



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:45 AM UTC

PDB ID : 6TGH / pdb_00006tgh
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

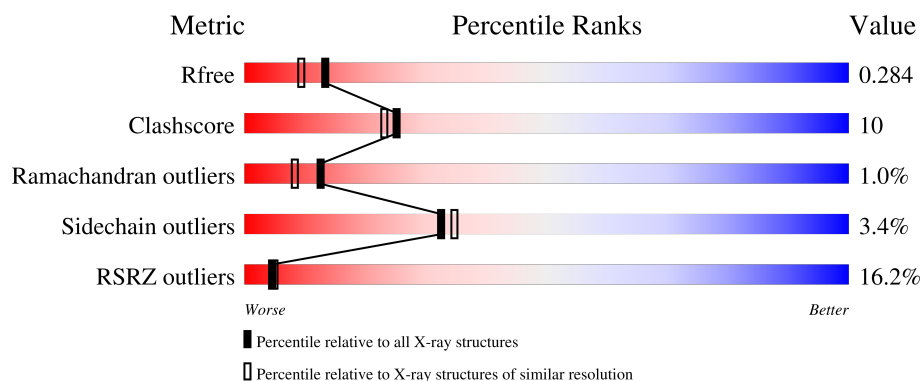
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 $\leq 5\%$. 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	415	22% 70%25%..
1	B	415	3% 86%12%..
1	C	415	30% 72%23%..
1	D	415	9% 85%13%. .

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			

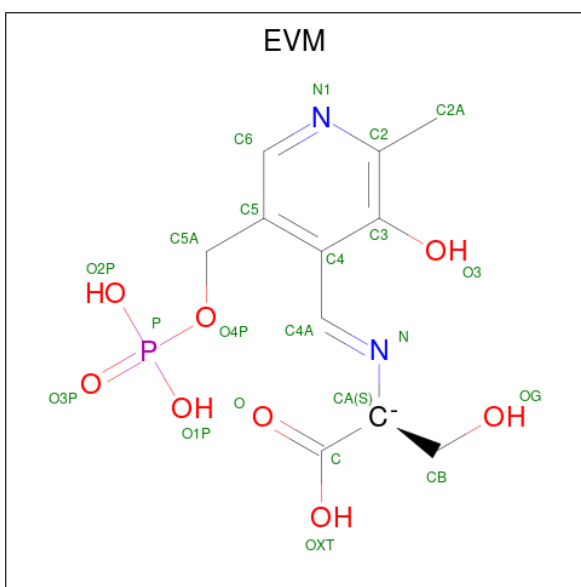
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

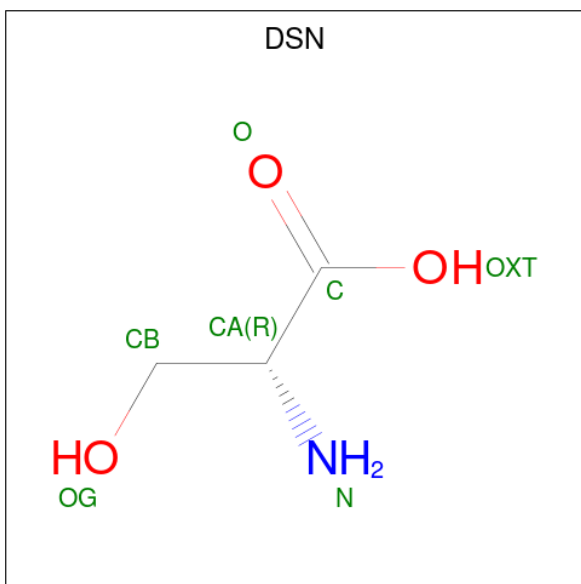
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is L-Serine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methylene] (CCD ID: EVM) (formula: C₁₁H₁₄N₂O₈P) (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 (CCD ID: DSN) (formula: $C_3H_7NO_3$) (labeled as "Ligand of Interest" by depositor).



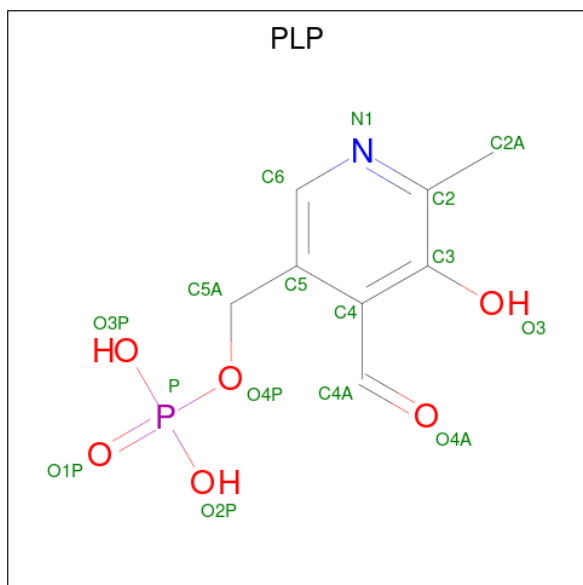
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			7	3	1	3		

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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 (CCD ID: 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.

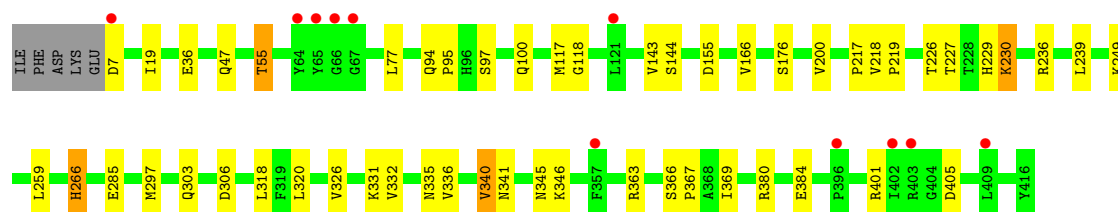
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	94	Total	O	0	0
			94	94		
6	C	101	Total	O	0	0
			101	101		
6	B	114	Total	O	0	0
			114	114		
6	D	72	Total	O	0	0
			72	72		

- Molecule 1: Serine hydroxymethyltransferase



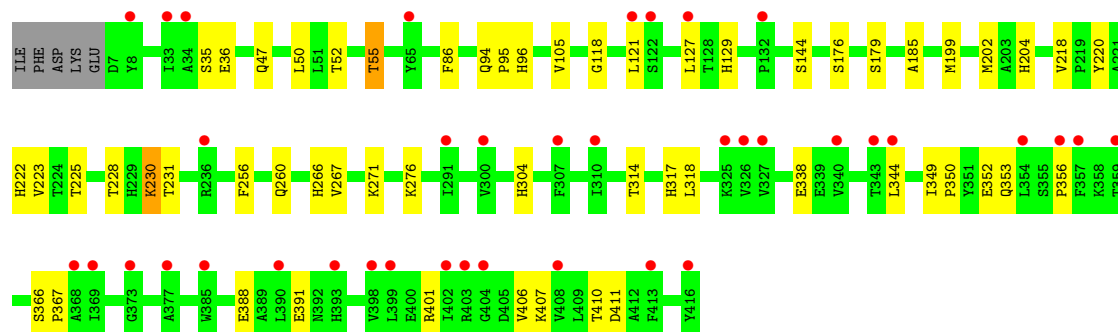
- Molecule 1: Serine hydroxymethyltransferase

Chain B:  3% 86% 12% ..



- Molecule 1: Serine hydroxymethyltransferase

Chain D:  9% 85% 13% .



4 Data and refinement statistics

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 47.76 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.76-2.12) 99.5 (47.76-2.12)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.97%)	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)	0.36 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: EVM, PLP, NA, DSN

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	1.14	1/3190 (0.0%)	1.57	15/4332 (0.3%)
1	B	1.07	1/3190 (0.0%)	1.45	2/4332 (0.0%)
1	C	1.20	7/3189 (0.2%)	1.59	9/4330 (0.2%)
1	D	1.05	0/3189	1.51	1/4330 (0.0%)
All	All	1.12	9/12758 (0.1%)	1.53	27/17324 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	ILE	C-O	7.91	1.33	1.23
1	C	377	ALA	C-O	6.58	1.31	1.24
1	B	200	VAL	C-O	5.70	1.30	1.24
1	C	301	PHE	C-O	5.62	1.31	1.24
1	C	379	SER	C-O	5.33	1.30	1.24
1	A	381	GLN	C-O	5.24	1.30	1.24
1	C	287	GLY	C-O	5.15	1.29	1.23
1	C	217	PRO	C-O	-5.14	1.17	1.24
1	C	378	GLU	C-O	5.08	1.29	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	PRO	CA-C-N	8.30	125.47	120.24
1	C	217	PRO	C-N-CA	8.30	125.47	120.24
1	C	20	ASP	CB-CA-C	7.45	121.78	110.08
1	A	217	PRO	CA-C-N	7.42	124.91	120.24
1	A	217	PRO	C-N-CA	7.42	124.91	120.24
1	A	228	THR	N-CA-C	-6.54	104.78	112.89
1	C	18	ALA	N-CA-C	-6.11	105.95	113.41
1	A	71	ILE	N-CA-C	-5.92	105.08	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	PRO	CA-C-N	5.72	123.84	120.24
1	B	217	PRO	C-N-CA	5.72	123.84	120.24
1	A	413	PHE	CB-CA-C	5.58	116.44	108.68
1	A	227	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	267	VAL	N-CA-C	-5.38	105.14	111.00
1	D	222	HIS	N-CA-C	-5.29	105.41	111.07
1	C	29[A]	ASN	CA-CB-CG	5.28	117.88	112.60
1	C	29[B]	ASN	CA-CB-CG	5.28	117.88	112.60
1	C	410	THR	CA-C-N	5.19	128.00	120.79
1	C	410	THR	C-N-CA	5.19	128.00	120.79
1	C	302	ASN	O-C-N	5.08	127.31	122.07
1	A	411	ASP	CA-C-N	5.06	127.37	120.54
1	A	411	ASP	C-N-CA	5.06	127.37	120.54
1	A	257	PRO	CA-C-N	5.03	125.67	119.99
1	A	257	PRO	C-N-CA	5.03	125.67	119.99
1	A	148	ASP	CA-C-N	5.02	126.97	120.44
1	A	148	ASP	C-N-CA	5.02	126.97	120.44
1	A	388	GLU	CA-C-N	5.02	127.00	120.28
1	A	388	GLU	C-N-CA	5.02	127.00	120.28

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	98	0
1	B	3128	0	3108	34	0
1	C	3120	0	3092	92	0
1	D	3120	0	3093	38	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	5	0
3	B	22	0	0	3	0
4	C	7	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	7	0	6	2	0
5	C	15	0	7	1	0
5	D	15	0	6	3	0
6	A	94	0	0	5	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	243	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 (243) 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:B:230:LYS:HZ1	3:B:502:EVM:C4A	1.91	0.82
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:C:366:SER:O	1:C:370:THR:OG1	2.03	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
1:C:366:SER:H	1:C:367:PRO:HD3	1.59	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:A:230:LYS:HZ1	3:A:502:EVM:C4A	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HZ1	3:A:502:EVM:C4	2.10	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: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:372:ARG:C	6:C:604:HOH:O	2.45	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:297:MET:HE2	1:B:369:ILE:HD11	1.83	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:A:318:LEU:HD12	1:A:318:LEU:C	2.31	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:A:44:MET:O	1:A:45:ALA:C	2.49	0.56
1:C:366:SER:N	1:C:367:PRO:CD	2.68	0.56
1:C:318:LEU:HD12	1:C:318:LEU:C	2.31	0.55
1:A:27:GLN:HG2	6:A:603:HOH:O	2.07	0.55
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:345:ASN:C	1:C:346:LYS:O	2.50	0.54
1:C:317:HIS:NE2	1:C:318:LEU:HD23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:185:ALA:HA	1:D:220:TYR:CD1	2.43	0.53
1:C:19:ILE:O	1:C:19:ILE:HG22	2.08	0.53
1:A:227:THR:HB	1:A:229:HIS:CE1	2.43	0.53
1:A:229:HIS:O	1:A:230:LYS:HB2	2.08	0.53
1:B:318:LEU:C	1:B:318:LEU:HD12	2.34	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:322:ASP:OD1	1:A:322:ASP:C	2.53	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:155:ASP:C	1:A:155:ASP:OD1	2.53	0.52
1:A:352:GLU:OE2	1:A:360:SER:OG	2.28	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:326:VAL:O	1:A:326:VAL:HG12	2.10	0.51
1:D:366:SER:N	1:D:367:PRO:HD3	2.25	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:D:318:LEU:C	1:D:318:LEU:HD12	2.36	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:256:PHE:C	1:D:256:PHE:CD2	2.91	0.48
1:D:406:VAL:O	1:D:410:THR:HG23	2.13	0.48
1:C:382:ILE:HG22	1:C:386:MET:HE3	1.94	0.48
1:D:86:PHE:CD1	1:D:202:MET:HE1	2.49	0.48
1:A:8:TYR:HB2	1:C:42:ALA:HB2	1.96	0.48
1:C:50:LEU:HD12	1:C:50:LEU:C	2.38	0.48
1:B:118:GLY:O	1:B:144:SER:HA	2.13	0.48
1:A:19:ILE:O	1:A:20:ASP:C	2.57	0.48
1:C:176:SER:HA	1:C:204:HIS:CD2	2.49	0.48
1:C:349:ILE:O	1:C:350:PRO:C	2.56	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:C:229:HIS:C	1:C:230:LYS:HG3	2.39	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: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
1:B:331:LYS:HE3	1:B:335:ASN:HD21	1.79	0.46
1:A:56:ALA:O	1:A:57:GLU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:HIS:O	1:D:231:THR:OG1	2.27	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:C:37:ASN:CG	1:C:233:ARG:HG3	2.40	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: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:C:298:ALA:O	1:C:299:ASP:C	2.60	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:A:55:THR:HG23	1:C:36:GLU:CD	2.42	0.44
1:C:244:ASP:OD1	1:C:244:ASP:C	2.61	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:A:388:GLU:CD	1:A:401:ARG:HH12	2.25	0.43
1:C:19:ILE:O	1:C:19:ILE:CG2	2.66	0.43
1:A:50:LEU:HB3	1:C:44:MET:SD	2.59	0.43
1:A:290:VAL:HG13	1:A:366:SER:OG	2.17	0.43
1:B:332:VAL:O	1:B:336:VAL:HG23	2.17	0.43
1:D:176:SER:HA	1:D:204:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:GLU:OE2	1:A:26:GLN:NE2	2.43	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: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:D:349:ILE:O	1:D:350:PRO:C	2.62	0.42
1:A:61:GLY:C	1:A:62:LYS:HG3	2.43	0.42
1:C:341:ASN:CB	1:C:406:VAL:HG11	2.46	0.42
1:C:345:ASN:O	1:C:346:LYS:C	2.62	0.42
1:D:94:GLN:O	1:D:95:PRO:C	2.62	0.42
1:A:297:MET:HE2	1:A:369:ILE:HD11	2.02	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:D:129:HIS:CE1	5:D:502:PLP:H2A3	2.55	0.41
1:B:218:VAL:N	1:B:219:PRO:CD	2.84	0.41
1:A:387:VAL:O	1:A:388:GLU:C	2.63	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:70:VAL:HG11	1:C:21:ALA:C	2.45	0.41
1:A:293:ASN:OD1	1:A:379:SER:OG	2.36	0.41
1:B:155:ASP:C	1:B:155:ASP:OD1	2.63	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:CE1	1:D:202:MET:HE1	2.55	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:344:LEU:HD21	1:A:386:MET:HE3	2.03	0.40
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
1:A:265:GLU:OE1	1:A:265:GLU:HA	2.20	0.40
1:C:229:HIS:HD1	1:C:236:ARG:HA	1.85	0.40
1:C:50:LEU:C	1:C:50:LEU:CD1	2.94	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%)	7 3
1	B	409/415 (99%)	395 (97%)	13 (3%)	1 (0%)	43 44
1	C	409/415 (99%)	367 (90%)	35 (9%)	7 (2%)	7 3
1	D	409/415 (99%)	390 (95%)	17 (4%)	2 (0%)	24 22
All	All	1636/1660 (99%)	1511 (92%)	108 (7%)	17 (1%)	12 8

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

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Mol	Chain	Res	Type
1	B	230	LYS
1	D	230	LYS
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 ⓘ

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%)	317 (97%)	11 (3%)	32	35
1	B	328/332 (99%)	317 (97%)	11 (3%)	32	35
1	C	328/332 (99%)	311 (95%)	17 (5%)	21	19
1	D	328/332 (99%)	321 (98%)	7 (2%)	47	54
All	All	1312/1328 (99%)	1266 (96%)	46 (4%)	32	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	24	GLU
1	A	29	ASN
1	A	55	THR
1	A	73	VAL
1	A	77	LEU
1	A	134	SER
1	A	281	PRO

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Mol	Chain	Res	Type
1	A	340	VAL
1	A	381	GLN
1	A	393	HIS
1	C	14	GLU
1	C	15	LEU
1	C	19	ILE
1	C	28	ASN
1	C	29[A]	ASN
1	C	29[B]	ASN
1	C	71	ILE
1	C	121	LEU
1	C	165	GLU
1	C	167	ARG
1	C	179	SER
1	C	338	GLU
1	C	355	SER
1	C	366	SER
1	C	382	ILE
1	C	387	VAL
1	C	407	LYS
1	B	19	ILE
1	B	47	GLN
1	B	55	THR
1	B	77	LEU
1	B	166	VAL
1	B	249	LYS
1	B	259	LEU
1	B	266	HIS
1	B	285	GLU
1	B	340	VAL
1	B	346	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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	266	HIS
1	A	304	HIS
1	A	341	ASN
1	A	381	GLN
1	C	47	GLN
1	C	96	HIS
1	C	260	GLN
1	C	266	HIS
1	C	304	HIS
1	C	341	ASN
1	C	345	ASN
1	C	347	ASN
1	C	381	GLN
1	C	393	HIS
1	B	17	ASN
1	B	266	HIS
1	B	335	ASN
1	B	341	ASN
1	B	345	ASN
1	B	381	GLN
1	D	17	ASN
1	D	47	GLN
1	D	141	ASN
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 oligosaccharides 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
5	PLP	C	503	1	15,15,16	2.94	6 (40%)	21,22,23	2.00	5 (23%)
4	DSN	D	501	-	4,6,6	1.05	0	2,7,7	1.16	0
4	DSN	C	502	-	4,6,6	0.95	0	2,7,7	2.26	1 (50%)
3	EVM	A	502	-	22,22,22	2.88	4 (18%)	27,31,31	3.17	11 (40%)
3	EVM	B	502	-	22,22,22	2.69	4 (18%)	27,31,31	2.83	13 (48%)
5	PLP	D	502	1	15,15,16	3.09	6 (40%)	21,22,23	2.21	9 (42%)

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
5	PLP	C	503	1	-	0/6/6/8	0/1/1/1
4	DSN	D	501	-	-	2/6/6/6	-
4	DSN	C	502	-	-	4/6/6/6	-
3	EVM	A	502	-	-	6/17/17/17	0/1/1/1
3	EVM	B	502	-	-	7/17/17/17	0/1/1/1
5	PLP	D	502	1	-	0/6/6/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	EVM	C3-C2	9.10	1.50	1.41
3	B	502	EVM	C3-C2	8.82	1.50	1.41
5	C	503	PLP	C3-C2	7.95	1.49	1.41
5	D	502	PLP	C5-C4	7.87	1.49	1.40
5	D	502	PLP	C3-C2	6.79	1.48	1.41
3	B	502	EVM	C4-C3	6.09	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	EVM	C4-C5	6.08	1.50	1.42
5	C	503	PLP	C5-C4	5.59	1.46	1.40
3	A	502	EVM	C4-C3	5.57	1.50	1.41
3	B	502	EVM	C4-C5	4.17	1.47	1.42
5	D	502	PLP	C3-C4	3.67	1.47	1.40
5	C	503	PLP	C3-C4	3.13	1.46	1.40
5	C	503	PLP	C2-N1	2.92	1.39	1.33
5	D	502	PLP	C4A-C4	-2.78	1.46	1.51
3	A	502	EVM	C4-C4A	2.76	1.52	1.46
5	C	503	PLP	C6-C5	2.65	1.43	1.37
5	C	503	PLP	C4A-C4	-2.31	1.47	1.51
5	D	502	PLP	C2-N1	2.18	1.37	1.33
5	D	502	PLP	C6-C5	2.16	1.42	1.37
3	B	502	EVM	C4-C4A	2.09	1.51	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	EVM	CA-N-C4A	11.92	134.47	116.77
3	B	502	EVM	CA-N-C4A	6.41	126.29	116.77
3	A	502	EVM	O4P-C5A-C5	5.70	120.05	109.36
5	C	503	PLP	C2A-C2-C3	-4.94	115.02	120.80
5	D	502	PLP	C5A-C5-C6	4.90	127.35	119.36
3	B	502	EVM	C5A-C5-C6	4.77	127.13	119.36
3	A	502	EVM	C3-C4-C5	-4.76	114.45	118.28
3	B	502	EVM	C4-C3-C2	-4.65	117.53	120.14
3	B	502	EVM	C3-C4-C4A	4.49	128.51	120.40
3	B	502	EVM	C5-C4-C4A	-4.46	114.60	121.47
3	B	502	EVM	O4P-C5A-C5	3.96	116.79	109.36
3	B	502	EVM	O2P-P-O4P	-3.88	96.55	106.67
5	C	503	PLP	C2A-C2-N1	3.50	124.24	117.64
3	A	502	EVM	O2P-P-O4P	-3.50	97.55	106.67
5	C	503	PLP	C5A-C5-C4	-3.35	116.03	122.64
5	D	502	PLP	C2A-C2-C3	-3.29	116.94	120.80
5	D	502	PLP	C2A-C2-N1	3.28	123.81	117.64
5	D	502	PLP	C5A-C5-C4	-3.14	116.44	122.64
5	C	503	PLP	C5A-C5-C6	3.09	124.40	119.36
4	C	502	DSN	OXT-C-O	-3.09	117.07	124.08
3	A	502	EVM	C4-C3-C2	-3.07	118.42	120.14
3	B	502	EVM	C-CA-N	-3.02	100.77	108.22
3	A	502	EVM	C2A-C2-C3	-3.00	117.29	120.80
5	D	502	PLP	O4P-C5A-C5	2.91	114.81	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	EVM	C6-N1-C2	2.81	124.29	119.20
3	B	502	EVM	C2A-C2-N1	2.78	122.88	117.64
5	D	502	PLP	O3-C3-C2	2.76	123.30	117.58
3	A	502	EVM	O4P-P-O3P	2.74	113.85	106.44
3	B	502	EVM	C2A-C2-C3	-2.74	117.59	120.80
5	D	502	PLP	C6-N1-C2	2.69	124.07	119.20
5	C	503	PLP	O3-C3-C2	2.61	122.99	117.58
3	A	502	EVM	O2P-P-O1P	2.56	117.39	107.80
3	A	502	EVM	C2A-C2-N1	2.38	122.12	117.64
3	A	502	EVM	C4-C4A-N	-2.35	118.10	122.73
3	B	502	EVM	C3-C4-C5	-2.34	116.40	118.28
5	D	502	PLP	C6-C5-C4	-2.30	116.21	118.10
3	A	502	EVM	C6-N1-C2	2.09	122.99	119.20
5	D	502	PLP	C4A-C4-C3	-2.06	117.09	120.52
3	B	502	EVM	C4-C4A-N	-2.02	118.77	122.73

There are no chirality outliers.

All (19) torsion outliers are listed below:

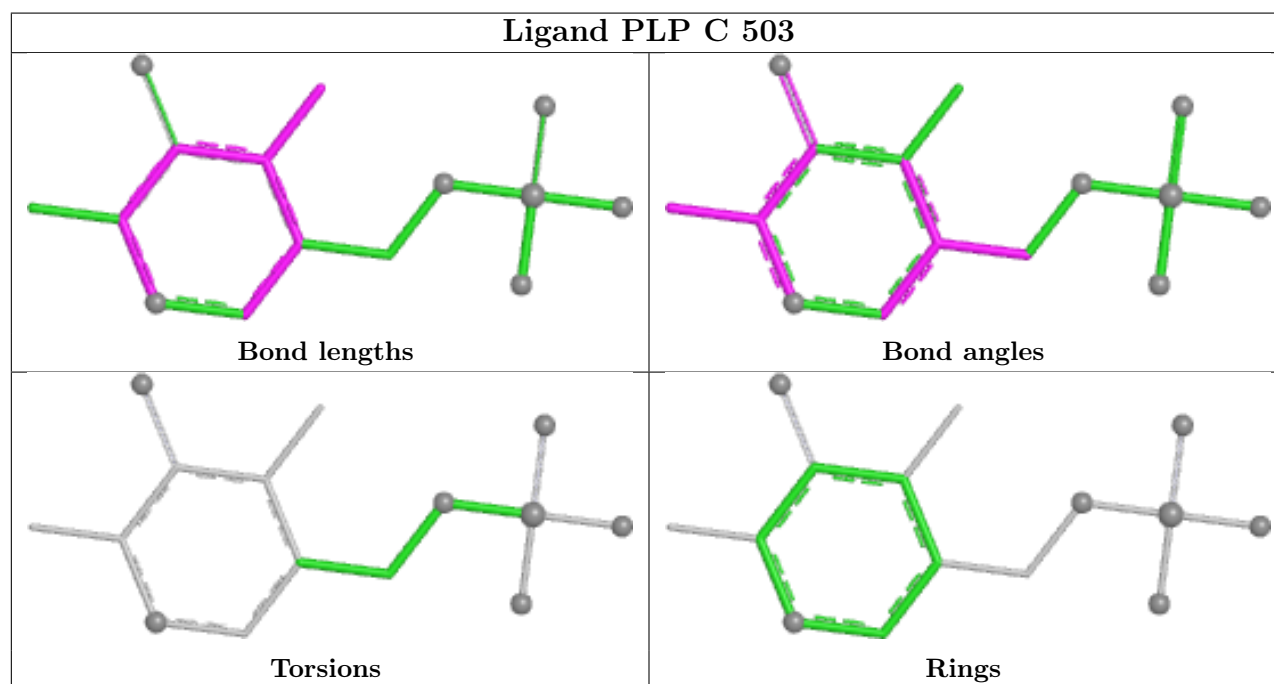
Mol	Chain	Res	Type	Atoms
3	A	502	EVM	CB-CA-N-C4A
3	A	502	EVM	C5A-O4P-P-O1P
3	A	502	EVM	C5A-O4P-P-O2P
3	A	502	EVM	C5A-O4P-P-O3P
3	A	502	EVM	N-CA-CB-OG
3	B	502	EVM	CB-CA-N-C4A
3	B	502	EVM	C5A-O4P-P-O1P
3	B	502	EVM	C5A-O4P-P-O2P
3	B	502	EVM	C5A-O4P-P-O3P
3	B	502	EVM	N-CA-CB-OG
4	C	502	DSN	O-C-CA-CB
4	C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

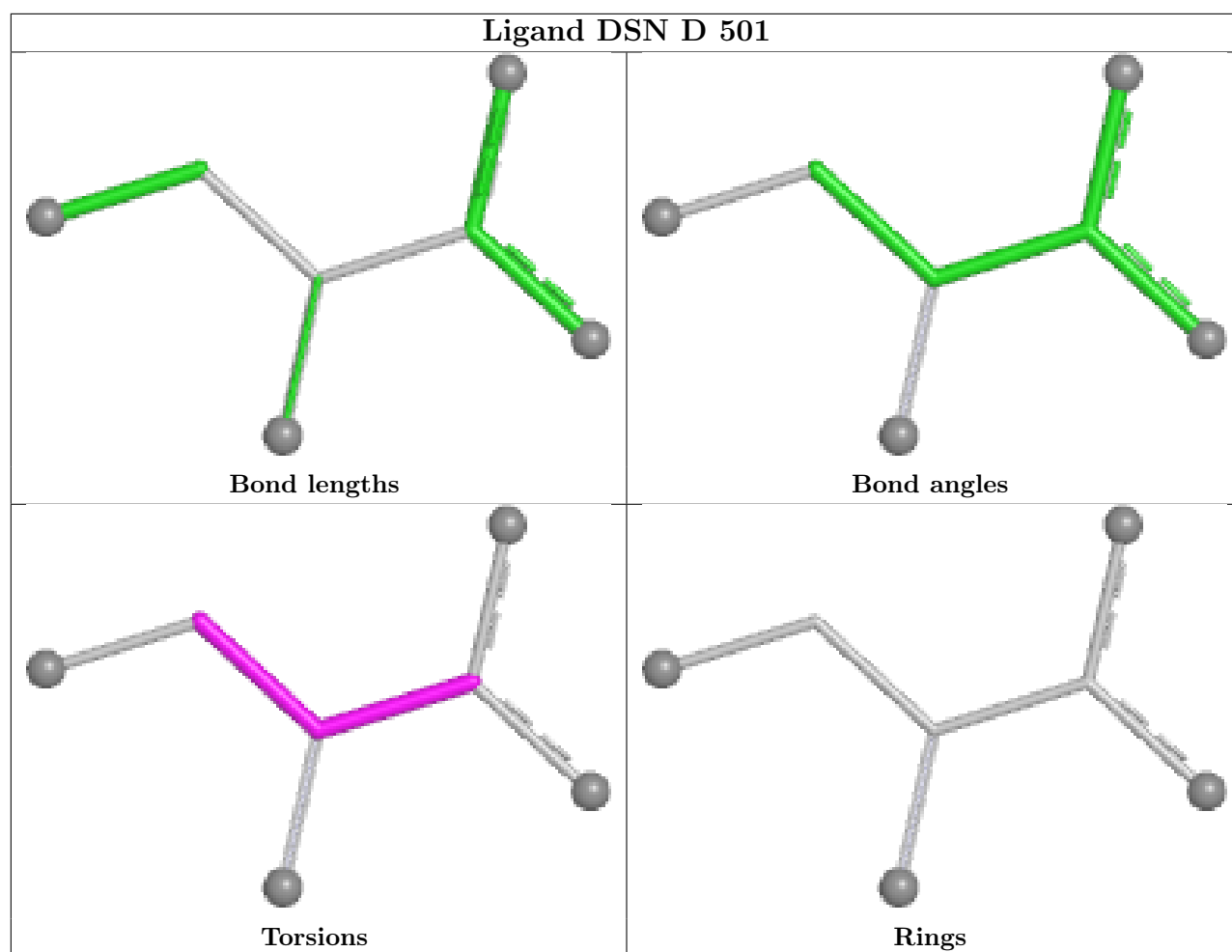
There are no ring outliers.

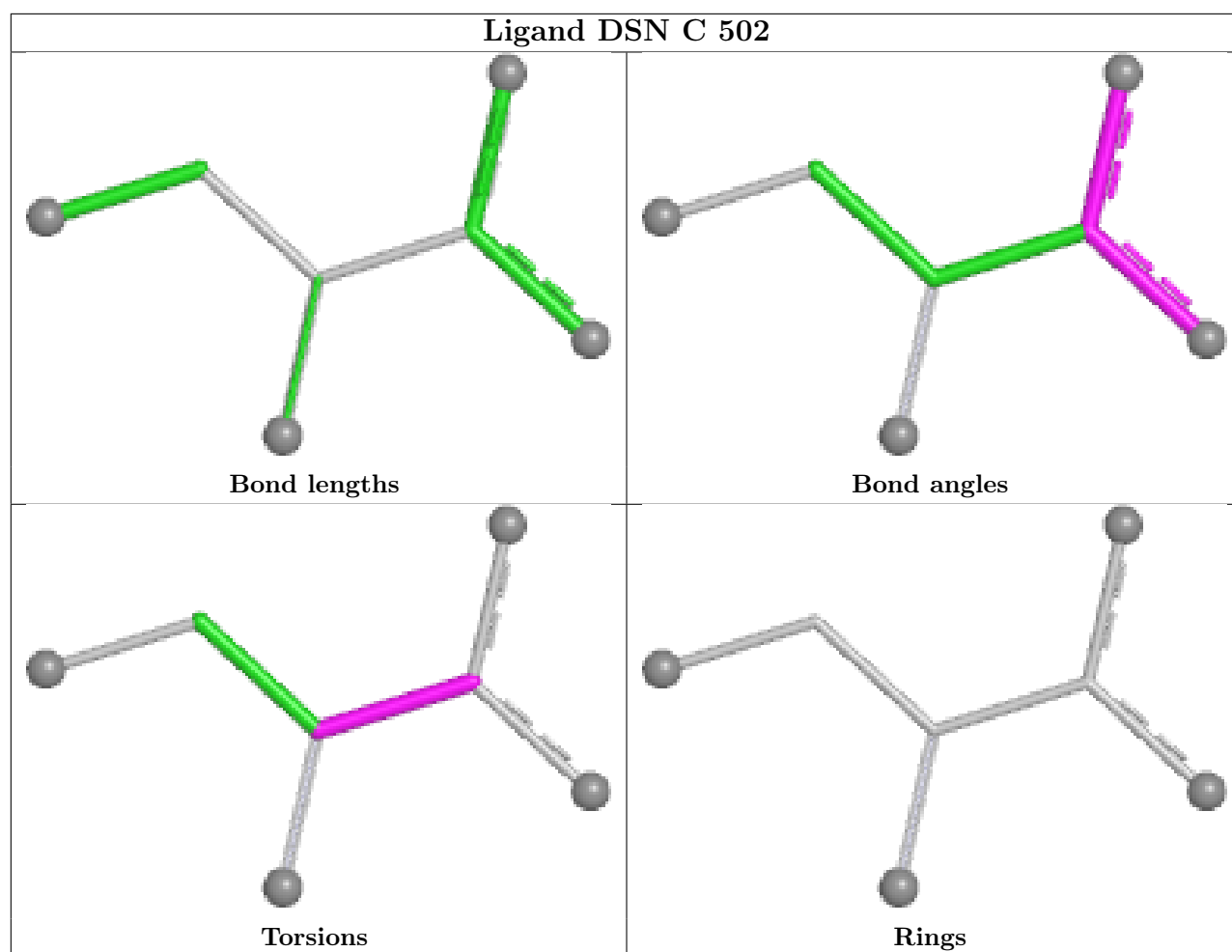
6 monomers are involved in 13 short contacts:

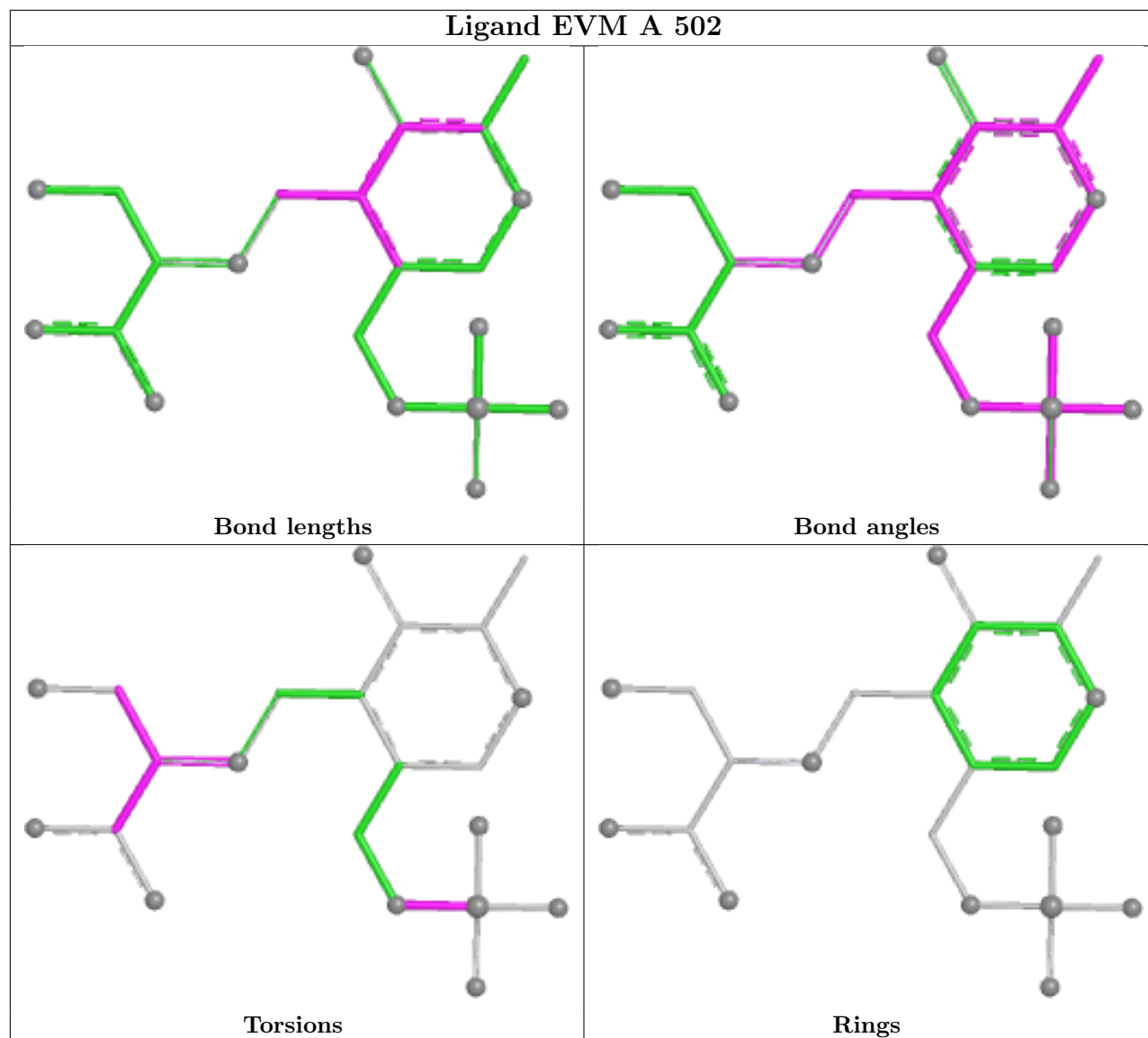
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	503	PLP	1	0
4	D	501	DSN	2	0
4	C	502	DSN	2	0
3	A	502	EVM	5	0
3	B	502	EVM	3	0
5	D	502	PLP	3	0

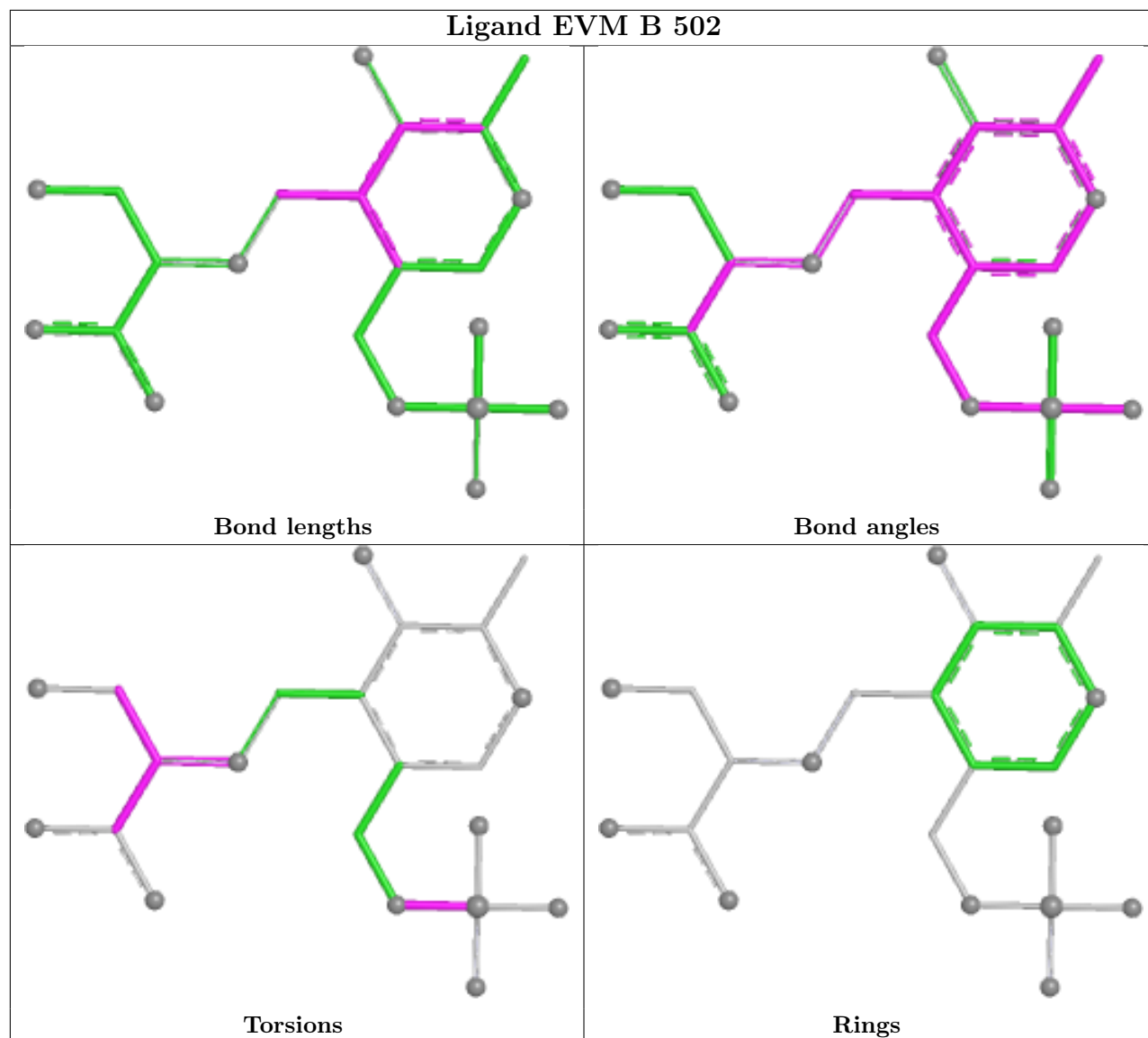
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

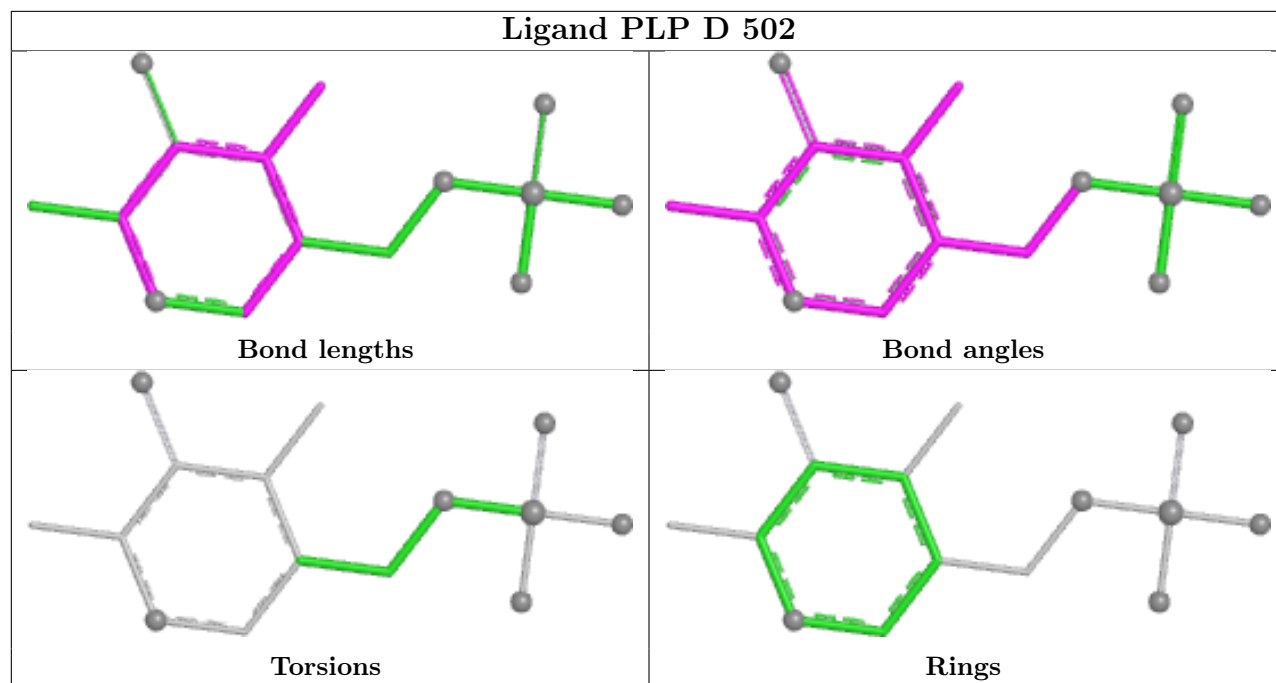












5.7 Other polymers [i](#)

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	410/415 (98%)	1.18	92 (22%) 2 2	28, 52, 90, 112	1 (0%)
1	B	410/415 (98%)	0.46	11 (2%) 56 59	28, 51, 75, 122	1 (0%)
1	C	410/415 (98%)	1.49	125 (30%) 1 1	35, 57, 87, 110	1 (0%)
1	D	410/415 (98%)	0.97	38 (9%) 14 15	40, 65, 93, 109	1 (0%)
All	All	1640/1660 (98%)	1.03	266 (16%) 4 5	28, 56, 89, 122	4 (0%)

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	413	PHE	7.5
1	A	398	VAL	7.3
1	C	387	VAL	7.2
1	C	398	VAL	6.8
1	D	121	LEU	6.3
1	C	390	LEU	6.3
1	C	414	PRO	6.0
1	C	307	PHE	5.9
1	C	321	VAL	5.9
1	C	408	VAL	5.6
1	C	415	LEU	5.5
1	A	307	PHE	5.3
1	C	402	ILE	5.1
1	C	362	ILE	5.0
1	C	336	VAL	5.0
1	C	30	ILE	5.0
1	A	387	VAL	4.9
1	C	409	LEU	4.9
1	A	390	LEU	4.8
1	C	300	VAL	4.8
1	C	32	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	342	ILE	4.7
1	A	414	PRO	4.7
1	C	357	PHE	4.6
1	C	407	LYS	4.6
1	A	409	LEU	4.5
1	C	323	VAL	4.5
1	D	357	PHE	4.3
1	A	393	HIS	4.3
1	C	399	LEU	4.3
1	C	383	ALA	4.2
1	C	121	LEU	4.2
1	A	65	TYR	4.2
1	C	11	PHE	4.2
1	C	21	ALA	4.2
1	C	338	GLU	4.2
1	C	332	VAL	4.2
1	A	357	PHE	4.2
1	A	402	ILE	4.1
1	C	326	VAL	4.1
1	C	327	VAL	4.1
1	A	337	LEU	4.0
1	C	379	SER	4.0
1	C	382	ILE	4.0
1	A	121	LEU	3.9
1	C	380	ARG	3.9
1	C	412	ALA	3.9
1	C	301	PHE	3.9
1	C	369	ILE	3.9
1	C	385	TRP	3.8
1	A	69	ALA	3.8
1	C	324	THR	3.8
1	A	362	ILE	3.8
1	C	337	LEU	3.7
1	C	123	ALA	3.7
1	C	386	MET	3.7
1	A	413	PHE	3.7
1	A	377	ALA	3.7
1	A	401	ARG	3.6
1	A	382	ILE	3.6
1	C	334	GLN	3.6
1	A	342	ILE	3.6
1	A	64	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	389	ALA	3.5
1	C	331	LYS	3.5
1	C	333	ALA	3.5
1	A	415	LEU	3.5
1	A	8	TYR	3.4
1	A	300	VAL	3.4
1	C	13	PRO	3.4
1	C	33	ILE	3.4
1	C	389	ALA	3.4
1	A	396	PRO	3.4
1	D	307	PHE	3.4
1	C	341	ASN	3.3
1	A	305	PRO	3.3
1	A	296	ALA	3.3
1	C	372	ARG	3.3
1	A	332	VAL	3.3
1	C	133	VAL	3.3
1	C	18	ALA	3.2
1	B	65	TYR	3.2
1	C	392	ASN	3.2
1	B	121	LEU	3.2
1	A	336	VAL	3.2
1	D	408	VAL	3.2
1	C	354	LEU	3.2
1	C	304	HIS	3.2
1	C	406	VAL	3.2
1	A	399	LEU	3.2
1	C	8	TYR	3.2
1	A	373	GLY	3.2
1	C	356	PRO	3.2
1	A	306	ASP	3.1
1	D	8	TYR	3.1
1	D	416	TYR	3.1
1	C	388	GLU	3.1
1	C	393	HIS	3.1
1	C	404	GLY	3.1
1	C	353	GLN	3.1
1	A	327	VAL	3.1
1	A	408	VAL	3.1
1	C	275	LEU	3.1
1	A	304	HIS	3.1
1	A	407	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	374	MET	3.1
1	A	28	ASN	3.1
1	C	403	ARG	3.1
1	C	306	ASP	3.1
1	D	300	VAL	3.1
1	C	375	GLY	3.1
1	C	340	VAL	3.1
1	C	376	GLU	3.0
1	A	340	VAL	3.0
1	A	324	THR	3.0
1	A	394	ASP	3.0
1	C	325	LYS	3.0
1	D	356	PRO	3.0
1	C	303	GLN	2.9
1	C	384	GLU	2.9
1	D	354	LEU	2.9
1	A	321	VAL	2.9
1	C	330	GLY	2.9
1	D	291	ILE	2.9
1	C	410	THR	2.9
1	A	412	ALA	2.9
1	C	23	ALA	2.9
1	A	323	VAL	2.9
1	A	71	ILE	2.9
1	A	380	ARG	2.9
1	A	392	ASN	2.9
1	A	23	ALA	2.9
1	C	320	LEU	2.8
1	A	384	GLU	2.8
1	C	296	ALA	2.8
1	A	11	PHE	2.8
1	D	377	ALA	2.8
1	D	344	LEU	2.8
1	D	127	LEU	2.8
1	C	343	THR	2.8
1	C	358	LYS	2.8
1	C	397	GLU	2.7
1	A	55	THR	2.7
1	A	122	SER	2.7
1	A	355	SER	2.7
1	A	385	TRP	2.7
1	A	9	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	2.7
1	C	359	THR	2.7
1	C	416	TYR	2.7
1	C	368	ALA	2.7
1	A	32	LEU	2.7
1	A	50	LEU	2.7
1	D	122	SER	2.7
1	A	397	GLU	2.6
1	A	405	ASP	2.6
1	A	30	ILE	2.6
1	A	73	VAL	2.6
1	A	369	ILE	2.6
1	C	38	VAL	2.6
1	C	391	GLU	2.6
1	C	28	ASN	2.6
1	A	301	PHE	2.6
1	D	310	ILE	2.6
1	C	297	MET	2.6
1	C	10	ALA	2.6
1	C	377	ALA	2.6
1	C	322	ASP	2.6
1	C	308	ARG	2.6
1	A	70	VAL	2.6
1	D	340	VAL	2.6
1	C	395	LYS	2.6
1	C	310	ILE	2.5
1	C	335	ASN	2.5
1	A	383	ALA	2.5
1	C	122	SER	2.5
1	C	396	PRO	2.5
1	C	16	TRP	2.5
1	C	124	GLY	2.5
1	C	361	GLY	2.5
1	B	67	GLY	2.5
1	D	325	LYS	2.5
1	A	309	VAL	2.5
1	C	309	VAL	2.5
1	C	24	GLU	2.5
1	C	305	PRO	2.5
1	D	132	PRO	2.5
1	C	401	ARG	2.5
1	B	357	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	353	GLN	2.4
1	C	26	GLN	2.4
1	D	373	GLY	2.4
1	D	413	PHE	2.4
1	C	7	ASP	2.4
1	D	327	VAL	2.4
1	D	398	VAL	2.4
1	D	402	ILE	2.4
1	D	65	TYR	2.4
1	C	346	LYS	2.4
1	A	416	TYR	2.4
1	B	396	PRO	2.4
1	D	34	ALA	2.4
1	A	354	LEU	2.4
1	A	375	GLY	2.4
1	C	373	GLY	2.4
1	A	326	VAL	2.4
1	A	403	ARG	2.4
1	C	355	SER	2.4
1	D	385	TRP	2.4
1	C	27	GLN	2.3
1	C	329	ASN	2.3
1	C	394	ASP	2.3
1	D	326	VAL	2.3
1	A	45	ALA	2.3
1	C	45	ALA	2.3
1	D	399	LEU	2.3
1	C	132	PRO	2.3
1	A	18	ALA	2.3
1	C	69	ALA	2.3
1	D	368	ALA	2.3
1	A	297	MET	2.3
1	C	31	GLU	2.3
1	A	13	PRO	2.3
1	B	403	ARG	2.3
1	C	42	ALA	2.3
1	C	15	LEU	2.3
1	D	369	ILE	2.2
1	A	406	VAL	2.2
1	A	341	ASN	2.2
1	A	411	ASP	2.2
1	A	374	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	381	GLN	2.2
1	C	128	THR	2.2
1	A	7	ASP	2.2
1	B	7	ASP	2.2
1	A	308	ARG	2.2
1	D	236	ARG	2.2
1	A	276	LYS	2.2
1	D	343	THR	2.2
1	D	404	GLY	2.2
1	C	50	LEU	2.2
1	A	400	GLU	2.1
1	D	33	ILE	2.1
1	A	404	GLY	2.1
1	C	381	GLN	2.1
1	A	333	ALA	2.1
1	B	409	LEU	2.1
1	D	390	LEU	2.1
1	A	376	GLU	2.1
1	B	402	ILE	2.1
1	D	403	ARG	2.1
1	C	276	LYS	2.1
1	C	400	GLU	2.1
1	C	49	THR	2.1
1	D	393	HIS	2.1
1	C	298	ALA	2.1
1	C	51	LEU	2.1
1	A	388	GLU	2.1
1	B	64	TYR	2.1
1	D	359	THR	2.1
1	A	339	GLU	2.0
1	A	325	LYS	2.0
1	C	364	VAL	2.0
1	A	329	ASN	2.0
1	C	234	GLY	2.0
1	B	66	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

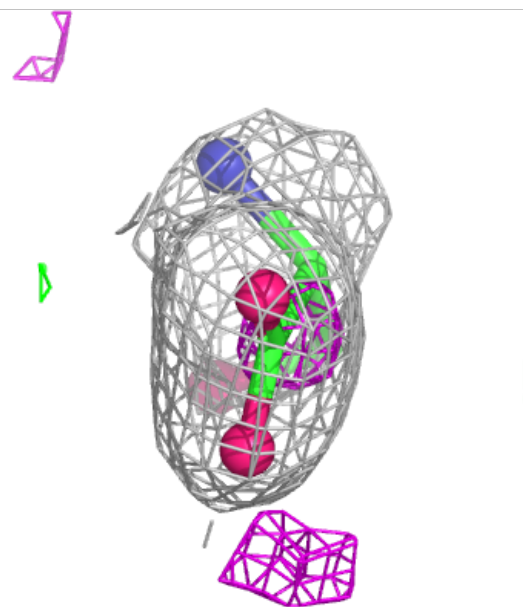
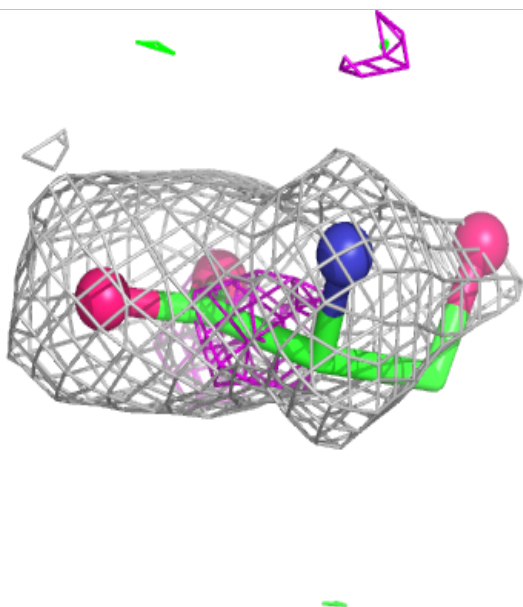
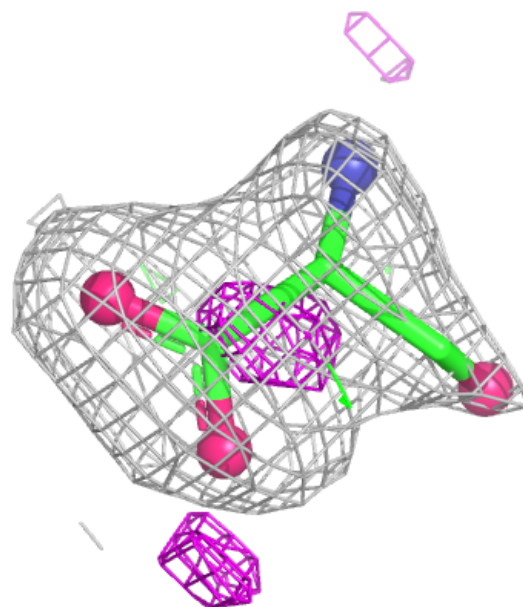
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DSN	C	502	7/7	0.83	0.17	50,75,87,91	0
4	DSN	D	501	7/7	0.85	0.18	65,92,98,109	0
5	PLP	C	503	15/16	0.88	0.16	42,71,79,95	0
3	EVM	A	502	22/22	0.91	0.16	43,70,82,95	0
5	PLP	D	502	15/16	0.91	0.14	64,89,97,98	0
3	EVM	B	502	22/22	0.92	0.13	48,63,84,90	0
2	NA	A	501	1/1	0.93	0.18	48,48,48,48	0
2	NA	B	501	1/1	0.95	0.16	48,48,48,48	0
2	NA	C	501	1/1	0.97	0.21	49,49,49,49	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.

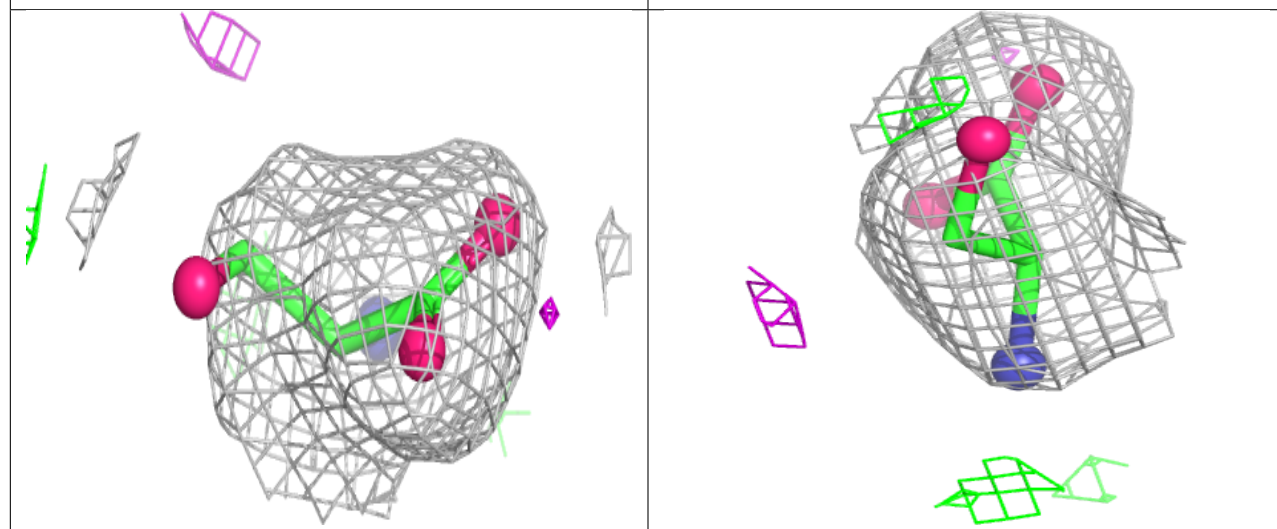
Electron density around DSN C 502:

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



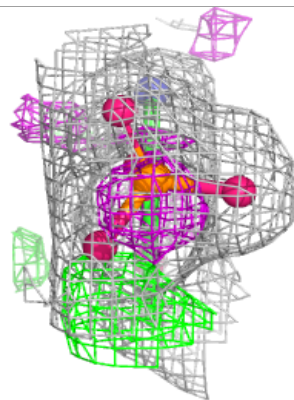
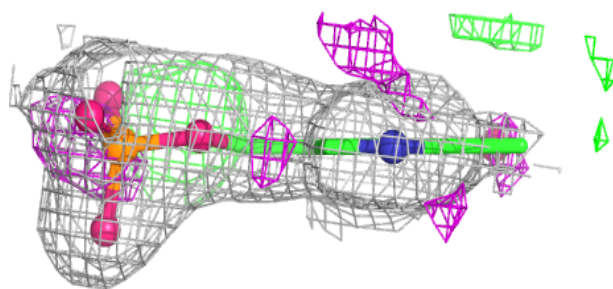
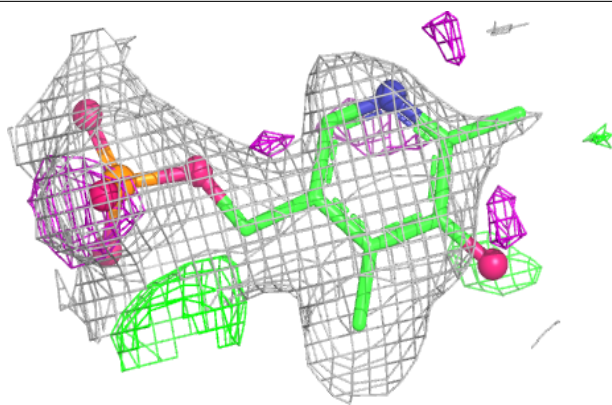
Electron density around DSN D 501:

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



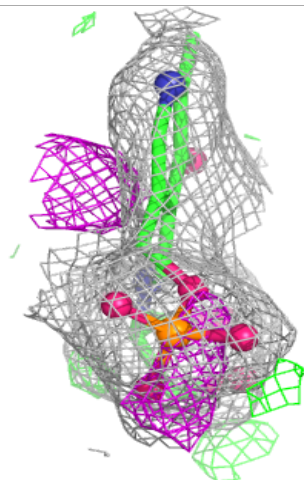
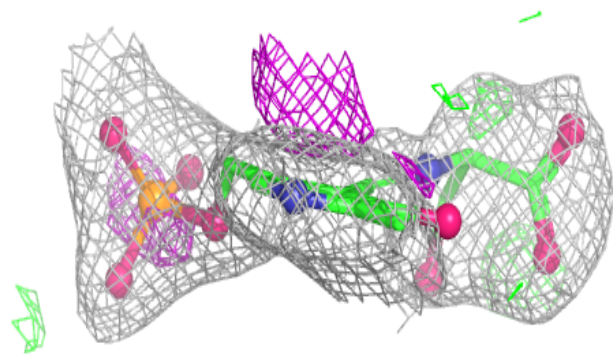
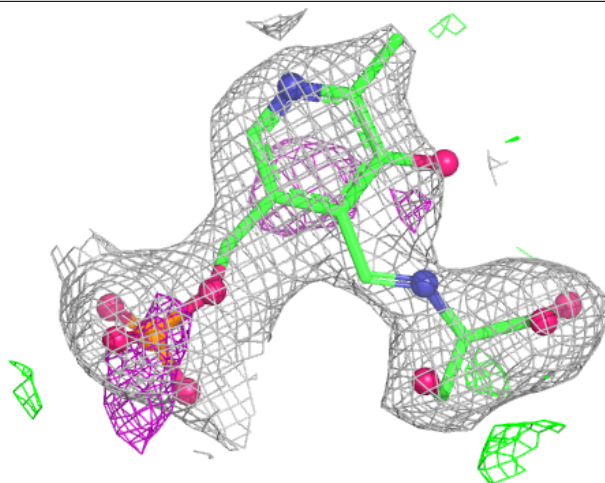
Electron density around PLP C 503:

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



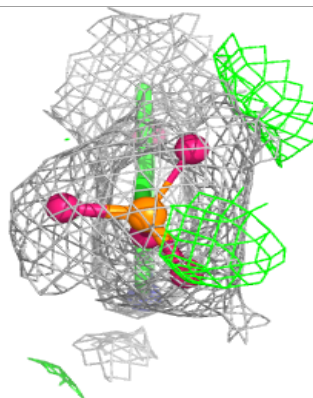
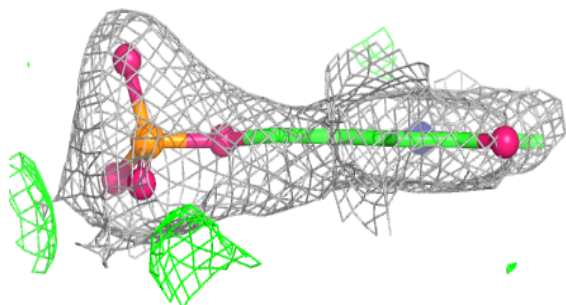
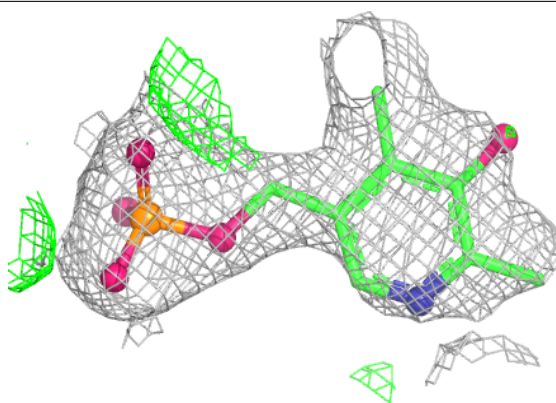
Electron density around EVM A 502:

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



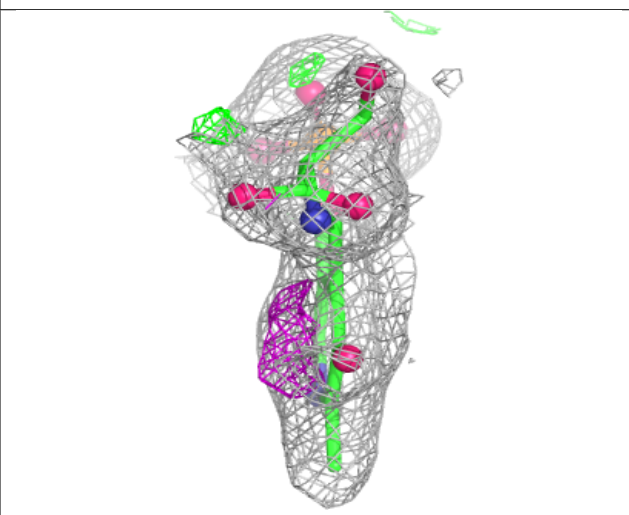
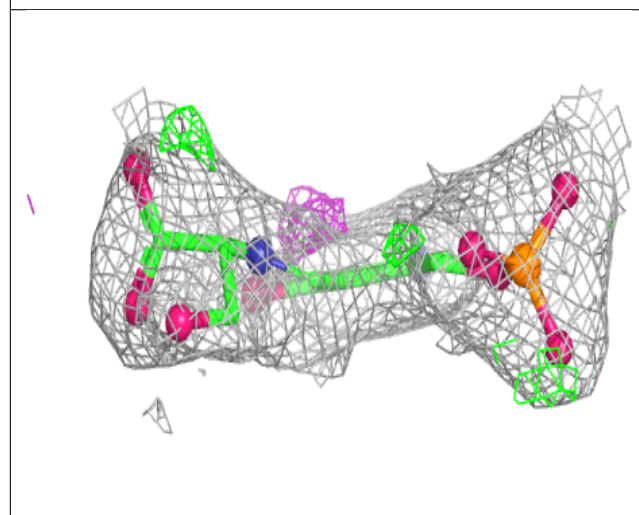
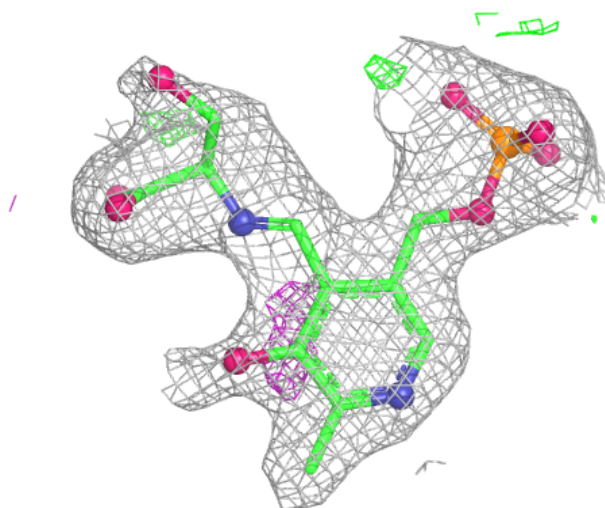
Electron density around PLP D 502:

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



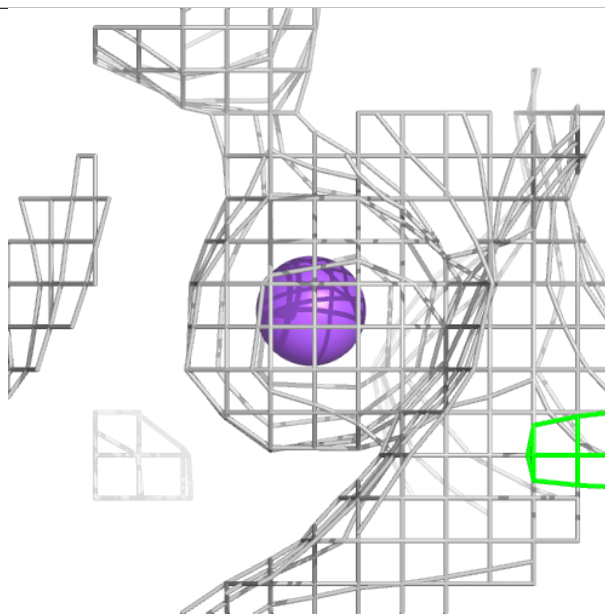
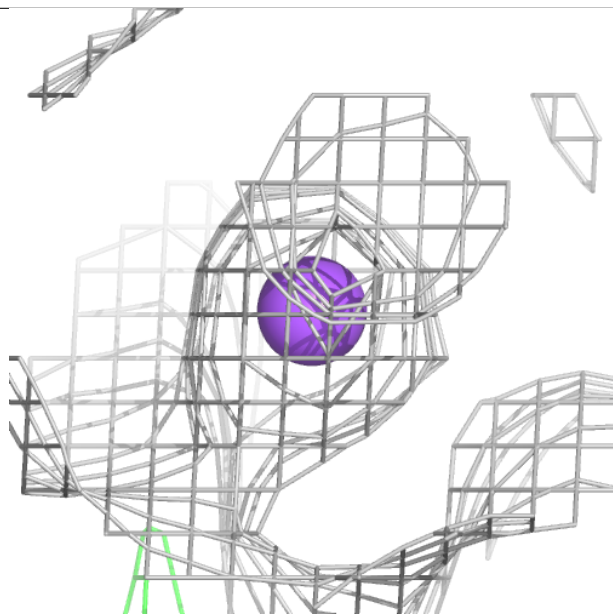
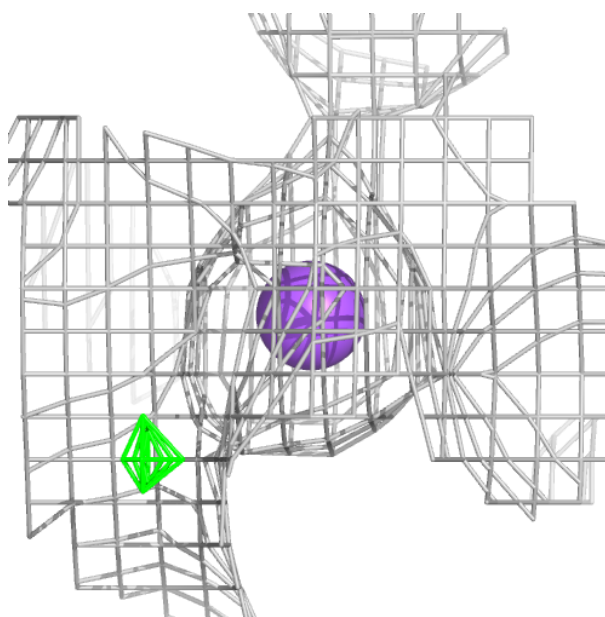
Electron density around EVM B 502:

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



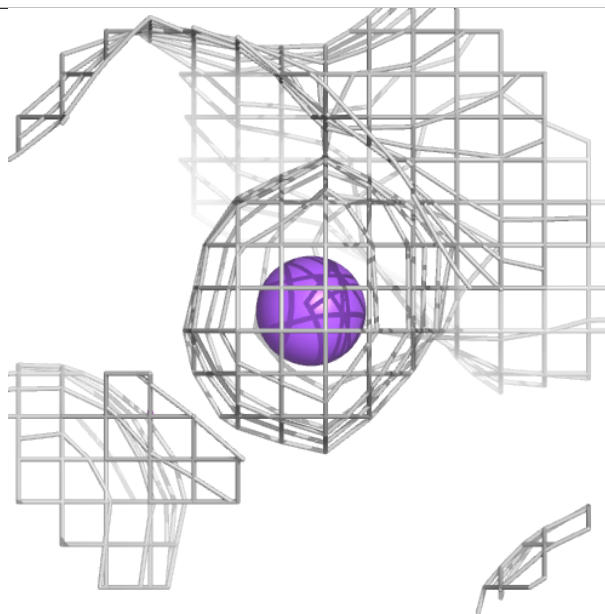
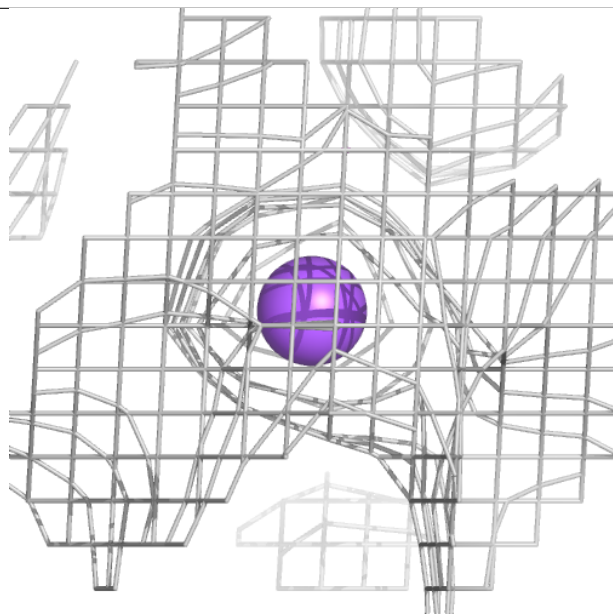
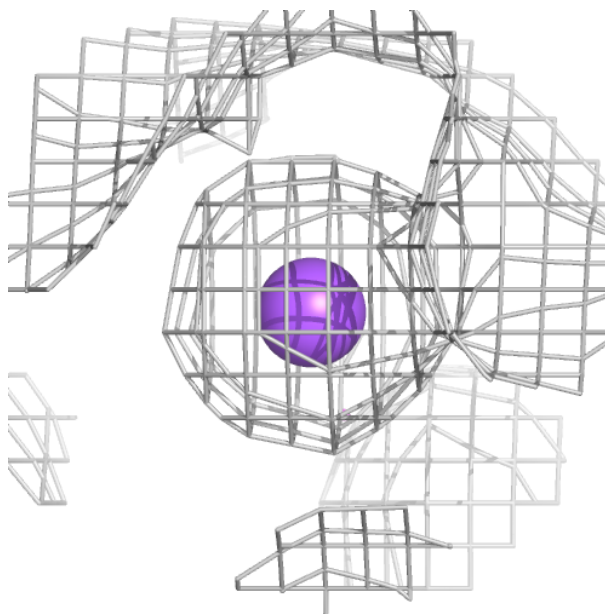
Electron density around NA A 501:

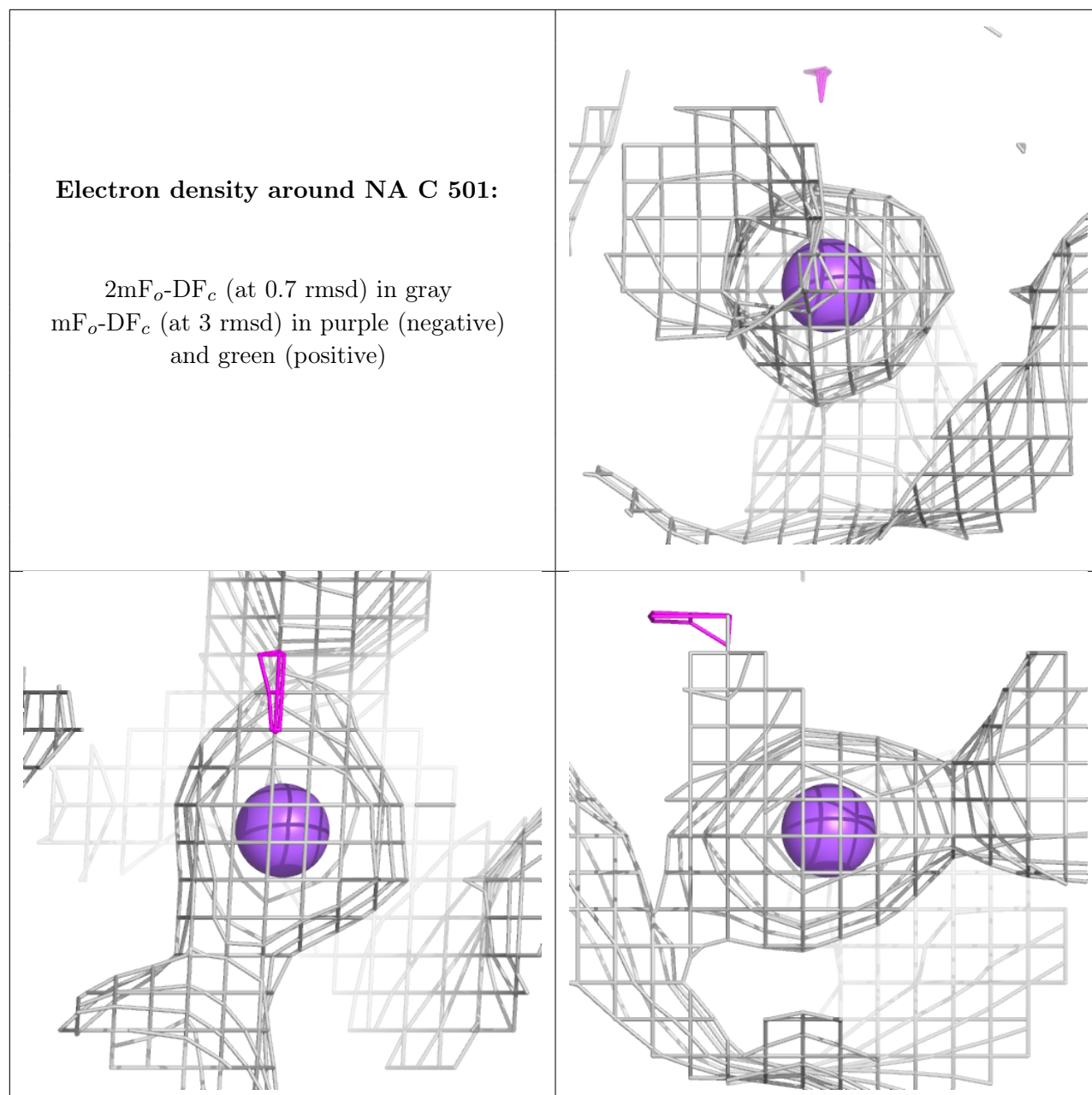
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.