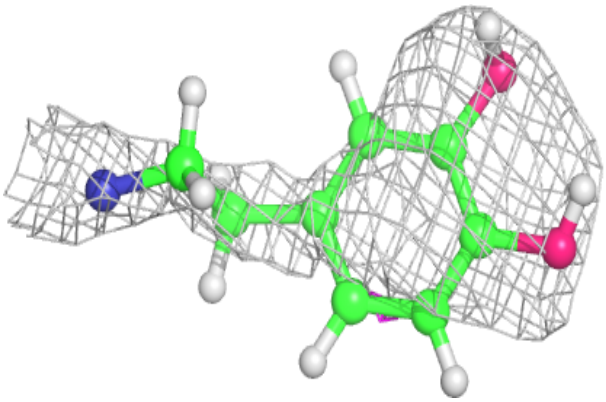
Electron density around LDP B 703:

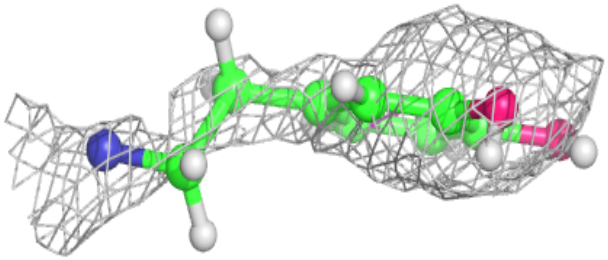
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

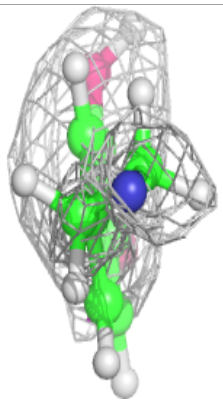


Electron density around LDP C 702:

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

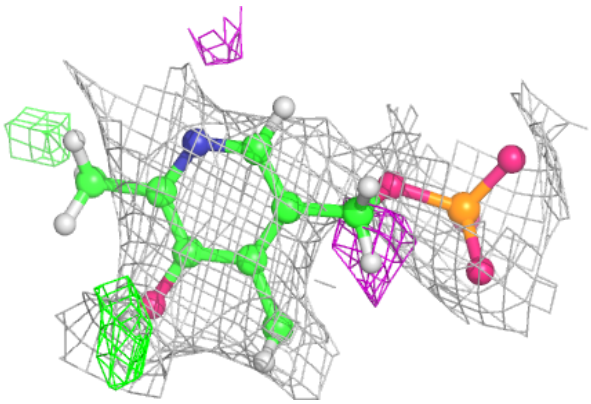


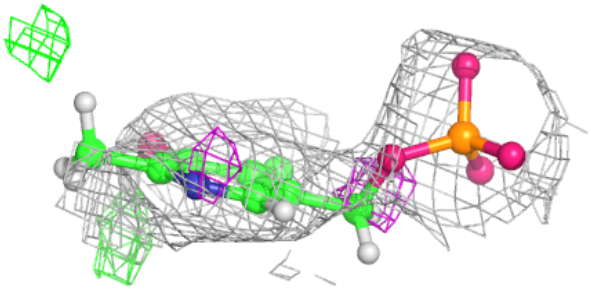


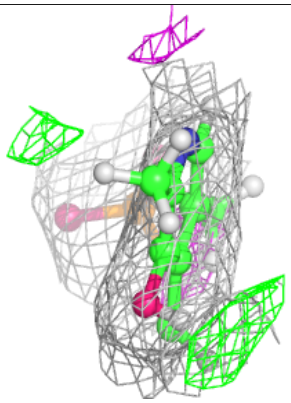


Electron density around PLP B 702:

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

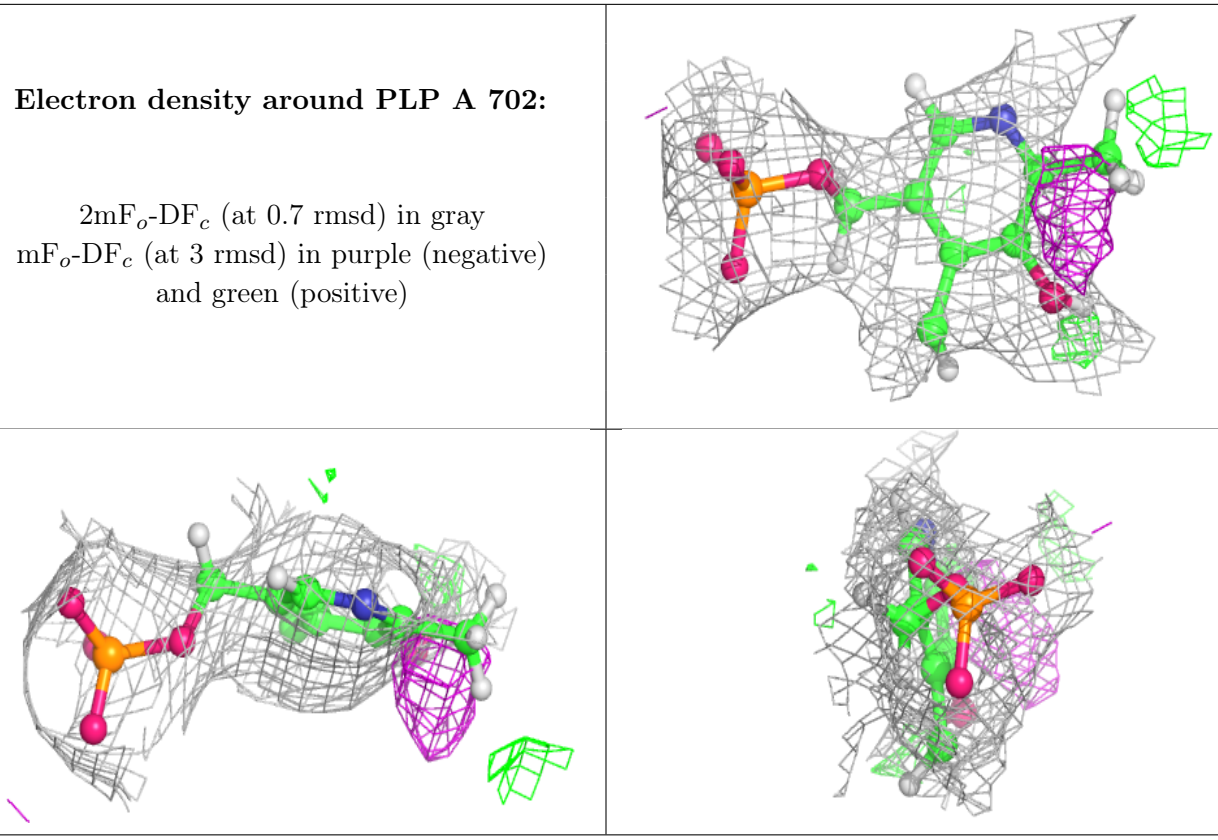






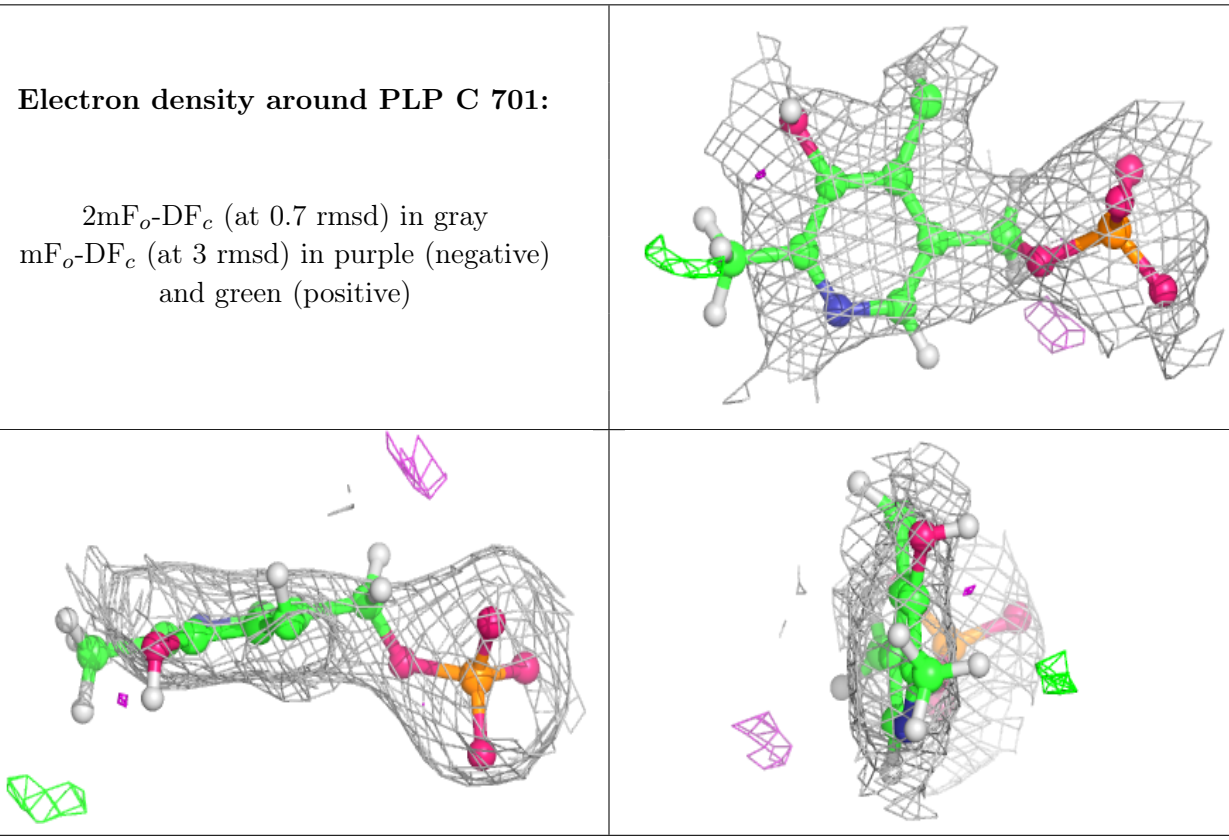
Electron density around PLP A 702:

$2mF_o$-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 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.