Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 02:24 pm GMT

PDB ID	:	6TGH
Title	:	SHMT from Streptococcus thermophilus Tyr55Thr variant in complex with D-Serine both as external aldimine and as non-covalent complex
Authors	:	Petrillo, G.; Hernandez, K.; Bujons, J.; Clapes, P.; Uson, I.
Deposited on	:	2019-11-15
Resolution	:	2.12 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:

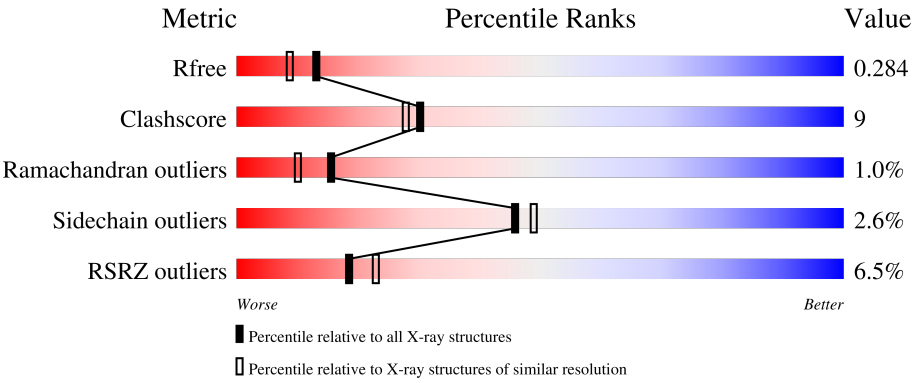
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	415	6% 73% 24%
1	B	415	3% 87% 11%
1	C	415	10% 74% 22%
1	D	415	7% 87% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12968 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	1	0
			3128	1979	538	602	9			
1	C	410	Total	C	N	O	S	0	1	0
			3120	1975	536	600	9			
1	B	410	Total	C	N	O	S	0	1	0
			3128	1979	538	602	9			
1	D	410	Total	C	N	O	S	0	1	0
			3120	1975	536	600	9			

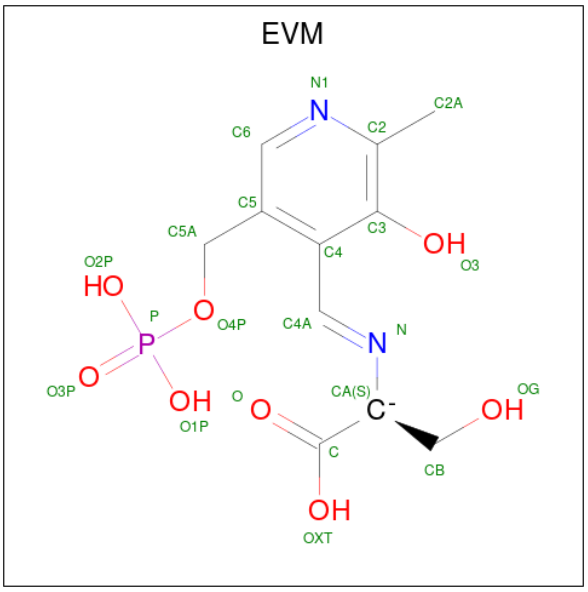
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	THR	TYR	engineered mutation	UNP Q5MCK9
C	55	THR	TYR	engineered mutation	UNP Q5MCK9
B	55	THR	TYR	engineered mutation	UNP Q5MCK9
D	55	THR	TYR	engineered mutation	UNP Q5MCK9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

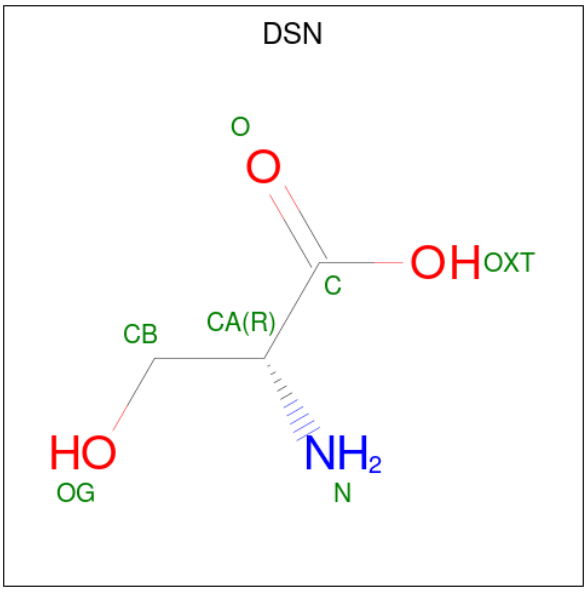
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is L-Serine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene] (three-letter code: EVM) (formula: $C_{11}H_{14}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 4 is D-SERINE (three-letter code: DSN) (formula: $C_3H_7NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			7	3	1	3		

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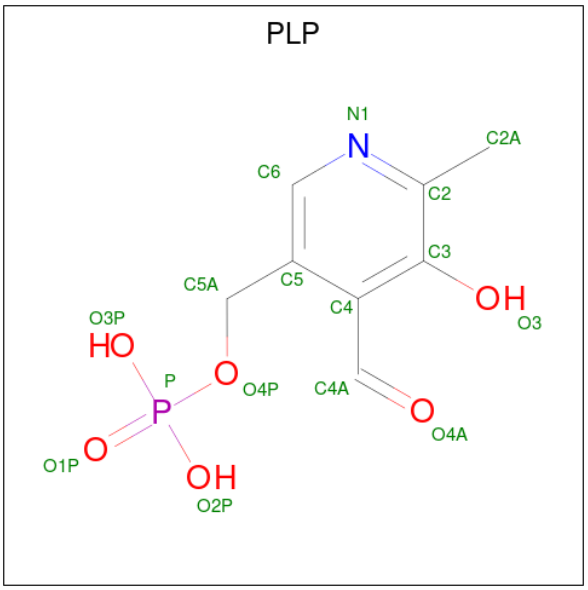
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 5 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
5	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

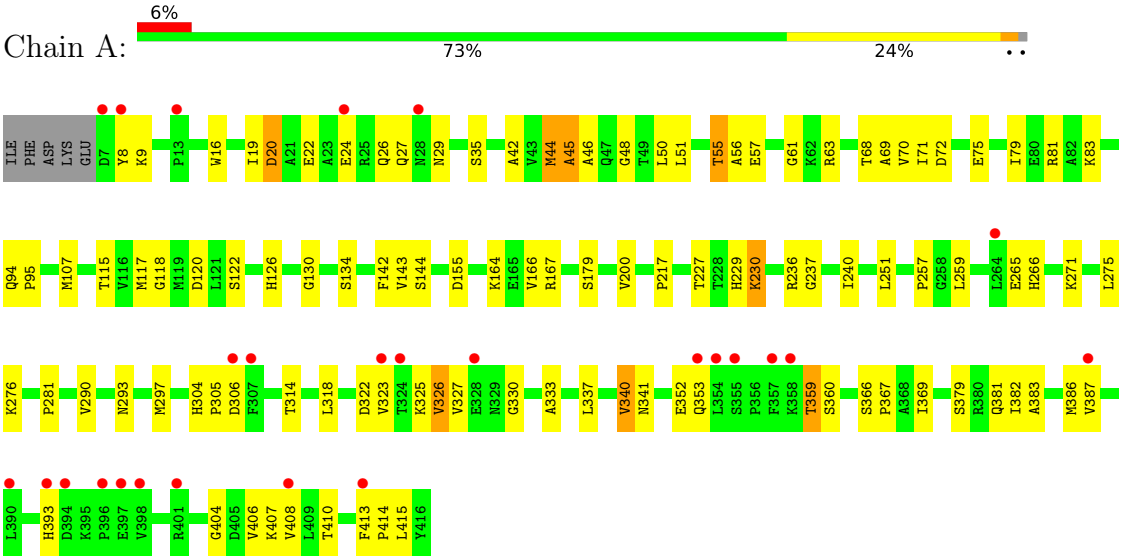
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	94	Total	O	0	0
			94	94		
6	C	101	Total	O	0	0
			101	101		
6	B	114	Total	O	0	0
			114	114		
6	D	72	Total	O	0	0
			72	72		

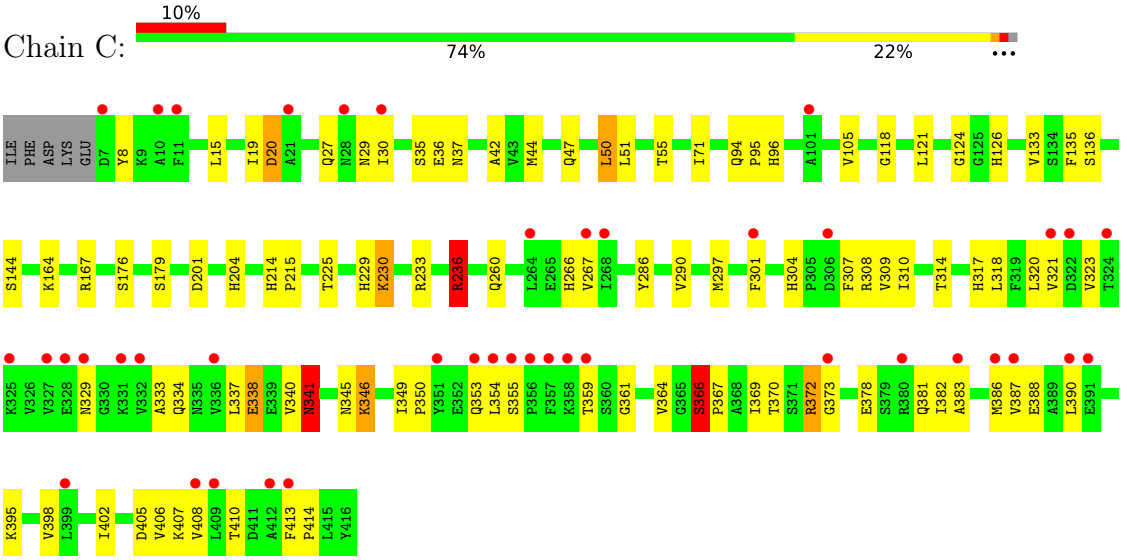
3 Residue-property plots (i)

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

• Molecule 1: Serine hydroxymethyltransferase

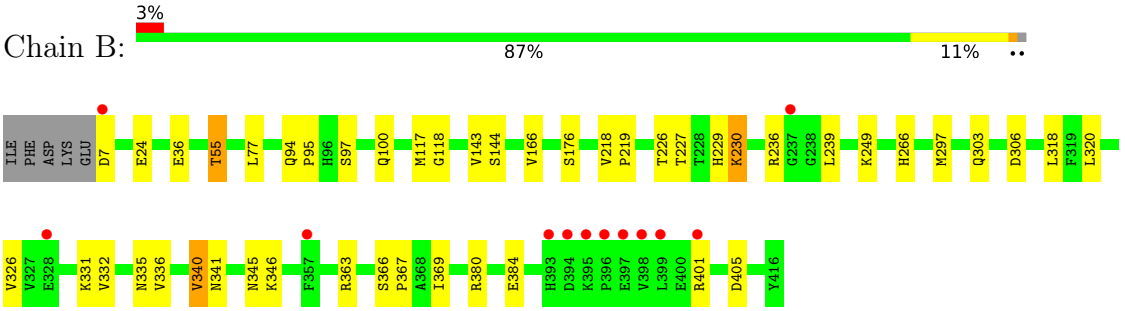


• Molecule 1: Serine hydroxymethyltransferase



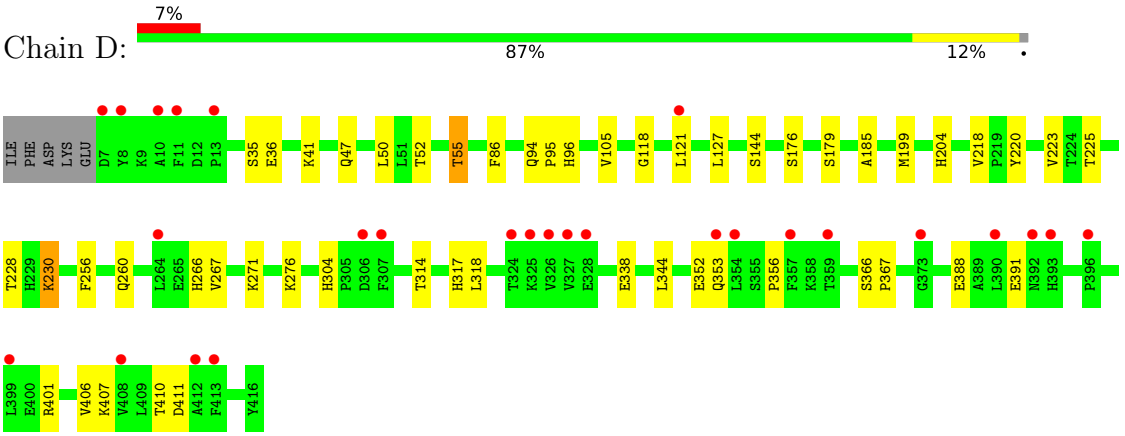
• Molecule 1: Serine hydroxymethyltransferase

Chain B:



• Molecule 1: Serine hydroxymethyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.79Å 112.93Å 131.92Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	47.76 – 2.12 47.71 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.76-2.12) 99.3 (47.71-2.12)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.237 , 0.284 0.239 , 0.284	Depositor DCC
R_{free} test set	8296 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.010 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.011 for 1/2*h+3/2*k,1/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12968	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: DSN, PLP, NA, EVM

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	0.77	0/3190	0.93	0/4332
1	B	0.72	0/3190	0.83	0/4332
1	C	0.81	1/3189 (0.0%)	0.93	3/4330 (0.1%)
1	D	0.69	0/3189	0.82	0/4330
All	All	0.75	1/12758 (0.0%)	0.88	3/17324 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	ILE	C-O	5.12	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	236	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	372	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	20	ASP	CB-CA-C	5.69	121.78	110.40

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	3128	0	3108	94	0
1	B	3128	0	3108	35	0
1	C	3120	0	3092	88	0
1	D	3120	0	3093	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	22	0	0	6	0
3	B	22	0	0	5	0
4	C	7	0	6	2	0
4	D	7	0	6	2	0
5	C	15	0	7	3	0
5	D	15	0	6	2	0
6	A	94	0	0	6	0
6	B	114	0	0	3	0
6	C	101	0	0	8	0
6	D	72	0	0	0	0
All	All	12968	0	12426	232	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 9.

All (232) 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:20:ASP:HA	6:C:605:HOH:O	1.36	1.21
1:A:326:VAL:O	1:A:327:VAL:HG13	1.67	0.94
4:D:501:DSN:HA	5:D:502:PLP:C4A	1.96	0.93
1:C:337:LEU:O	1:C:340:VAL:HG22	1.71	0.89
1:A:325:LYS:O	1:A:326:VAL:HG23	1.74	0.87
1:A:55:THR:HG22	1:C:236:ARG:HH22	1.40	0.87
1:C:304:HIS:HA	6:C:635:HOH:O	1.77	0.85
1:C:353:GLN:HA	6:C:601:HOH:O	1.77	0.84
1:A:322:ASP:OD1	1:A:323:VAL:N	2.11	0.84
1:A:55:THR:HG22	1:C:236:ARG:NH2	2.02	0.74
1:A:366:SER:N	1:A:367:PRO:HD3	2.03	0.73
4:C:502:DSN:HA	5:C:503:PLP:C4A	2.18	0.73
1:A:75:GLU:OE1	1:A:265:GLU:OE2	2.07	0.72
1:C:96:HIS:H	1:C:260:GLN:HE22	1.39	0.71
1:A:27:GLN:HB3	6:A:603:HOH:O	1.90	0.71
1:A:107:MET:SD	1:A:259:LEU:CD1	2.79	0.70
1:C:341:ASN:HB2	1:C:406:VAL:HG11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:SER:H	1:C:367:PRO:HD3	1.59	0.68
1:C:366:SER:O	1:C:370:THR:OG1	2.03	0.68
1:B:230:LYS:NZ	3:B:502:EVM:C4A	2.57	0.68
1:D:96:HIS:H	1:D:260:GLN:HE22	1.41	0.67
1:C:301:PHE:CE1	1:C:383:ALA:HB1	2.31	0.66
1:C:307:PHE:CE2	1:C:387:VAL:HG22	2.31	0.65
1:A:382:ILE:O	1:A:386:MET:HG3	1.97	0.64
1:A:325:LYS:O	1:A:326:VAL:CG2	2.46	0.64
1:C:334:GLN:NE2	1:C:338:GLU:OE2	2.31	0.64
1:B:55:THR:HG23	1:D:36:GLU:OE2	1.97	0.64
1:A:230:LYS:HZ1	3:A:502:EVM:C4	2.11	0.63
1:A:55:THR:CG2	1:C:236:ARG:HH22	2.10	0.63
1:C:179:SER:HB2	1:C:314:THR:HA	1.79	0.63
1:B:36:GLU:OE2	1:D:55:THR:CG2	2.47	0.62
1:C:382:ILE:HG22	1:C:386:MET:CE	2.30	0.62
1:C:378:GLU:O	1:C:381:GLN:HB3	2.00	0.62
1:C:373:GLY:HA3	6:C:604:HOH:O	1.99	0.61
1:A:366:SER:N	1:A:367:PRO:CD	2.63	0.61
1:A:120:ASP:OD2	1:A:122:SER:HB3	2.01	0.60
1:A:61:GLY:N	1:A:72:ASP:OD2	2.26	0.60
1:C:266:HIS:CD2	1:C:266:HIS:H	2.19	0.59
1:A:330:GLY:N	1:A:359:THR:O	2.28	0.59
1:D:366:SER:N	1:D:367:PRO:CD	2.66	0.59
1:B:230:LYS:HZ1	3:B:502:EVM:C4A	2.16	0.59
1:A:266:HIS:CD2	1:A:266:HIS:H	2.21	0.58
1:A:337:LEU:O	1:A:340:VAL:HG22	2.03	0.58
1:A:236:ARG:HH22	1:C:55:THR:HB	1.67	0.58
1:A:230:LYS:NZ	3:A:502:EVM:C4A	2.66	0.58
1:A:326:VAL:O	1:A:327:VAL:CG1	2.45	0.58
1:A:366:SER:H	1:A:367:PRO:HD3	1.68	0.58
1:C:410:THR:O	1:C:413:PHE:O	2.22	0.57
1:A:407:LYS:HG3	6:A:645:HOH:O	2.03	0.56
1:C:35:SER:HB3	4:C:502:DSN:OXT	2.05	0.56
1:C:27:GLN:OE1	1:C:27:GLN:HA	2.04	0.56
1:A:22:GLU:HG2	1:C:51:LEU:HD23	1.87	0.56
1:C:47:GLN:HE21	1:C:267:VAL:HG22	1.71	0.56
1:C:94:GLN:N	1:C:95:PRO:CD	2.69	0.56
1:A:326:VAL:O	1:A:326:VAL:CG1	2.54	0.56
1:C:366:SER:N	1:C:367:PRO:CD	2.68	0.56
1:A:27:GLN:HG2	6:A:603:HOH:O	2.07	0.55
1:C:372:ARG:C	6:C:604:HOH:O	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:THR:HG21	1:D:271:LYS:HG2	1.89	0.55
1:A:107:MET:SD	1:A:259:LEU:HD13	2.46	0.54
1:C:19:ILE:O	1:C:19:ILE:HG22	2.08	0.54
1:C:317:HIS:NE2	1:C:318:LEU:HD23	2.22	0.54
1:C:329:ASN:HB3	1:C:354:LEU:HD13	1.89	0.53
1:C:366:SER:H	1:C:367:PRO:CD	2.21	0.53
1:A:68:THR:O	1:A:70:VAL:N	2.41	0.53
1:A:240:ILE:CG2	1:A:251:LEU:HD13	2.39	0.53
1:C:124:GLY:O	1:C:176:SER:N	2.36	0.53
1:B:401:ARG:HD2	1:B:405:ASP:OD2	2.07	0.53
1:A:229:HIS:O	1:A:230:LYS:HB2	2.08	0.53
1:D:185:ALA:HA	1:D:220:TYR:CD1	2.43	0.53
1:A:227:THR:HB	1:A:229:HIS:CE1	2.43	0.53
1:B:345:ASN:HD21	1:B:363:ARG:HH21	1.57	0.53
1:D:47:GLN:HE21	1:D:267:VAL:HG22	1.74	0.52
1:A:236:ARG:NH2	1:C:55:THR:HB	2.24	0.52
1:C:405:ASP:O	1:C:408:VAL:HB	2.10	0.52
1:A:230:LYS:HZ1	3:A:502:EVM:C4A	2.23	0.52
1:A:410:THR:O	1:A:413:PHE:O	2.28	0.52
1:C:229:HIS:ND1	1:C:236:ARG:HA	2.24	0.52
1:B:36:GLU:OE2	1:D:55:THR:HG22	2.10	0.51
1:A:318:LEU:HD12	1:A:318:LEU:C	2.31	0.51
1:A:326:VAL:O	1:A:326:VAL:HG12	2.10	0.51
1:A:44:MET:O	1:A:45:ALA:C	2.49	0.51
1:D:366:SER:N	1:D:367:PRO:HD3	2.25	0.51
1:C:318:LEU:HD12	1:C:318:LEU:C	2.31	0.51
1:B:266:HIS:H	1:B:266:HIS:CD2	2.27	0.51
1:A:117:MET:HA	1:A:143:VAL:O	2.10	0.51
1:A:240:ILE:HG21	1:A:251:LEU:HD13	1.92	0.50
1:C:388:GLU:HG2	1:C:402:ILE:HD11	1.92	0.50
1:C:301:PHE:HB2	1:C:309:VAL:HG23	1.94	0.50
1:A:352:GLU:OE2	1:A:353:GLN:N	2.45	0.50
1:C:405:ASP:OD2	1:C:405:ASP:N	2.43	0.50
1:A:404:GLY:O	1:A:408:VAL:HG23	2.12	0.49
1:C:345:ASN:C	1:C:346:LYS:O	2.50	0.49
1:A:118:GLY:O	1:A:144:SER:HA	2.12	0.49
1:C:310:ILE:HB	1:C:320:LEU:HB2	1.95	0.49
1:C:382:ILE:HG22	1:C:386:MET:HE3	1.94	0.49
1:B:94:GLN:N	1:B:95:PRO:CD	2.76	0.49
1:A:55:THR:HG23	1:C:36:GLU:OE1	2.13	0.49
1:C:126:HIS:HB2	5:C:503:PLP:H2A3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLN:HA	1:B:303:GLN:OE1	2.13	0.49
1:A:164:LYS:O	1:A:167:ARG:NE	2.43	0.49
1:D:199:MET:HA	1:D:223:VAL:O	2.12	0.49
1:B:266:HIS:HE1	1:D:47:GLN:NE2	2.11	0.49
1:D:388:GLU:OE2	1:D:401:ARG:NH1	2.45	0.49
4:D:501:DSN:CA	5:D:502:PLP:C4A	2.83	0.49
1:B:340:VAL:HG23	1:B:340:VAL:O	2.13	0.48
1:D:118:GLY:O	1:D:144:SER:HA	2.14	0.48
1:D:406:VAL:O	1:D:410:THR:HG23	2.13	0.48
1:A:8:TYR:HB2	1:C:42:ALA:HB2	1.96	0.48
1:B:118:GLY:O	1:B:144:SER:HA	2.13	0.48
1:B:318:LEU:C	1:B:318:LEU:HD12	2.34	0.48
1:C:176:SER:HA	1:C:204:HIS:CD2	2.49	0.48
1:A:304:HIS:CD2	1:A:306:ASP:H	2.31	0.47
1:C:94:GLN:N	1:C:95:PRO:HD3	2.29	0.47
1:C:301:PHE:HB2	1:C:309:VAL:CG2	2.43	0.47
1:A:48:GLY:HA2	1:C:44:MET:O	2.14	0.47
1:A:322:ASP:OD1	1:A:322:ASP:C	2.53	0.47
1:B:7:ASP:HA	6:B:648:HOH:O	2.14	0.47
1:D:353:GLN:HA	1:D:353:GLN:NE2	2.29	0.47
1:A:352:GLU:OE2	1:A:360:SER:OG	2.28	0.47
1:A:155:ASP:C	1:A:155:ASP:OD1	2.53	0.47
1:A:383:ALA:O	1:A:387:VAL:HG23	2.14	0.47
1:C:373:GLY:CA	6:C:604:HOH:O	2.61	0.47
1:A:27:GLN:O	1:A:410:THR:HB	2.14	0.47
1:D:266:HIS:CD2	1:D:266:HIS:H	2.32	0.47
1:A:9:LYS:HA	1:A:16:TRP:CD1	2.49	0.47
1:A:27:GLN:CG	6:A:603:HOH:O	2.63	0.47
1:A:35:SER:O	1:A:230:LYS:HG2	2.15	0.47
1:C:323:VAL:HG22	1:C:361:GLY:HA2	1.96	0.47
1:B:366:SER:N	1:B:367:PRO:CD	2.78	0.47
1:A:130:GLY:HA3	1:A:142:PHE:CG	2.50	0.47
1:A:325:LYS:O	1:A:326:VAL:CB	2.63	0.47
1:C:27:GLN:OE1	1:C:372:ARG:NH2	2.49	0.46
1:C:301:PHE:HE1	1:C:383:ALA:HB1	1.80	0.46
1:A:22:GLU:HG2	1:C:51:LEU:CD2	2.46	0.46
1:B:97:SER:OG	1:B:100:GLN:OE1	2.31	0.46
1:C:333:ALA:O	1:C:337:LEU:HG	2.15	0.46
1:D:52:THR:HA	1:D:266:HIS:CD2	2.51	0.46
1:A:179:SER:HB2	1:A:314:THR:HA	1.97	0.46
1:C:297:MET:SD	1:C:364:VAL:HG11	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LYS:HE3	1:B:335:ASN:HD21	1.79	0.46
1:D:318:LEU:C	1:D:318:LEU:HD12	2.36	0.46
1:A:75:GLU:O	1:A:79:ILE:HG13	2.16	0.46
1:C:340:VAL:O	1:C:341:ASN:HB2	2.15	0.46
1:D:317:HIS:NE2	1:D:318:LEU:HD23	2.31	0.46
1:A:44:MET:O	1:A:46:ALA:N	2.49	0.46
1:C:96:HIS:HD2	6:C:636:HOH:O	1.98	0.46
1:A:230:LYS:NZ	3:A:502:EVM:C4	2.78	0.45
1:A:44:MET:SD	1:C:50:LEU:HB3	2.56	0.45
1:B:117:MET:HA	1:B:143:VAL:O	2.16	0.45
1:B:227:THR:HB	1:B:229:HIS:CE1	2.50	0.45
1:D:94:GLN:N	1:D:95:PRO:CD	2.79	0.45
1:C:395:LYS:O	1:C:398:VAL:HB	2.17	0.45
1:A:330:GLY:O	1:A:333:ALA:HB3	2.17	0.45
1:C:382:ILE:CG2	1:C:386:MET:CE	2.95	0.45
1:C:321:VAL:O	1:C:361:GLY:HA3	2.16	0.45
1:B:230:LYS:HZ2	3:B:502:EVM:C4	2.29	0.45
1:A:115:THR:HG21	1:A:166:VAL:CG1	2.46	0.45
1:C:229:HIS:O	1:C:230:LYS:HG3	2.16	0.45
1:D:35:SER:O	1:D:230:LYS:HA	2.16	0.45
1:C:164:LYS:O	1:C:167:ARG:HD3	2.17	0.45
1:B:100:GLN:NE2	6:B:609:HOH:O	2.49	0.45
1:B:236:ARG:HH12	1:D:55:THR:HB	1.81	0.45
1:C:307:PHE:CD2	1:C:387:VAL:HG22	2.51	0.44
1:B:236:ARG:NH1	1:D:55:THR:HB	2.31	0.44
1:B:401:ARG:NH2	1:B:405:ASP:OD2	2.49	0.44
1:C:20:ASP:CA	6:C:605:HOH:O	2.21	0.44
1:B:380:ARG:O	1:B:384:GLU:HG2	2.17	0.44
1:C:96:HIS:N	1:C:260:GLN:HE22	2.11	0.44
1:D:36:GLU:OE2	1:D:36:GLU:HA	2.18	0.44
1:D:256:PHE:CD2	1:D:256:PHE:C	2.91	0.44
1:B:176:SER:OG	3:B:502:EVM:O3	2.36	0.43
1:A:81:ARG:CZ	1:A:276:LYS:HD3	2.48	0.43
1:A:341:ASN:HB2	1:A:406:VAL:HG11	2.00	0.43
1:C:19:ILE:O	1:C:19:ILE:CG2	2.66	0.43
1:C:50:LEU:HD12	1:C:50:LEU:C	2.38	0.43
1:A:50:LEU:HB3	1:C:44:MET:SD	2.59	0.43
1:A:83:LYS:NZ	6:A:607:HOH:O	2.50	0.43
1:A:290:VAL:HG13	1:A:366:SER:OG	2.17	0.43
1:A:19:ILE:O	1:A:20:ASP:C	2.57	0.43
1:B:332:VAL:O	1:B:336:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:SER:HA	1:D:204:HIS:CD2	2.54	0.43
1:A:257:PRO:HG2	1:C:133:VAL:HB	2.00	0.43
1:A:143:VAL:HG11	1:A:166:VAL:HG21	2.00	0.43
1:A:227:THR:HB	1:A:229:HIS:ND1	2.34	0.43
1:A:297:MET:HE2	1:A:369:ILE:HD11	2.00	0.43
1:C:201:ASP:CG	5:C:503:PLP:H2A2	2.39	0.43
1:C:349:ILE:O	1:C:350:PRO:C	2.56	0.43
1:A:22:GLU:OE2	1:A:26:GLN:NE2	2.43	0.43
1:C:229:HIS:C	1:C:230:LYS:HG3	2.39	0.43
1:A:304:HIS:HA	1:A:305:PRO:HD3	1.89	0.43
1:C:286:TYR:O	1:C:290:VAL:HG23	2.19	0.43
1:A:230:LYS:HZ3	3:A:502:EVM:C4A	2.31	0.42
1:B:230:LYS:HZ2	3:B:502:EVM:C4A	2.32	0.42
1:C:406:VAL:O	1:C:410:THR:HG23	2.19	0.42
1:C:214:HIS:ND1	1:C:215:PRO:HD2	2.35	0.42
1:C:105:VAL:HG21	1:C:225:THR:CG2	2.49	0.42
1:C:333:ALA:HA	1:C:390:LEU:CD2	2.49	0.42
1:C:341:ASN:CB	1:C:406:VAL:HG11	2.46	0.42
1:A:200:VAL:HG11	1:A:217:PRO:HB3	2.01	0.42
1:D:179:SER:HB2	1:D:314:THR:HA	2.02	0.42
1:D:407:LYS:O	1:D:411:ASP:OD2	2.37	0.42
1:A:26:GLN:O	1:A:415:LEU:HD22	2.19	0.42
1:A:94:GLN:N	1:A:95:PRO:CD	2.82	0.42
1:A:27:GLN:CB	6:A:603:HOH:O	2.59	0.41
1:A:107:MET:SD	1:A:259:LEU:HD11	2.57	0.41
1:C:317:HIS:CE1	1:C:318:LEU:HD23	2.55	0.41
1:B:218:VAL:N	1:B:219:PRO:CD	2.84	0.41
1:A:56:ALA:O	1:A:57:GLU:C	2.59	0.41
1:A:126:HIS:CD2	3:A:502:EVM:C4	3.04	0.41
1:A:227:THR:HA	1:A:237:GLY:O	2.19	0.41
1:A:265:GLU:OE1	1:A:265:GLU:HA	2.20	0.41
1:A:293:ASN:OD1	1:A:379:SER:OG	2.36	0.41
1:B:226:THR:CG2	1:B:239:LEU:HD23	2.51	0.41
1:B:320:LEU:CD2	1:B:363:ARG:HB2	2.50	0.41
1:D:86:PHE:HB3	1:D:218:VAL:HG21	2.02	0.41
1:A:63:ARG:NH2	1:A:71:ILE:HG22	2.35	0.41
1:C:297:MET:HE1	1:C:369:ILE:CD1	2.50	0.41
1:D:121:LEU:H	1:D:121:LEU:HD22	1.85	0.41
1:A:51:LEU:HD23	1:A:71:ILE:CD1	2.51	0.41
1:C:37:ASN:CG	1:C:233:ARG:HG3	2.40	0.41
1:B:297:MET:CE	1:B:369:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:ND2	6:B:615:HOH:O	2.54	0.41
1:D:105:VAL:HG21	1:D:225:THR:CG2	2.51	0.41
1:A:42:ALA:HB2	1:C:8:TYR:HB2	2.03	0.41
1:C:118:GLY:O	1:C:144:SER:HA	2.20	0.41
1:A:271:LYS:O	1:A:275:LEU:HG	2.21	0.40
1:C:135:PHE:CG	1:C:136:SER:N	2.89	0.40
1:D:304:HIS:NE2	1:D:391:GLU:OE1	2.54	0.40
1:B:306:ASP:HB3	1:B:326:VAL:CG2	2.51	0.40
1:A:27:GLN:HE22	1:A:414:PRO:HA	1.86	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	409/415 (99%)	359 (88%)	43 (10%)	7 (2%)	9 4
1	B	409/415 (99%)	395 (97%)	13 (3%)	1 (0%)	47 48
1	C	409/415 (99%)	367 (90%)	35 (9%)	7 (2%)	9 4
1	D	409/415 (99%)	390 (95%)	17 (4%)	2 (0%)	29 25
All	All	1636/1660 (99%)	1511 (92%)	108 (7%)	17 (1%)	15 10

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	LYS
1	A	326	VAL
1	C	230	LYS
1	C	308	ARG
1	B	230	LYS
1	D	230	LYS

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Mol	Chain	Res	Type
1	A	69	ALA
1	A	20	ASP
1	C	346	LYS
1	C	359	THR
1	A	359	THR
1	C	414	PRO
1	D	352	GLU
1	A	44	MET
1	C	341	ASN
1	A	45	ALA
1	C	366	SER

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	328/332 (99%)	320 (98%)	8 (2%)	49	52
1	B	328/332 (99%)	321 (98%)	7 (2%)	53	57
1	C	328/332 (99%)	316 (96%)	12 (4%)	34	34
1	D	328/332 (99%)	320 (98%)	8 (2%)	49	52
All	All	1312/1328 (99%)	1277 (97%)	35 (3%)	46	47

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	29	ASN
1	A	55	THR
1	A	134	SER
1	A	281	PRO
1	A	340	VAL
1	A	381	GLN
1	A	393	HIS
1	C	15	LEU
1	C	29[A]	ASN

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Mol	Chain	Res	Type
1	C	29[B]	ASN
1	C	50	LEU
1	C	71	ILE
1	C	121	LEU
1	C	236	ARG
1	C	338	GLU
1	C	341	ASN
1	C	355	SER
1	C	366	SER
1	C	407	LYS
1	B	24	GLU
1	B	55	THR
1	B	77	LEU
1	B	166	VAL
1	B	249	LYS
1	B	340	VAL
1	B	346	LYS
1	D	41	LYS
1	D	50	LEU
1	D	55	THR
1	D	127	LEU
1	D	276	LYS
1	D	338	GLU
1	D	344	LEU
1	D	356	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	304	HIS
1	A	341	ASN
1	A	345	ASN
1	A	347	ASN
1	A	381	GLN
1	C	17	ASN
1	C	47	GLN
1	C	96	HIS
1	C	260	GLN
1	C	266	HIS
1	C	341	ASN
1	C	345	ASN

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Mol	Chain	Res	Type
1	C	347	ASN
1	B	17	ASN
1	B	47	GLN
1	B	266	HIS
1	B	335	ASN
1	B	341	ASN
1	B	345	ASN
1	B	347	ASN
1	D	17	ASN
1	D	47	GLN
1	D	260	GLN
1	D	266	HIS
1	D	335	ASN
1	D	341	ASN
1	D	345	ASN
1	D	353	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 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	EVM	B	502	-	22,22,22	2.86	4 (18%)	27,31,31	2.79	12 (44%)
4	DSN	D	501	-	5,6,6	0.97	0	5,7,7	1.16	0
5	PLP	D	502	1	15,15,16	3.13	6 (40%)	20,22,23	2.13	9 (45%)
3	EVM	A	502	-	22,22,22	3.07	4 (18%)	27,31,31	3.15	11 (40%)
5	PLP	C	503	1	15,15,16	2.98	6 (40%)	20,22,23	1.86	4 (20%)
4	DSN	C	502	-	5,6,6	0.82	0	5,7,7	1.97	2 (40%)

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	EVM	B	502	-	-	7/17/17/17	0/1/1/1
4	DSN	D	501	-	-	1/6/6/6	-
5	PLP	D	502	1	-	0/6/6/8	0/1/1/1
3	EVM	A	502	-	-	6/17/17/17	0/1/1/1
5	PLP	C	503	1	-	0/6/6/8	0/1/1/1
4	DSN	C	502	-	-	4/6/6/6	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	EVM	C3-C2	9.50	1.50	1.40
3	B	502	EVM	C3-C2	9.21	1.50	1.40
5	C	503	PLP	C3-C2	8.31	1.49	1.40
5	D	502	PLP	C5-C4	8.05	1.49	1.40
5	D	502	PLP	C3-C2	7.11	1.48	1.40
3	B	502	EVM	C4-C3	6.86	1.51	1.40
3	A	502	EVM	C4-C5	6.72	1.50	1.42
3	A	502	EVM	C4-C3	6.30	1.50	1.40
5	C	503	PLP	C5-C4	5.73	1.46	1.40
3	B	502	EVM	C4-C5	4.61	1.47	1.42
5	D	502	PLP	C3-C4	3.37	1.47	1.40
3	A	502	EVM	C4-C4A	3.09	1.52	1.46
5	C	503	PLP	C3-C4	2.87	1.46	1.40
5	C	503	PLP	C2-N1	2.75	1.39	1.33
5	D	502	PLP	C4A-C4	-2.68	1.46	1.51
5	C	503	PLP	C6-C5	2.51	1.43	1.37
3	B	502	EVM	C4-C4A	2.34	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	PLP	C4A-C4	-2.23	1.47	1.51
5	D	502	PLP	C2-N1	2.05	1.37	1.33
5	D	502	PLP	C6-C5	2.04	1.42	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	EVM	CA-N-C4A	11.89	134.47	117.31
3	B	502	EVM	CA-N-C4A	6.22	126.29	117.31
3	A	502	EVM	O4P-C5A-C5	5.61	120.05	109.35
3	A	502	EVM	C3-C4-C5	-4.96	114.45	118.26
5	D	502	PLP	C5A-C5-C6	4.85	127.35	119.37
5	C	503	PLP	C2A-C2-C3	-4.75	115.02	120.89
3	B	502	EVM	C5A-C5-C6	4.72	127.13	119.37
3	B	502	EVM	C3-C4-C4A	4.34	128.51	120.41
3	B	502	EVM	C4-C3-C2	-4.30	117.53	120.19
3	B	502	EVM	C5-C4-C4A	-4.23	114.60	121.56
3	B	502	EVM	C-CA-N	-3.99	100.77	108.67
3	B	502	EVM	O4P-C5A-C5	3.90	116.79	109.35
3	B	502	EVM	O2P-P-O4P	-3.83	96.55	106.73
3	A	502	EVM	O2P-P-O4P	-3.45	97.55	106.73
5	C	503	PLP	C2A-C2-N1	3.37	124.24	117.67
5	D	502	PLP	C2A-C2-C3	-3.20	116.94	120.89
5	D	502	PLP	C2A-C2-N1	3.14	123.81	117.67
4	C	502	DSN	OXT-C-O	-3.09	117.07	124.09
5	C	503	PLP	C5A-C5-C6	3.06	124.40	119.37
4	C	502	DSN	OXT-C-CA	2.98	123.53	113.38
3	A	502	EVM	C2A-C2-C3	-2.91	117.29	120.89
3	A	502	EVM	C4-C3-C2	-2.86	118.42	120.19
5	D	502	PLP	O4P-C5A-C5	2.86	114.81	109.35
3	B	502	EVM	C6-N1-C2	2.76	124.29	119.17
3	B	502	EVM	C2A-C2-C3	-2.67	117.59	120.89
5	D	502	PLP	O3-C3-C2	2.67	123.30	117.49
3	B	502	EVM	C2A-C2-N1	2.67	122.88	117.67
5	D	502	PLP	C6-N1-C2	2.65	124.07	119.17
3	A	502	EVM	O4P-P-O3P	2.63	113.85	106.47
3	A	502	EVM	O2P-P-O1P	2.55	117.39	107.64
5	C	503	PLP	O3-C3-C2	2.52	122.99	117.49
5	D	502	PLP	C6-C5-C4	-2.48	116.21	118.16
3	B	502	EVM	C3-C4-C5	-2.43	116.40	118.26
3	A	502	EVM	C2A-C2-N1	2.28	122.12	117.67
3	A	502	EVM	C4-C4A-N	-2.21	118.10	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	EVM	C6-N1-C2	2.06	122.99	119.17
5	D	502	PLP	C4A-C4-C3	-2.01	117.09	120.50
5	D	502	PLP	C4-C3-C2	-2.01	117.10	120.07

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EVM	CB-CA-N-C4A
3	A	502	EVM	C5A-O4P-P-O1P
3	A	502	EVM	C5A-O4P-P-O2P
3	A	502	EVM	C5A-O4P-P-O3P
3	B	502	EVM	CB-CA-N-C4A
3	B	502	EVM	C5A-O4P-P-O1P
3	B	502	EVM	C5A-O4P-P-O2P
3	B	502	EVM	C5A-O4P-P-O3P
3	B	502	EVM	N-CA-CB-OG
4	C	502	DSN	O-C-CA-N
4	C	502	DSN	O-C-CA-CB
4	C	502	DSN	OXT-C-CA-CB
4	C	502	DSN	OXT-C-CA-N
3	B	502	EVM	OXT-C-CA-N
3	A	502	EVM	OXT-C-CA-N
3	A	502	EVM	N-CA-CB-OG
4	D	501	DSN	OXT-C-CA-N
3	B	502	EVM	C-CA-CB-OG

There are no ring outliers.

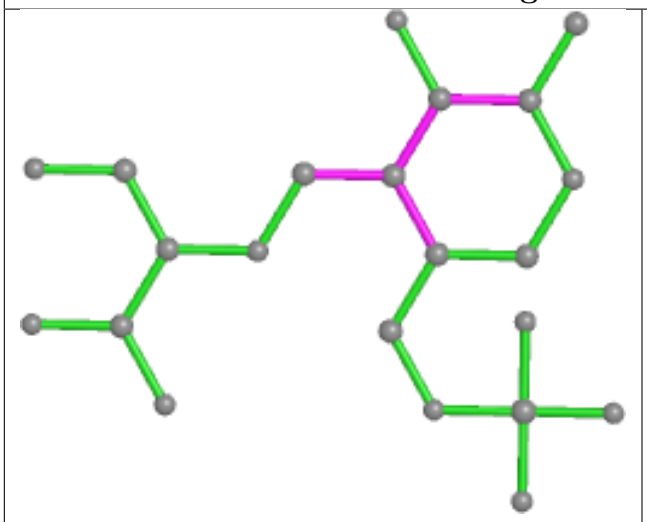
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EVM	5	0
4	D	501	DSN	2	0
5	D	502	PLP	2	0
3	A	502	EVM	6	0
5	C	503	PLP	3	0
4	C	502	DSN	2	0

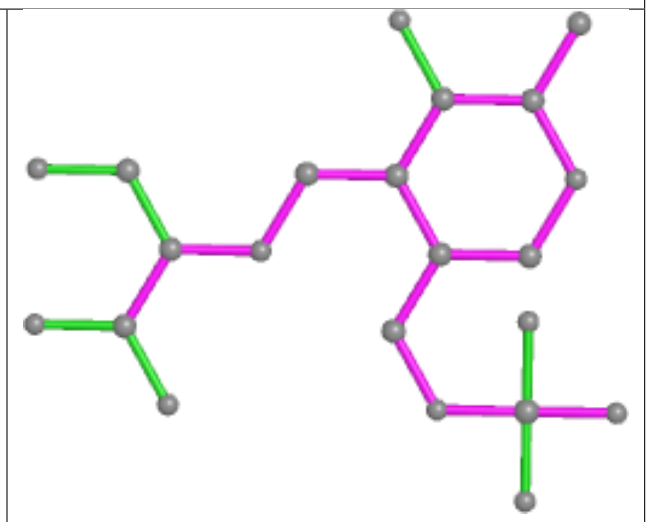
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

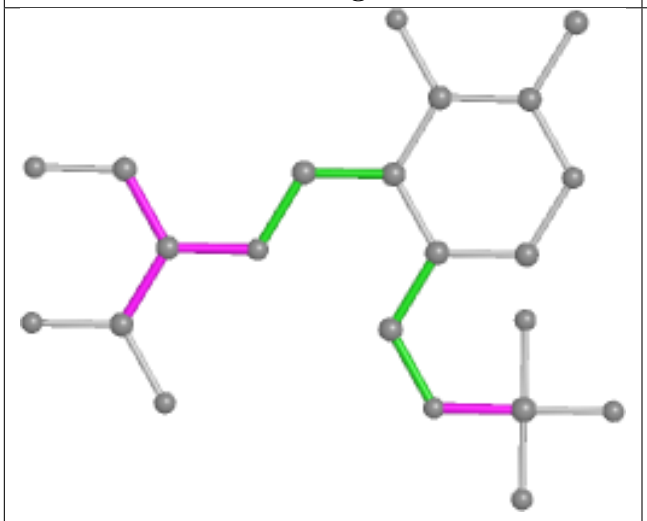
Ligand EVM B 502



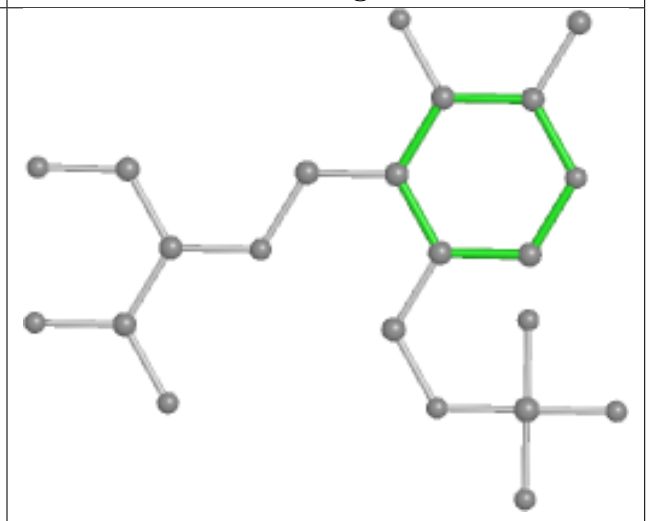
Bond lengths



Bond angles

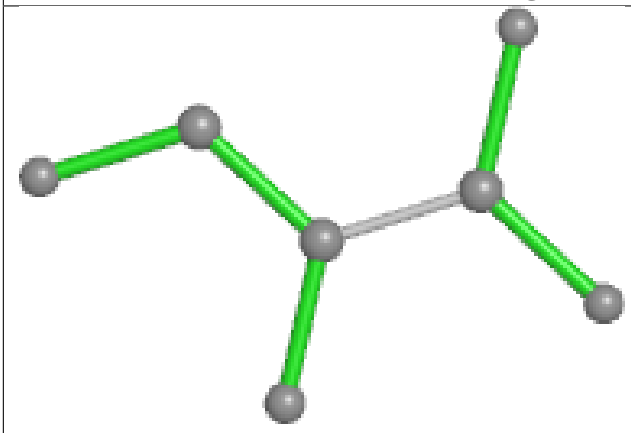


Torsions

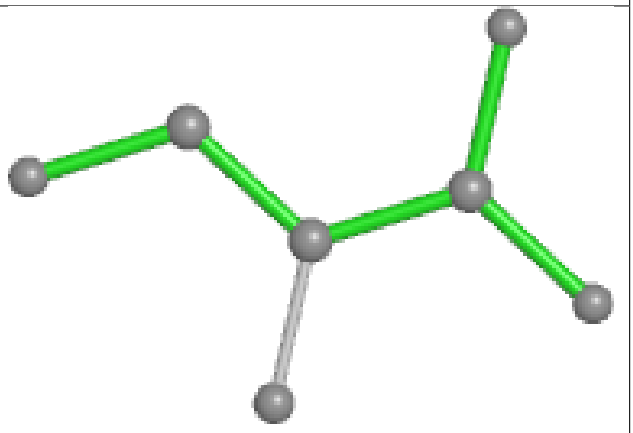


Rings

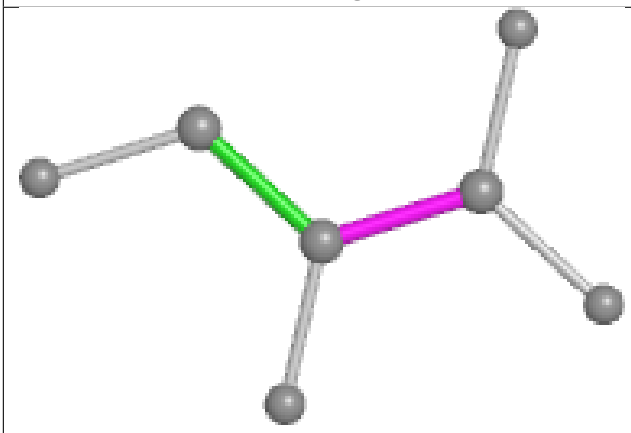
Ligand DSN D 501



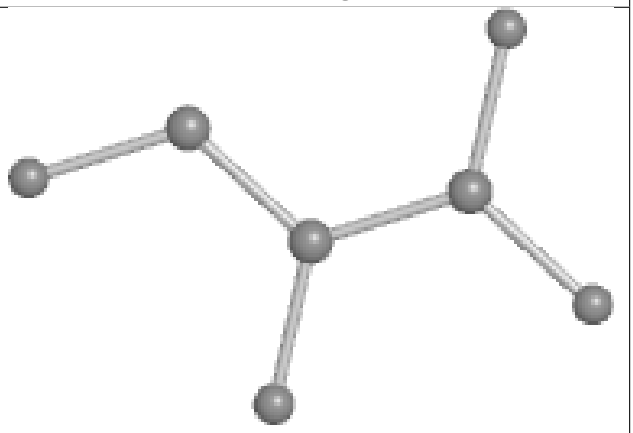
Bond lengths



Bond angles

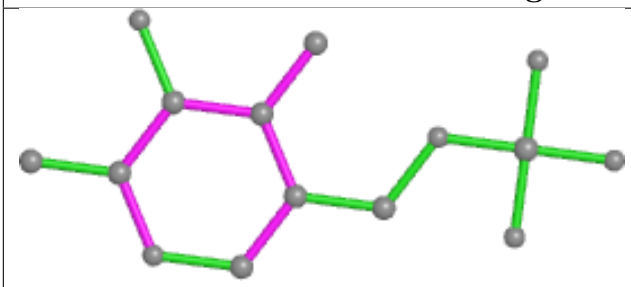


Torsions

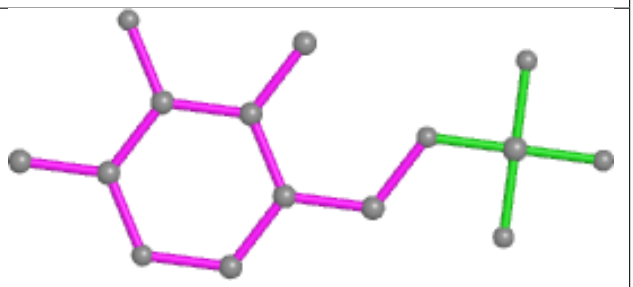


Rings

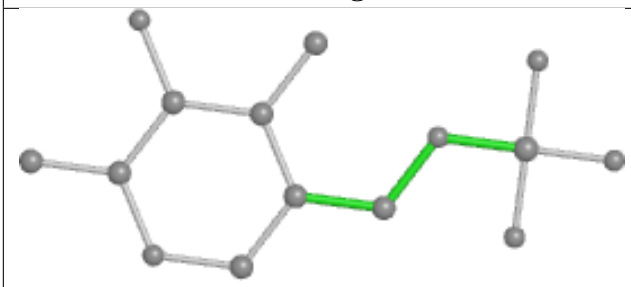
Ligand PLP D 502



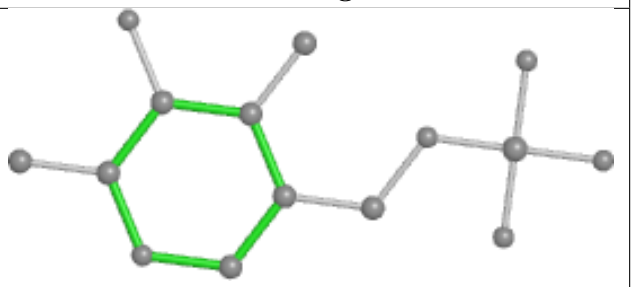
Bond lengths



Bond angles

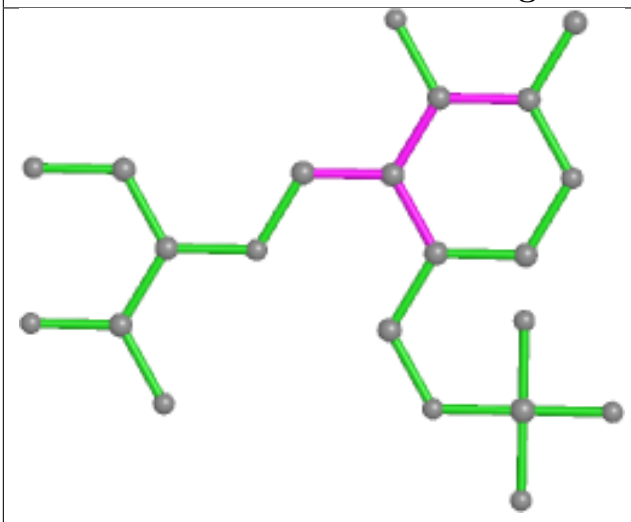


Torsions

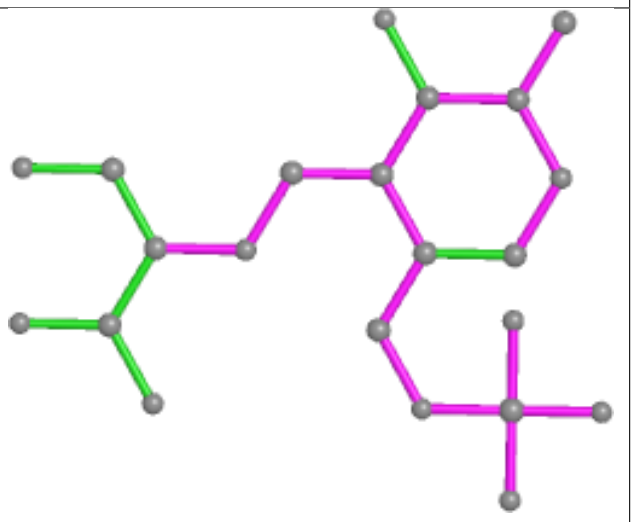


Rings

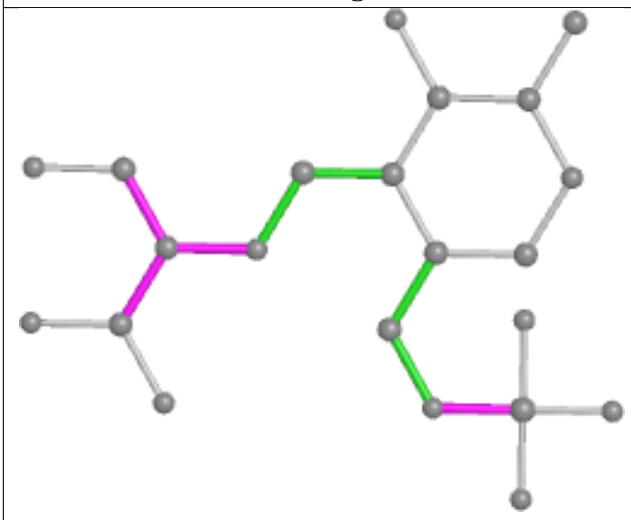
Ligand EVM A 502



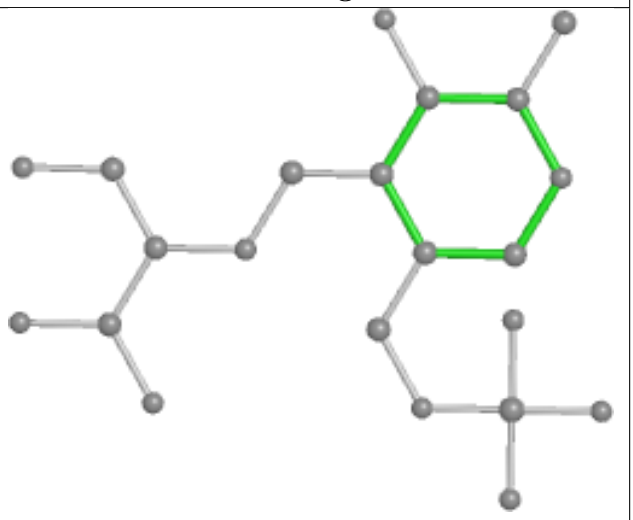
Bond lengths



Bond angles

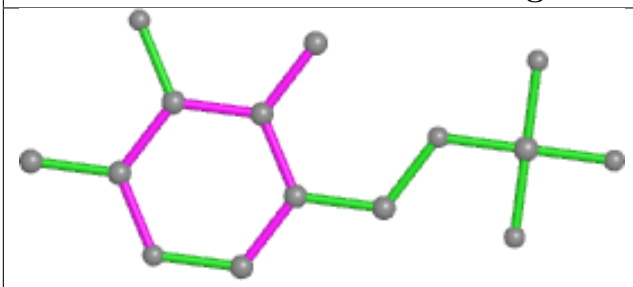


Torsions

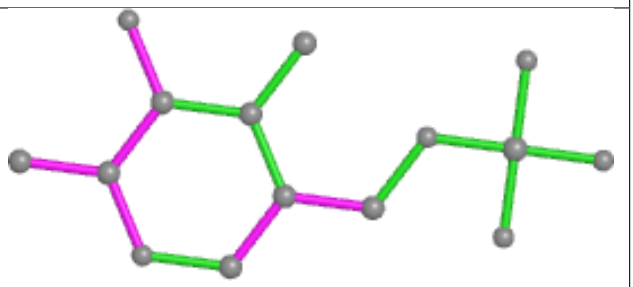


Rings

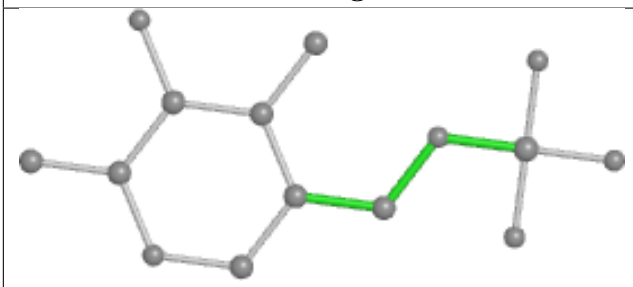
Ligand PLP C 503



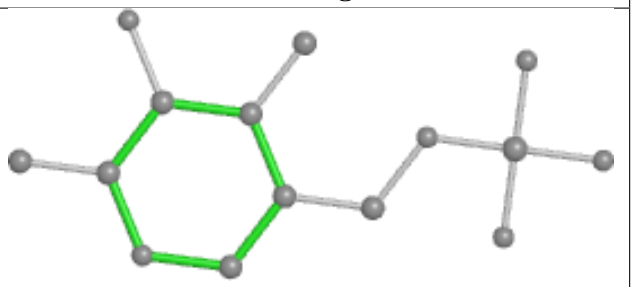
Bond lengths



Bond angles

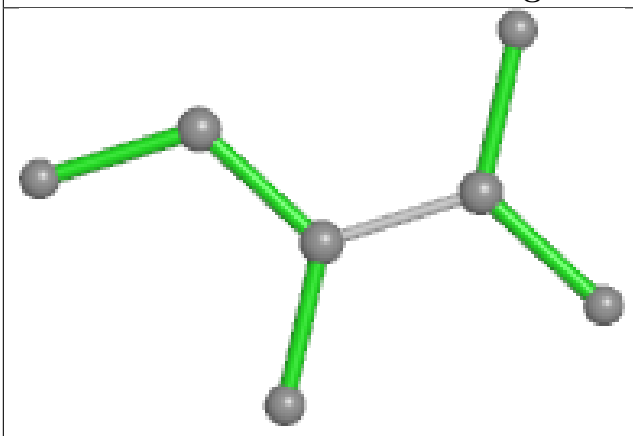


Torsions

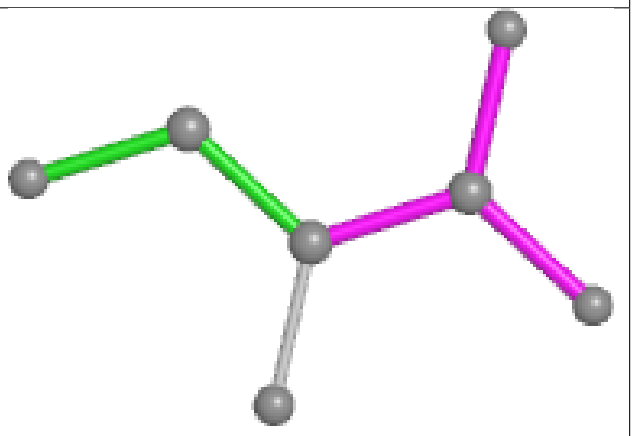


Rings

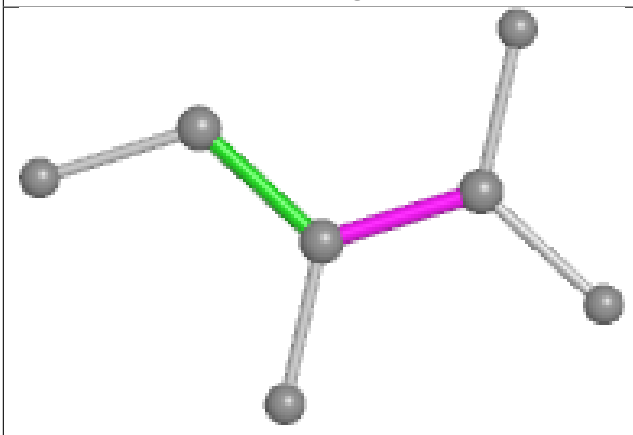
Ligand DSN C 502



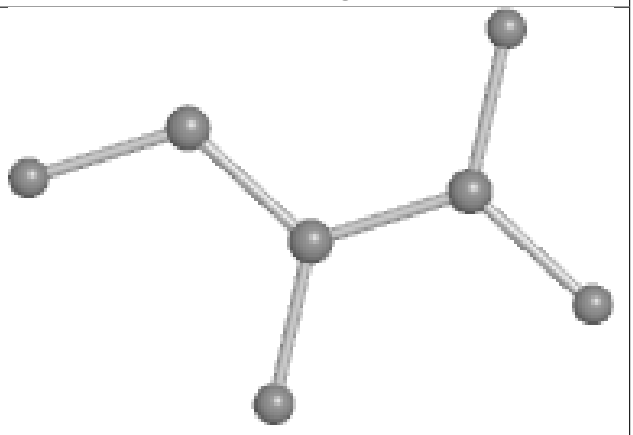
Bond lengths



Bond angles



Torsions



Rings

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	410/415 (98%)	0.40	26 (6%) 20 24	31, 52, 90, 112	0
1	B	410/415 (98%)	0.08	12 (2%) 51 57	34, 51, 75, 122	0
1	C	410/415 (98%)	0.60	42 (10%) 6 8	35, 57, 87, 110	0
1	D	410/415 (98%)	0.25	27 (6%) 18 22	40, 65, 93, 109	0
All	All	1640/1660 (98%)	0.33	107 (6%) 18 23	31, 56, 89, 122	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	390	LEU	6.8
1	C	387	VAL	5.7
1	C	353	GLN	5.6
1	A	390	LEU	5.5
1	C	357	PHE	5.1
1	C	413	PHE	5.0
1	D	354	LEU	4.9
1	D	357	PHE	4.7
1	D	8	TYR	4.4
1	C	324	THR	4.3
1	A	357	PHE	4.1
1	A	353	GLN	3.9
1	C	325	LYS	3.8
1	C	306	ASP	3.8
1	C	328	GLU	3.7
1	A	358	LYS	3.7
1	B	7	ASP	3.7
1	D	396	PRO	3.7
1	B	398	VAL	3.7
1	C	7	ASP	3.6
1	D	11	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	3.5
1	A	307	PHE	3.4
1	A	393	HIS	3.4
1	A	387	VAL	3.4
1	D	10	ALA	3.3
1	C	355	SER	3.3
1	A	408	VAL	3.3
1	A	306	ASP	3.2
1	A	8	TYR	3.2
1	D	408	VAL	3.2
1	A	328	GLU	3.1
1	D	307	PHE	3.1
1	C	10	ALA	3.1
1	C	380	ARG	3.1
1	B	394	ASP	3.1
1	A	394	ASP	3.0
1	C	267	VAL	3.0
1	C	358	LYS	2.9
1	C	21	ALA	2.9
1	A	355	SER	2.9
1	D	353	GLN	2.9
1	C	356	PRO	2.8
1	C	383	ALA	2.7
1	A	354	LEU	2.7
1	C	264	LEU	2.7
1	A	398	VAL	2.7
1	D	412	ALA	2.7
1	D	390	LEU	2.7
1	C	332	VAL	2.7
1	A	324	THR	2.7
1	C	359	THR	2.7
1	B	396	PRO	2.6
1	C	329	ASN	2.6
1	C	321	VAL	2.6
1	C	354	LEU	2.6
1	C	331	LYS	2.5
1	D	328	GLU	2.5
1	C	322	ASP	2.5
1	A	401	ARG	2.5
1	D	7	ASP	2.5
1	A	413	PHE	2.4
1	C	412	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	326	VAL	2.4
1	A	264	LEU	2.4
1	D	399	LEU	2.4
1	C	351	TYR	2.4
1	C	409	LEU	2.3
1	B	357	PHE	2.3
1	B	397	GLU	2.3
1	D	392	ASN	2.3
1	B	237	GLY	2.3
1	C	30	ILE	2.3
1	B	328	GLU	2.3
1	D	413	PHE	2.3
1	C	408	VAL	2.3
1	C	327	VAL	2.3
1	A	396	PRO	2.3
1	B	401	ARG	2.3
1	C	386	MET	2.2
1	A	28	ASN	2.2
1	D	13	PRO	2.2
1	D	393	HIS	2.2
1	D	327	VAL	2.2
1	B	393	HIS	2.2
1	A	24	GLU	2.2
1	C	101	ALA	2.2
1	A	13	PRO	2.2
1	C	11	PHE	2.2
1	C	391	GLU	2.2
1	D	121	LEU	2.2
1	D	264	LEU	2.2
1	C	373	GLY	2.1
1	D	359	THR	2.1
1	D	306	ASP	2.1
1	D	373	GLY	2.1
1	B	395	LYS	2.1
1	D	324	THR	2.1
1	D	325	LYS	2.1
1	C	399	LEU	2.1
1	C	268	ILE	2.0
1	C	28	ASN	2.0
1	C	336	VAL	2.0
1	C	301	PHE	2.0
1	A	397	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	399	LEU	2.0
1	A	323	VAL	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)

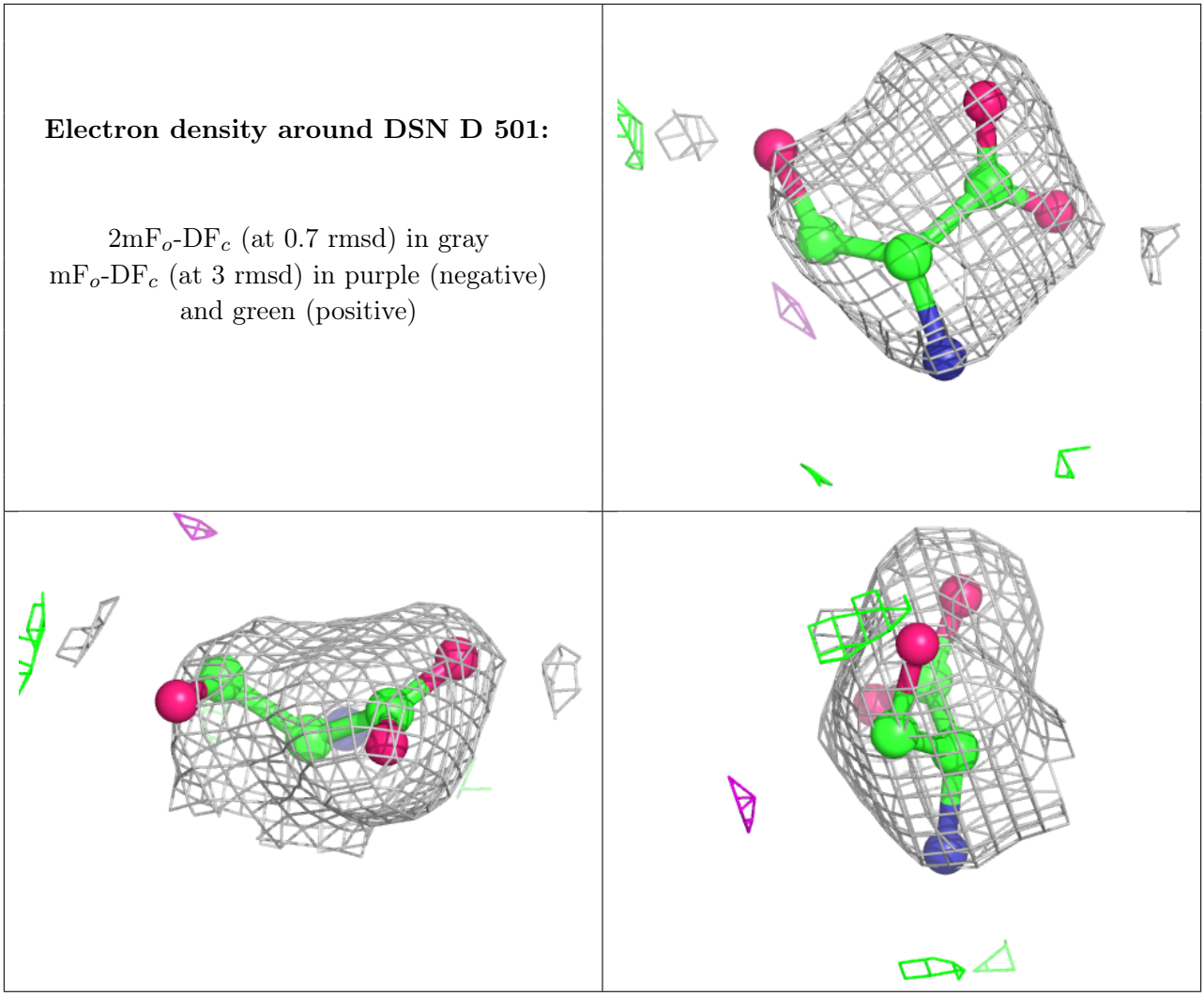
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	DSN	D	501	7/7	0.87	0.24	65,92,98,109	0
4	DSN	C	502	7/7	0.92	0.16	50,75,87,91	0
5	PLP	C	503	15/16	0.93	0.16	42,71,79,95	0
2	NA	C	501	1/1	0.94	0.08	49,49,49,49	0
3	EVM	A	502	22/22	0.94	0.17	43,70,82,95	0
3	EVM	B	502	22/22	0.94	0.17	48,63,84,90	0
2	NA	A	501	1/1	0.96	0.15	48,48,48,48	0
2	NA	B	501	1/1	0.97	0.11	48,48,48,48	0
5	PLP	D	502	15/16	0.97	0.13	64,89,97,98	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.

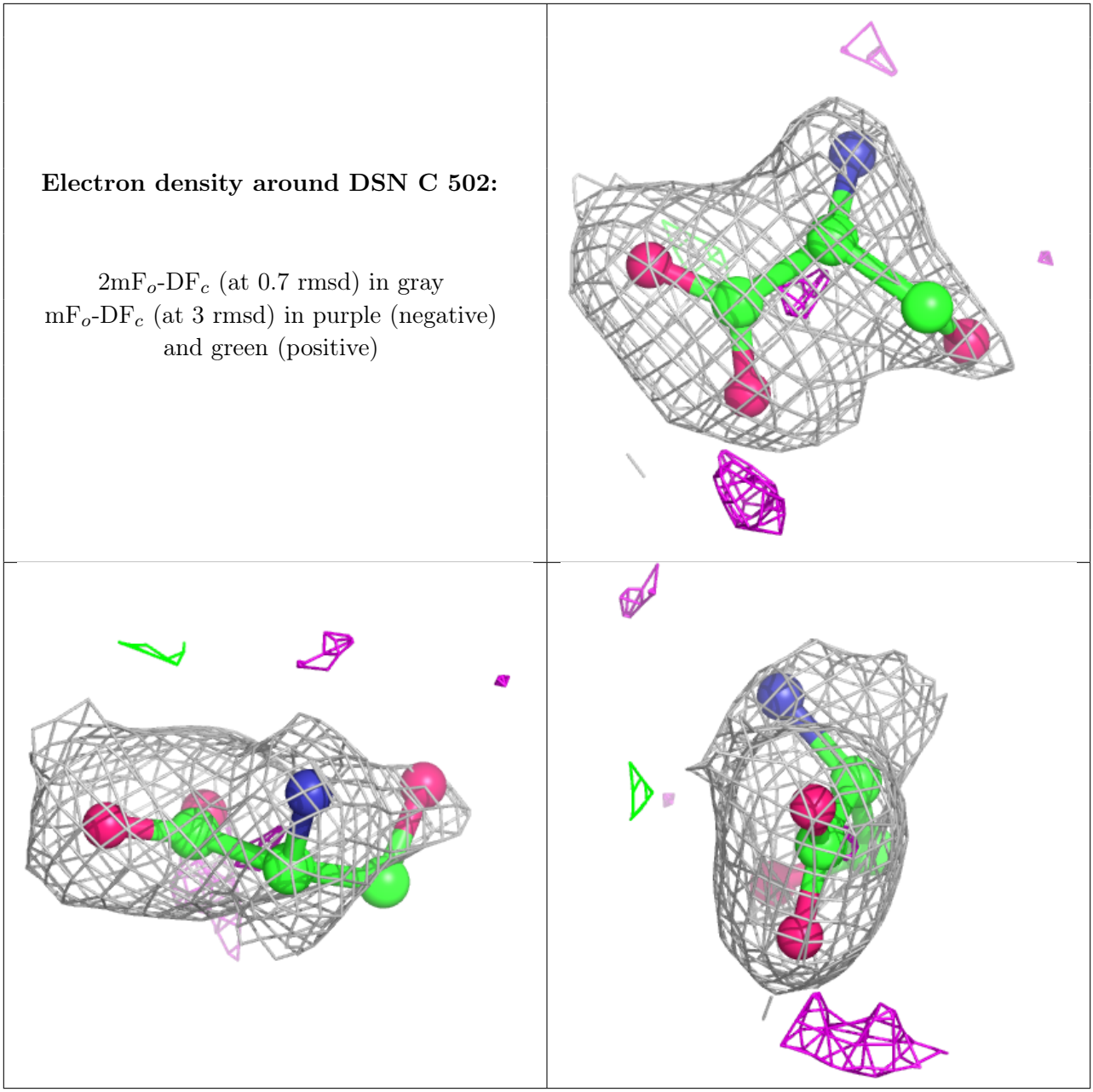
Electron density around DSN D 501:

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



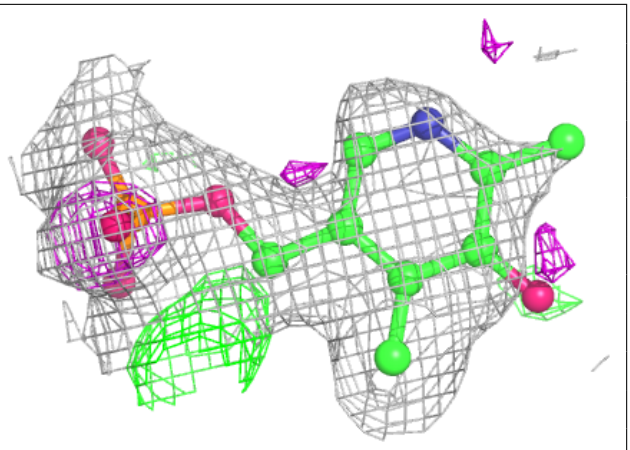
Electron density around DSN C 502:

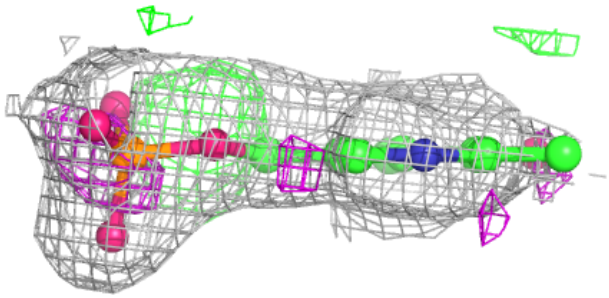
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

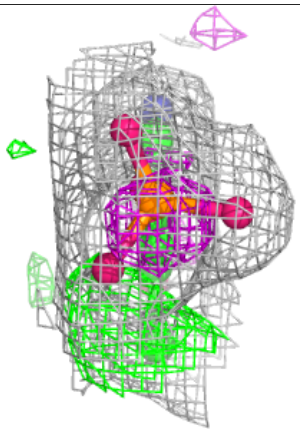


Electron density around PLP C 503:

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

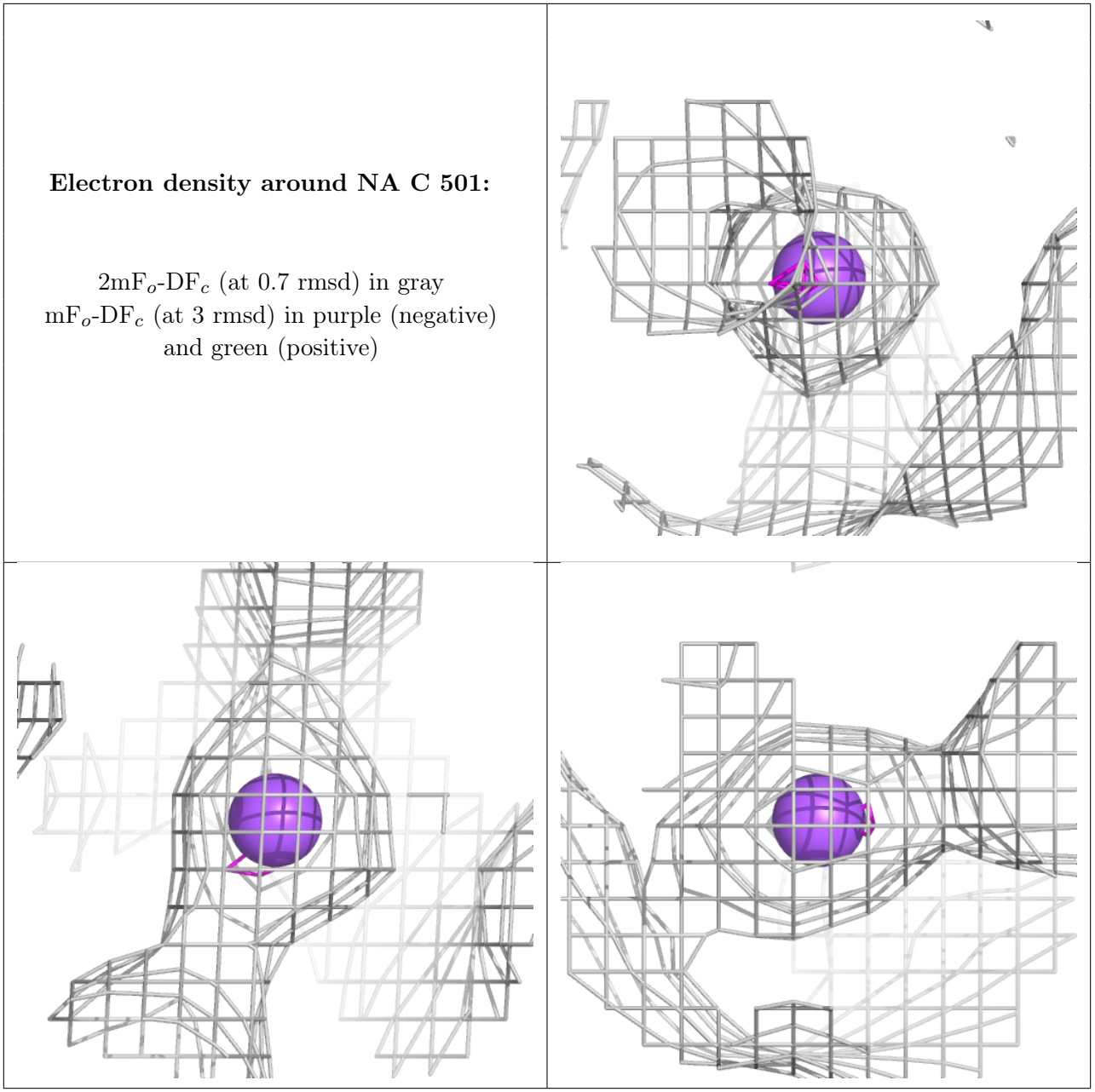






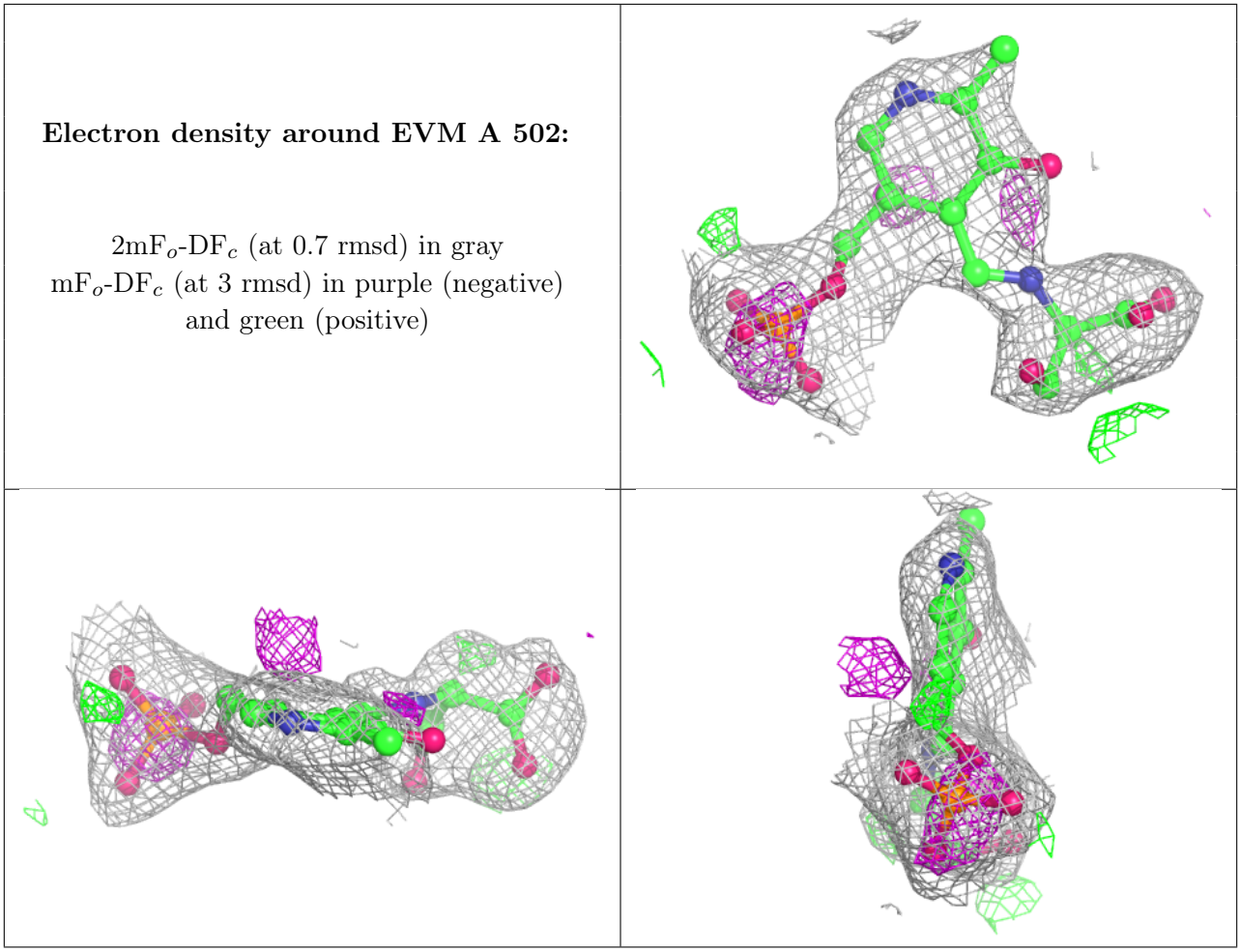
Electron density around NA C 501:

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



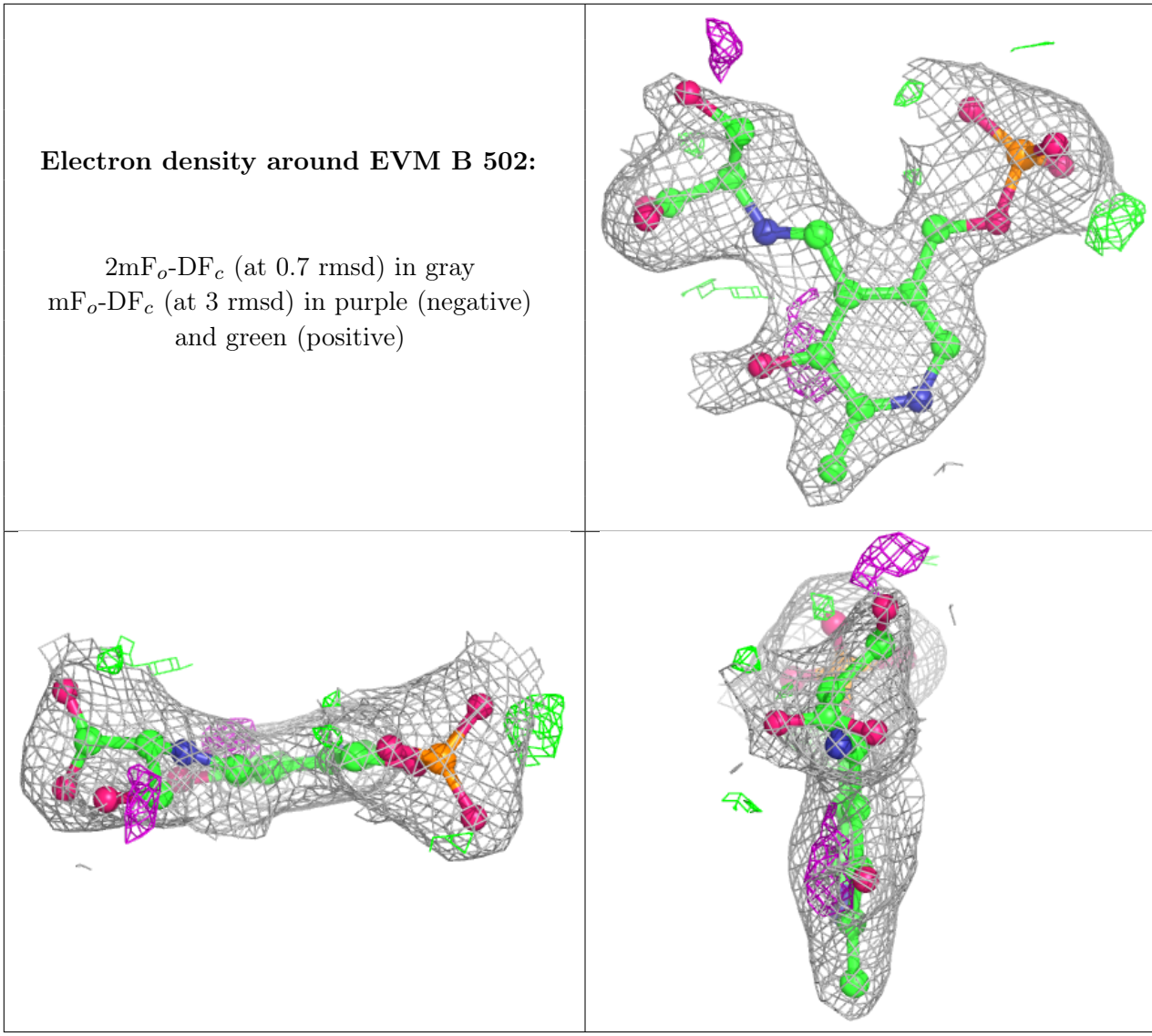
Electron density around EVM A 502:

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



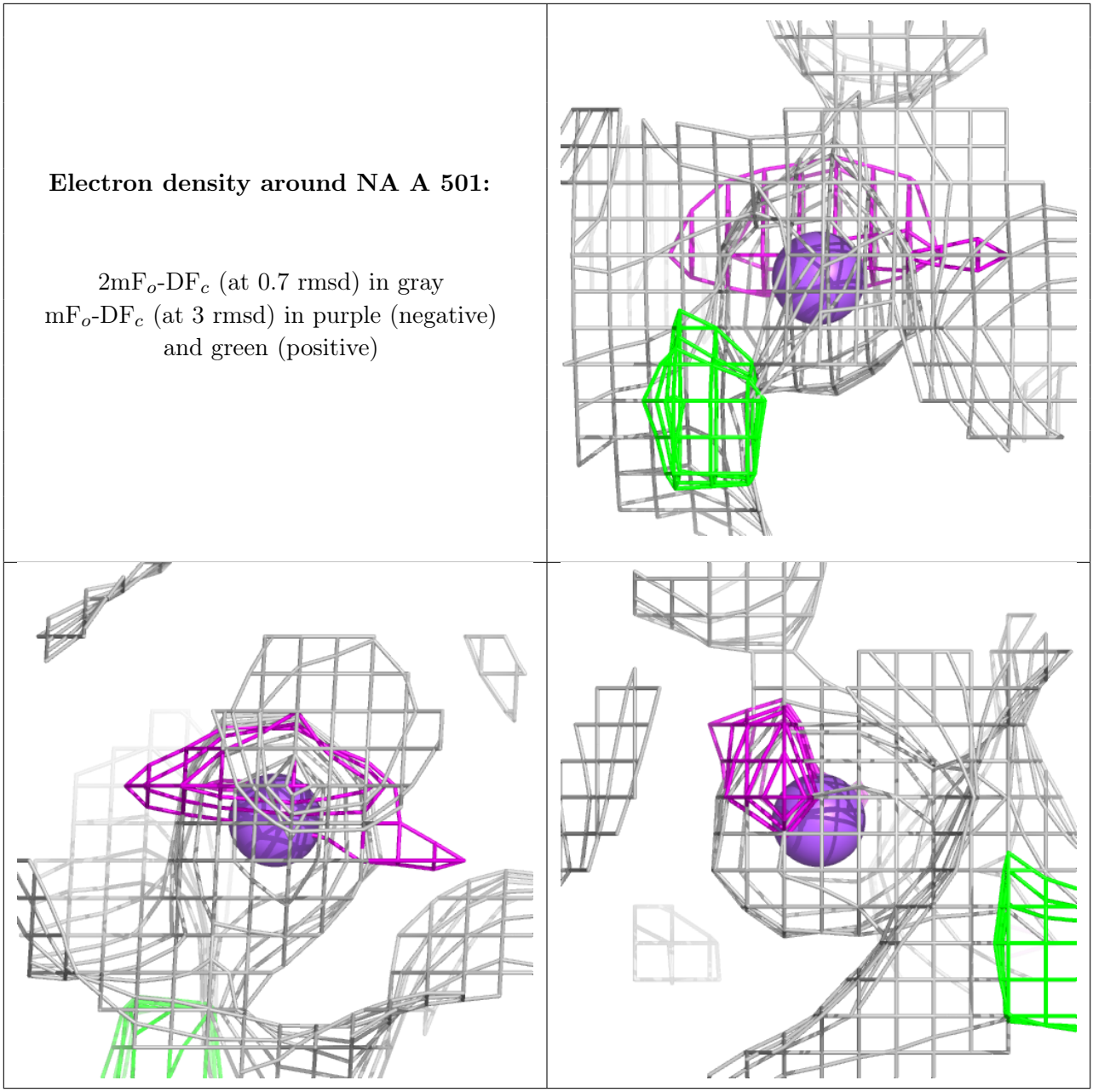
Electron density around EVM B 502:

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



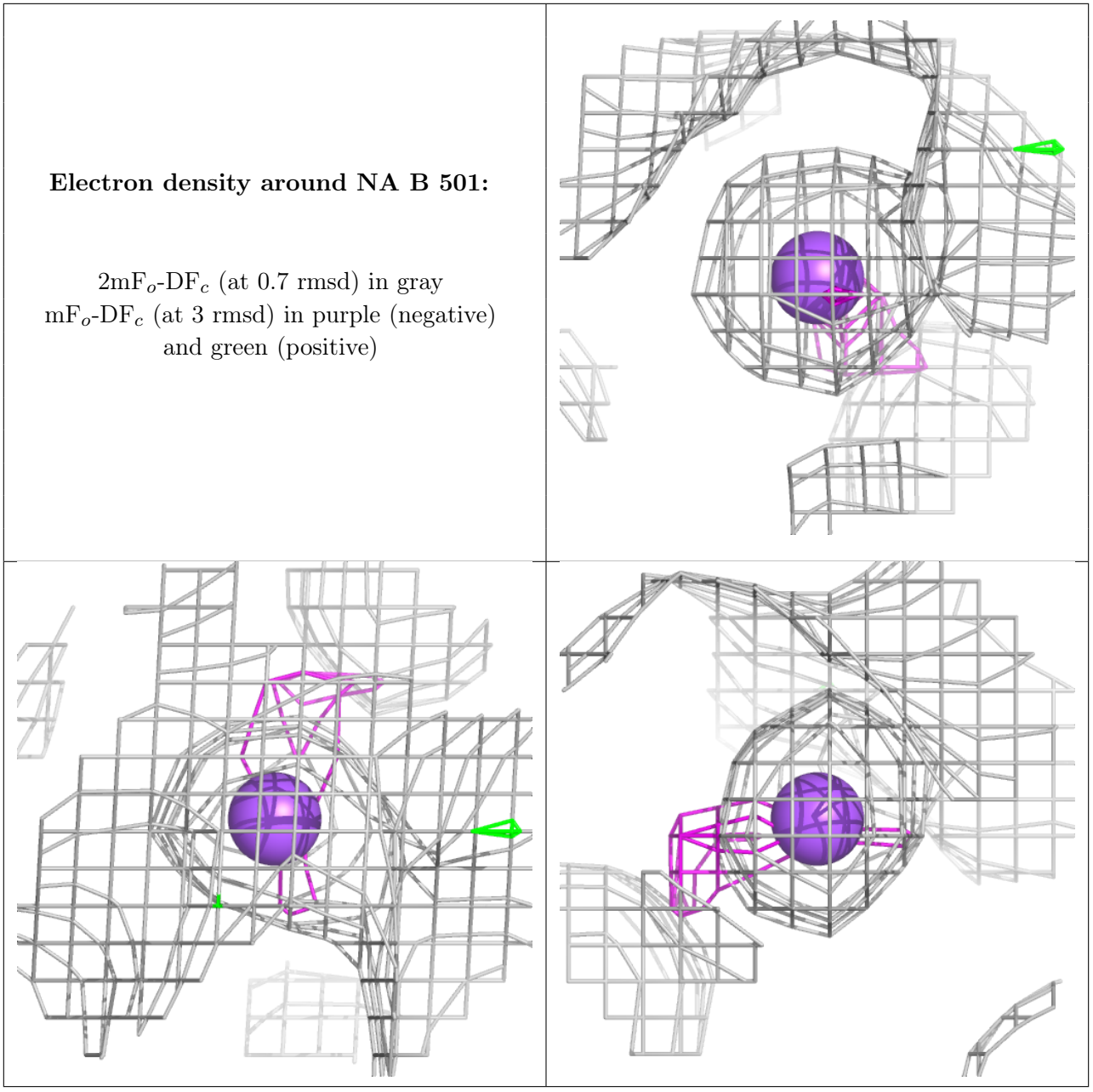
Electron density around NA A 501:

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



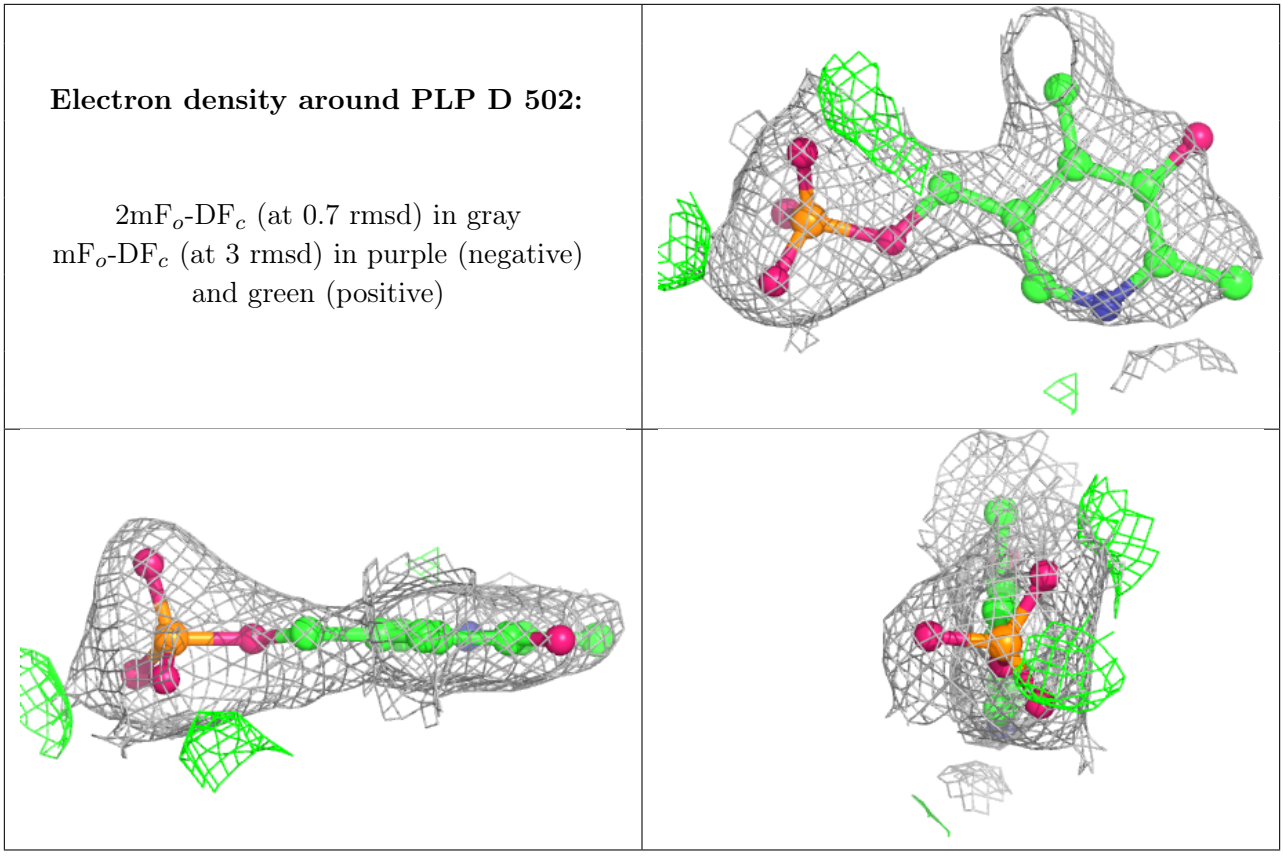
Electron density around NA B 501:

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



Electron density around PLP D 502:

$2mF_o$-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.