



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:48 PM UTC

PDB ID : 5XKD / pdb_00005xkd
Title : Crystal structure of dibenzothiophene sulfone monooxygenase BdsA in complex with FMN at 2.4 angstrom
Authors : Gu, L.; Su, T.; Liu, S.; Su, J.
Deposited on : 2017-05-07
Resolution : 2.39 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

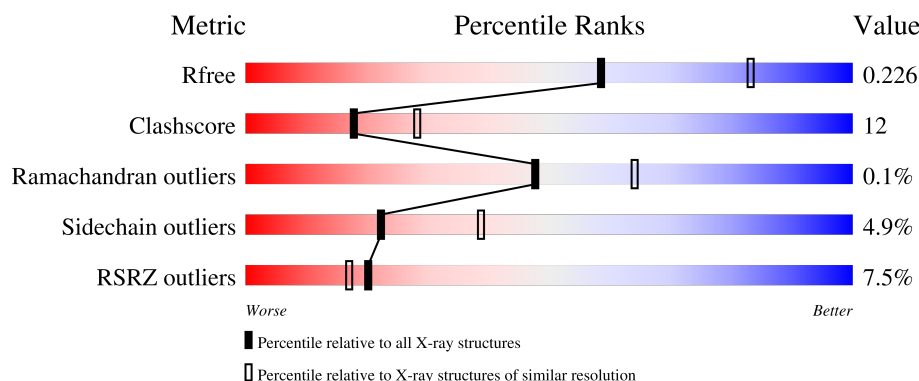
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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.

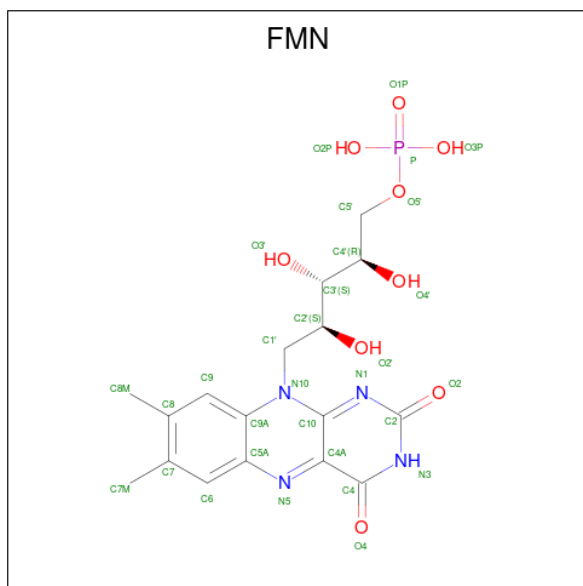
Mol	Chain	Length	Quality of chain
1	A	453	4% 82% 14% ...
1	B	453	5% 83% 12% ..
1	C	453	9% 79% 15% ..
1	D	453	12% 73% 20% ...

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 Dibenzothiophene desulfurization enzyme A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total 3451	C 2187	N 613	O 646	S 5	0	0	0
1	B	445	Total 3451	C 2187	N 613	O 646	S 5	0	0	0
1	C	445	Total 3451	C 2187	N 613	O 646	S 5	0	0	0
1	D	445	Total 3451	C 2187	N 613	O 646	S 5	0	0	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

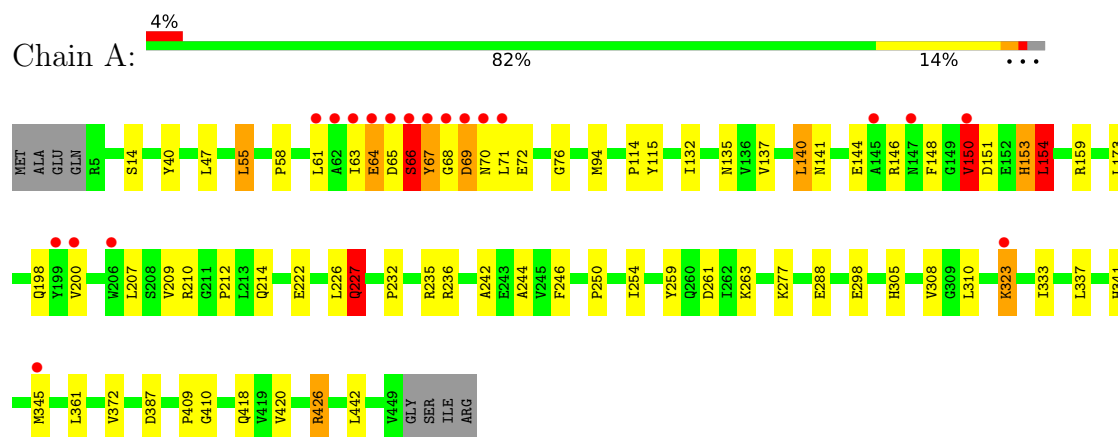
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	68	Total	O	0	0
			68	68		
3	C	68	Total	O	0	0
			68	68		
3	D	40	Total	O	0	0
			40	40		

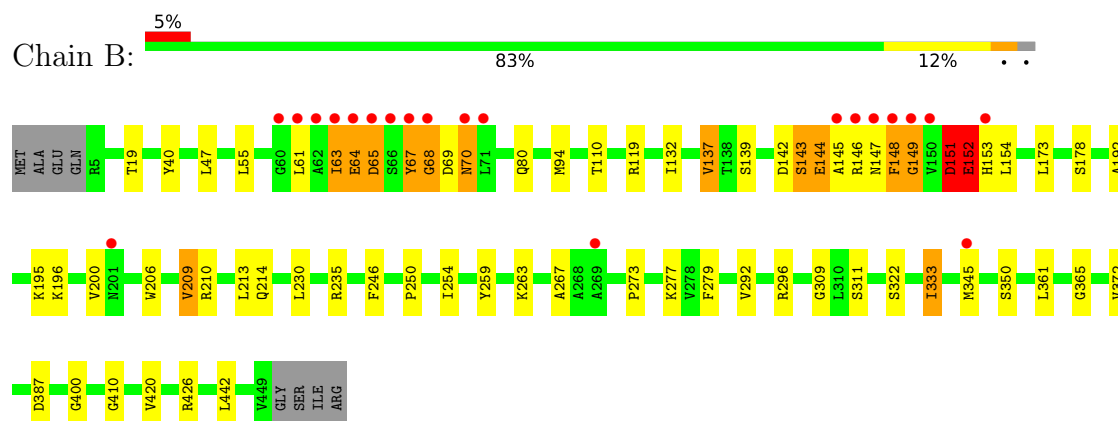
3 Residue-property plots [i](#)

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.

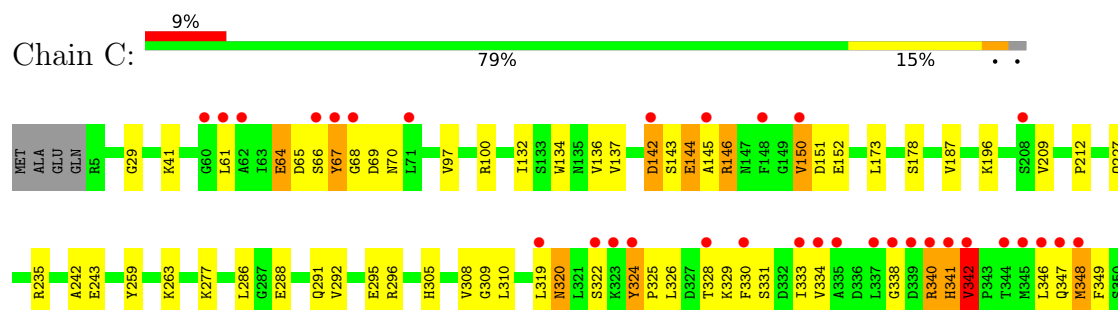
• Molecule 1: Dibenzothiophene desulfurization enzyme A

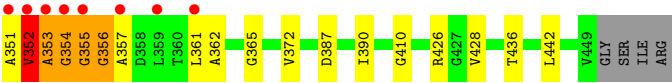


• Molecule 1: Dibenzothiophene desulfurization enzyme A

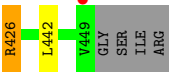
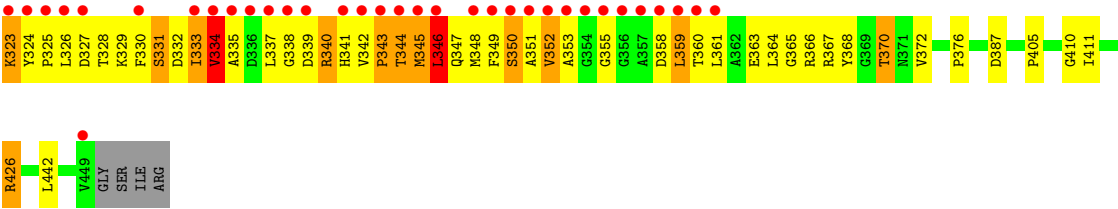
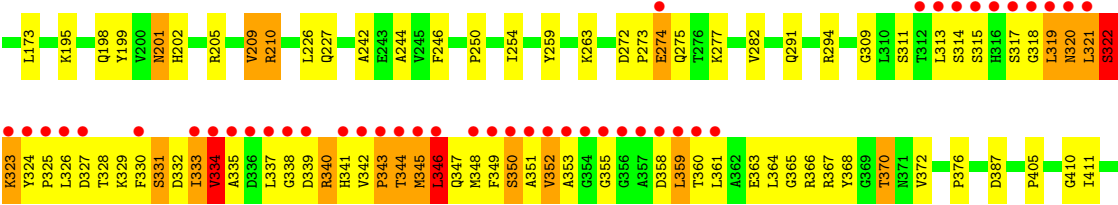
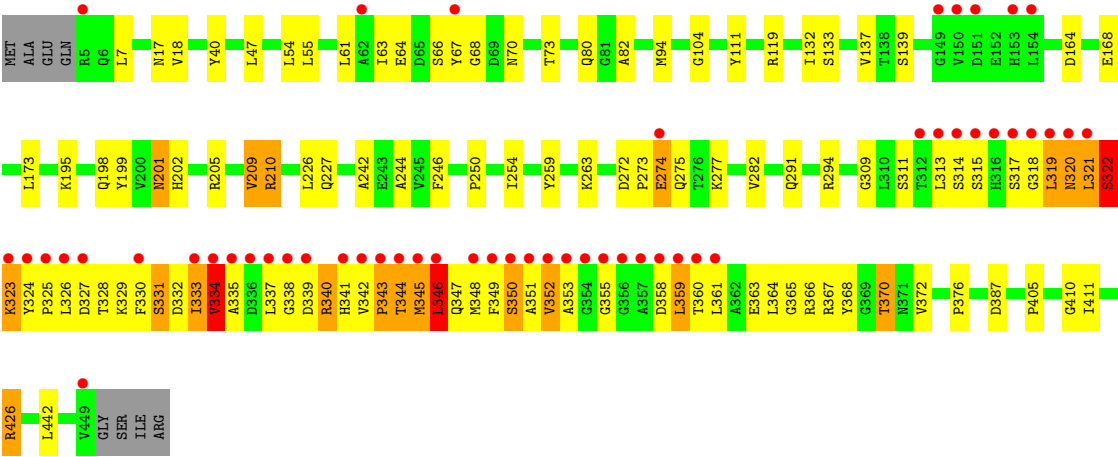


• Molecule 1: Dibenzothiophene desulfurization enzyme A





● Molecule 1: Dibenzothiophene desulfurization enzyme A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.62Å 175.89Å 84.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.39 48.25 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.25-2.39) 99.7 (48.25-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.181 , 0.221 0.190 , 0.226	Depositor DCC
R_{free} test set	3939 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14178	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: FMN

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	0.68	2/3533 (0.1%)	0.96	9/4803 (0.2%)
1	B	0.65	3/3533 (0.1%)	0.97	16/4803 (0.3%)
1	C	0.66	0/3533	0.98	18/4803 (0.4%)
1	D	0.63	0/3533	1.04	18/4803 (0.4%)
All	All	0.66	5/14132 (0.0%)	0.99	61/19212 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	420	VAL	CA-CB	9.39	1.58	1.54
1	A	420	VAL	CA-CB	6.41	1.57	1.54
1	A	153	HIS	CA-C	-5.84	1.47	1.53
1	B	19	THR	CA-C	5.35	1.55	1.52
1	B	148	PHE	CA-C	-5.08	1.45	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	353	ALA	N-CA-C	-14.65	95.31	111.28
1	C	355	GLY	N-CA-C	-13.04	98.01	115.36
1	D	210	ARG	N-CA-C	11.24	123.28	111.14
1	C	357	ALA	N-CA-C	10.27	124.08	110.53
1	B	63	ILE	CA-C-N	-9.96	109.52	122.77
1	B	63	ILE	C-N-CA	-9.96	109.52	122.77
1	A	154	LEU	N-CA-C	-9.56	94.09	109.76
1	A	227	GLN	CA-CB-CG	9.41	132.92	114.10
1	C	348	MET	N-CA-C	-9.15	102.11	113.18
1	B	144	GLU	N-CA-C	-8.65	101.85	111.28
1	B	68	GLY	N-CA-C	-8.61	88.33	113.30
1	B	148	PHE	N-CA-C	-8.59	102.80	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	324	TYR	N-CA-C	-8.21	94.94	108.82
1	D	410	GLY	N-CA-C	7.87	122.43	112.83
1	B	63	ILE	N-CA-C	-7.83	99.38	109.80
1	B	151	ASP	N-CA-C	7.66	122.80	113.38
1	A	148	PHE	N-CA-C	-7.45	103.92	113.16
1	B	152	GLU	N-CA-C	-6.92	99.65	109.96
1	C	142	ASP	N-CA-C	6.85	118.74	111.28
1	C	341	HIS	N-CA-C	6.83	119.62	110.88
1	A	72	GLU	N-CA-C	6.79	118.68	111.28
1	C	354	GLY	CA-C-O	6.76	127.83	120.66
1	D	350	SER	N-CA-C	-6.76	103.91	111.28
1	B	65	ASP	N-CA-C	-6.68	104.76	113.17
1	B	147	ASN	N-CA-C	6.59	118.13	111.07
1	D	318	GLY	N-CA-C	-6.55	106.19	115.30
1	D	344	THR	N-CA-C	6.27	118.11	111.28
1	D	335	ALA	N-CA-C	6.08	117.90	111.28
1	C	64	GLU	N-CA-C	-6.05	101.08	110.10
1	D	332	ASP	N-CA-C	-6.05	104.68	111.28
1	C	410	GLY	N-CA-C	6.04	120.20	112.83
1	D	322	SER	CA-C-N	-6.02	114.96	123.03
1	D	322	SER	C-N-CA	-6.02	114.96	123.03
1	C	342	VAL	CA-C-N	5.95	127.28	119.84
1	C	342	VAL	C-N-CA	5.95	127.28	119.84
1	D	346	LEU	N-CA-C	-5.88	104.87	111.28
1	D	317	SER	N-CA-C	-5.68	105.09	111.28
1	B	70	ASN	N-CA-C	5.63	117.65	108.76
1	A	66	SER	N-CA-C	5.62	117.41	111.28
1	D	355	GLY	N-CA-C	-5.59	106.94	115.66
1	D	345	MET	N-CA-C	-5.50	105.28	111.28
1	C	353	ALA	N-CA-C	5.49	116.94	111.07
1	B	410	GLY	N-CA-C	5.48	119.52	112.83
1	B	149	GLY	CA-C-N	-5.44	115.86	123.10
1	B	149	GLY	C-N-CA	-5.44	115.86	123.10
1	C	66	SER	CA-C-N	-5.42	115.46	123.05
1	C	66	SER	C-N-CA	-5.42	115.46	123.05
1	C	243	GLU	N-CA-C	-5.36	107.12	113.97
1	B	151	ASP	CA-C-N	-5.35	113.10	121.02
1	B	151	ASP	C-N-CA	-5.35	113.10	121.02
1	A	410	GLY	N-CA-C	5.27	119.26	112.83
1	A	227	GLN	CB-CG-CD	5.23	121.49	112.60
1	C	352	VAL	CA-C-N	-5.17	113.72	120.44
1	C	352	VAL	C-N-CA	-5.17	113.72	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	334	VAL	CB-CA-C	-5.11	105.34	112.04
1	A	70	ASN	N-CA-C	5.11	117.15	109.23
1	C	340	ARG	CA-C-N	-5.10	113.49	123.13
1	C	340	ARG	C-N-CA	-5.10	113.49	123.13
1	A	150	VAL	N-CA-C	5.06	116.65	108.85
1	D	319	LEU	CA-C-N	-5.01	116.11	122.77
1	D	319	LEU	C-N-CA	-5.01	116.11	122.77

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3451	0	3372	55	2
1	B	3451	0	3372	68	0
1	C	3451	0	3372	65	2
1	D	3451	0	3371	163	0
2	A	31	0	19	1	0
2	B	31	0	19	3	0
2	C	31	0	19	0	0
2	D	31	0	19	3	0
3	A	74	0	0	2	0
3	B	68	0	0	1	1
3	C	68	0	0	3	0
3	D	40	0	0	1	0
All	All	14178	0	13563	339	3

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 12.

All (339) 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:D:314:SER:OG	1:D:321:LEU:CD1	1.63	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:SER:HA	1:D:334:VAL:CG2	1.56	1.35
1:D:346:LEU:C	1:D:346:LEU:HD23	1.52	1.33
1:D:333:ILE:C	1:D:333:ILE:HD12	1.62	1.24
1:D:346:LEU:HD23	1:D:347:GLN:N	1.51	1.23
1:D:330:PHE:O	1:D:333:ILE:HG23	1.37	1.23
1:D:331:SER:C	1:D:334:VAL:HG23	1.60	1.23
1:D:333:ILE:HD12	1:D:333:ILE:O	1.35	1.22
1:D:359:LEU:HD21	1:D:363:GLU:CG	1.71	1.20
1:C:70:ASN:ND2	3:C:601:HOH:O	1.73	1.19
1:D:314:SER:HA	1:D:321:LEU:HD11	1.19	1.15
1:D:331:SER:O	1:D:334:VAL:HG23	1.43	1.15
1:D:319:LEU:HD23	1:D:320:ASN:N	1.61	1.15
1:A:66:SER:O	1:A:68:GLY:HA2	1.47	1.13
1:D:331:SER:HA	1:D:334:VAL:HG21	1.20	1.13
1:D:314:SER:CA	1:D:321:LEU:HD11	1.80	1.10
1:D:359:LEU:HD21	1:D:363:GLU:HG3	1.20	1.10
1:D:331:SER:CA	1:D:334:VAL:CG2	2.30	1.09
1:D:331:SER:CA	1:D:334:VAL:HG23	1.84	1.07
1:D:337:LEU:O	1:D:341:HIS:HB2	1.53	1.06
1:D:359:LEU:CD2	1:D:363:GLU:CG	2.33	1.05
1:D:330:PHE:C	1:D:333:ILE:HG23	1.83	1.03
1:D:314:SER:OG	1:D:321:LEU:HD12	0.85	1.02
1:B:142:ASP:O	1:B:145:ALA:HB3	1.64	0.97
1:D:359:LEU:HD23	1:D:363:GLU:HB3	1.45	0.97
1:D:346:LEU:C	1:D:346:LEU:CD2	2.29	0.96
1:D:319:LEU:HD23	1:D:319:LEU:C	1.89	0.96
1:D:333:ILE:C	1:D:333:ILE:CD1	2.33	0.95
1:D:346:LEU:CD2	1:D:347:GLN:N	2.30	0.95
1:C:67:TYR:HD1	1:C:67:TYR:O	1.47	0.95
1:A:222:GLU:OE2	3:A:601:HOH:O	1.85	0.94
1:D:359:LEU:CD2	1:D:363:GLU:HG3	1.93	0.94
1:B:387:ASP:OD1	1:B:426:ARG:NH2	2.01	0.93
1:C:67:TYR:CD2	1:C:322:SER:HB2	2.05	0.92
1:D:346:LEU:HD23	1:D:347:GLN:CA	1.99	0.92
1:D:331:SER:O	1:D:334:VAL:CG2	2.21	0.87
1:D:314:SER:CB	1:D:321:LEU:CD1	2.52	0.87
1:A:387:ASP:OD1	1:A:426:ARG:NH2	2.08	0.87
1:D:330:PHE:HA	1:D:333:ILE:CG2	2.05	0.87
1:D:314:SER:CB	1:D:321:LEU:HD12	2.04	0.86
1:A:67:TYR:CD2	1:A:67:TYR:O	2.29	0.85
1:D:67:TYR:CE1	1:D:322:SER:HA	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TYR:O	1:B:67:TYR:CD2	2.29	0.85
1:C:67:TYR:O	1:C:67:TYR:CD1	2.30	0.83
1:D:329:LYS:O	1:D:333:ILE:HG22	1.77	0.83
1:D:359:LEU:HD21	1:D:363:GLU:HG2	1.61	0.82
1:B:142:ASP:O	1:B:146:ARG:N	2.13	0.82
1:D:314:SER:CA	1:D:321:LEU:CD1	2.58	0.80
1:D:323:LYS:O	1:D:323:LYS:HD3	1.82	0.80
1:D:323:LYS:O	1:D:323:LYS:CD	2.30	0.80
1:C:387:ASP:OD1	1:C:426:ARG:NH2	2.16	0.79
1:D:323:LYS:O	1:D:323:LYS:CG	2.30	0.79
1:D:359:LEU:HD23	1:D:363:GLU:CB	2.13	0.79
1:C:310:LEU:HD21	1:C:361:LEU:HD13	1.64	0.79
1:C:325:PRO:HD2	1:C:328:THR:OG1	1.84	0.78
1:A:66:SER:O	1:A:68:GLY:CA	2.30	0.78
1:D:342:VAL:CG1	1:D:347:GLN:CG	2.62	0.77
1:D:342:VAL:HG12	1:D:347:GLN:CG	2.15	0.77
1:D:342:VAL:HG11	1:D:347:GLN:HG2	1.67	0.77
1:D:346:LEU:HD23	1:D:347:GLN:HA	1.67	0.77
1:D:345:MET:HG3	1:D:346:LEU:N	1.98	0.77
1:C:320:ASN:OD1	1:C:320:ASN:C	2.29	0.75
1:D:352:VAL:O	1:D:352:VAL:CG1	2.34	0.75
1:B:173:LEU:HD11	1:B:209:VAL:HG21	1.67	0.75
1:D:330:PHE:HA	1:D:333:ILE:HG21	1.68	0.75
1:D:337:LEU:HB3	1:D:341:HIS:O	1.87	0.75
1:D:319:LEU:C	1:D:319:LEU:CD2	2.61	0.74
1:C:67:TYR:CD1	1:C:67:TYR:C	2.65	0.73
1:D:330:PHE:CE2	1:D:350:SER:OG	2.41	0.73
1:A:210:ARG:CD	1:B:146:ARG:HD3	2.19	0.73
1:B:145:ALA:O	1:B:149:GLY:CA	2.36	0.72
1:B:145:ALA:O	1:B:149:GLY:HA2	1.88	0.72
1:C:142:ASP:O	1:C:146:ARG:HG2	1.87	0.72
1:A:210:ARG:HD3	1:B:146:ARG:HD3	1.71	0.72
1:D:342:VAL:HG12	1:D:347:GLN:HG3	1.70	0.71
1:A:66:SER:C	1:A:69:ASP:H	1.98	0.71
1:D:173:LEU:HD11	1:D:209:VAL:HG21	1.70	0.71
1:D:342:VAL:CG1	1:D:347:GLN:HG2	2.21	0.71
1:D:359:LEU:CD2	1:D:363:GLU:HG2	2.19	0.70
1:D:330:PHE:O	1:D:333:ILE:CG2	2.30	0.70
1:D:352:VAL:O	1:D:352:VAL:HG13	1.92	0.70
1:D:345:MET:HG3	1:D:346:LEU:H	1.53	0.70
1:A:66:SER:O	1:A:69:ASP:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:CD2	1:D:363:GLU:CB	2.70	0.69
1:D:331:SER:CA	1:D:334:VAL:HG21	2.10	0.69
1:D:359:LEU:HD23	1:D:363:GLU:CG	2.23	0.68
1:D:201:ASN:N	1:D:201:ASN:HD22	1.92	0.67
1:D:346:LEU:HD23	1:D:346:LEU:O	1.95	0.67
1:D:359:LEU:CD2	1:D:363:GLU:HB3	2.21	0.66
1:B:67:TYR:CE2	1:B:311:SER:HB2	2.31	0.66
1:D:348:MET:O	1:D:351:ALA:HB3	1.94	0.66
1:C:352:VAL:CG1	1:C:353:ALA:N	2.58	0.66
1:D:345:MET:CG	1:D:346:LEU:N	2.57	0.66
1:D:314:SER:CB	1:D:321:LEU:HD11	2.24	0.64
1:A:226:LEU:HD23	1:A:244:ALA:HB3	1.79	0.64
1:B:61:LEU:HD22	1:B:148:PHE:HE1	1.62	0.64
1:C:354:GLY:C	1:C:356:GLY:H	2.04	0.64
1:D:330:PHE:CA	1:D:333:ILE:HG23	2.27	0.64
1:D:320:ASN:HD22	1:D:320:ASN:H	1.46	0.64
1:D:323:LYS:O	1:D:323:LYS:HG3	1.96	0.64
1:D:329:LYS:O	1:D:333:ILE:CG2	2.46	0.64
1:C:61:LEU:HB2	1:C:144:GLU:HG3	1.80	0.63
1:D:205:ARG:HH11	1:D:205:ARG:HG3	1.62	0.63
1:B:67:TYR:CD2	1:B:67:TYR:C	2.76	0.63
1:C:352:VAL:HG12	1:C:353:ALA:N	2.14	0.62
1:D:330:PHE:CA	1:D:333:ILE:CG2	2.76	0.62
1:A:214:GLN:HG2	1:B:63:ILE:HG12	1.81	0.62
1:C:61:LEU:HB2	1:C:144:GLU:CG	2.30	0.61
1:A:61:LEU:N	1:A:144:GLU:OE2	2.31	0.61
1:A:65:ASP:O	1:A:69:ASP:HA	2.01	0.61
1:C:67:TYR:CG	1:C:322:SER:HB2	2.34	0.61
1:D:325:PRO:O	1:D:328:THR:OG1	2.18	0.61
1:C:351:ALA:O	1:C:355:GLY:N	2.34	0.60
1:D:342:VAL:HG11	1:D:347:GLN:CG	2.27	0.60
1:A:67:TYR:O	1:A:67:TYR:HD2	1.78	0.60
1:D:387:ASP:OD1	1:D:426:ARG:NH2	2.35	0.60
1:D:164:ASP:O	1:D:168:GLU:HG3	2.00	0.60
1:D:333:ILE:HG13	1:D:334:VAL:N	2.16	0.60
1:D:18:VAL:HG13	1:D:80:GLN:HA	1.83	0.59
1:D:320:ASN:N	1:D:320:ASN:HD22	2.01	0.59
1:B:67:TYR:CD2	1:B:311:SER:HA	2.37	0.59
1:B:142:ASP:O	1:B:145:ALA:CB	2.46	0.58
1:D:330:PHE:O	1:D:334:VAL:HG22	2.04	0.58
1:B:142:ASP:C	1:B:145:ALA:HB3	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASP:O	1:B:152:GLU:C	2.45	0.58
1:A:141:ASN:OD1	1:A:144:GLU:HG3	2.03	0.58
1:D:291:GLN:OE1	1:D:294:ARG:NH2	2.37	0.58
1:B:70:ASN:C	1:B:70:ASN:OD1	2.48	0.57
1:C:351:ALA:O	1:C:355:GLY:CA	2.53	0.57
1:D:250:PRO:HG2	1:D:254:ILE:HD12	1.87	0.56
1:A:150:VAL:HG13	1:A:151:ASP:N	2.19	0.56
1:B:350:SER:OG	3:B:601:HOH:O	2.16	0.56
1:B:61:LEU:HB2	1:B:144:GLU:HG2	1.87	0.56
1:D:67:TYR:CD1	1:D:322:SER:HA	2.40	0.56
1:B:173:LEU:HD23	1:B:200:VAL:HG21	1.88	0.55
1:C:324:TYR:N	1:C:324:TYR:CD2	2.73	0.55
1:A:310:LEU:HD11	1:A:361:LEU:HB3	1.88	0.55
1:C:324:TYR:H	1:C:324:TYR:HD2	1.53	0.55
1:A:214:GLN:HG2	1:B:63:ILE:CG1	2.36	0.55
1:D:320:ASN:N	1:D:320:ASN:ND2	2.55	0.55
1:C:348:MET:O	1:C:352:VAL:HB	2.07	0.55
1:D:349:PHE:CE2	1:D:368:TYR:HD2	2.24	0.55
1:D:333:ILE:O	1:D:333:ILE:CD1	2.30	0.54
1:B:230:LEU:O	1:B:235:ARG:NH1	2.40	0.54
1:D:327:ASP:HA	1:D:360:THR:CG2	2.36	0.54
1:B:142:ASP:HA	1:B:145:ALA:HB3	1.89	0.54
1:B:152:GLU:O	1:B:152:GLU:CG	2.55	0.54
1:B:145:ALA:O	1:B:149:GLY:N	2.39	0.54
1:D:346:LEU:CD2	1:D:347:GLN:HA	2.34	0.54
1:C:351:ALA:O	1:C:355:GLY:HA2	2.08	0.53
1:C:330:PHE:CD2	1:C:333:ILE:HD11	2.44	0.53
1:A:173:LEU:HD23	1:A:200:VAL:HG21	1.90	0.53
1:D:18:VAL:CG1	1:D:80:GLN:HA	2.39	0.53
1:C:331:SER:HA	1:C:334:VAL:HG22	1.91	0.53
1:D:338:GLY:O	1:D:341:HIS:N	2.36	0.53
1:B:143:SER:HA	1:B:146:ARG:HB2	1.91	0.53
1:D:330:PHE:O	1:D:334:VAL:CG2	2.56	0.53
1:D:344:THR:O	1:D:347:GLN:HB2	2.09	0.52
1:B:65:ASP:OD1	1:B:65:ASP:N	2.30	0.52
1:B:64:GLU:OE1	1:B:80:GLN:HB2	2.10	0.52
1:C:390:ILE:HG12	1:C:428:VAL:HG21	1.92	0.52
1:D:47:LEU:HD12	1:D:55:LEU:HD12	1.91	0.52
1:D:345:MET:SD	1:D:345:MET:C	2.93	0.52
1:D:333:ILE:CG1	1:D:334:VAL:N	2.68	0.52
1:A:114:PRO:HG3	1:A:207:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ASP:O	1:C:146:ARG:N	2.42	0.52
1:C:143:SER:HA	1:C:146:ARG:HG3	1.92	0.51
1:D:329:LYS:HB3	1:D:358:ASP:OD1	2.10	0.51
1:D:337:LEU:C	1:D:341:HIS:HB2	2.31	0.51
1:C:349:PHE:O	1:C:352:VAL:HG12	2.10	0.51
1:D:327:ASP:HA	1:D:360:THR:HG23	1.92	0.51
1:D:348:MET:O	1:D:351:ALA:N	2.43	0.51
1:B:151:ASP:OD2	1:B:151:ASP:C	2.53	0.51
1:D:205:ARG:HG3	1:D:205:ARG:NH1	2.25	0.51
1:D:338:GLY:O	1:D:339:ASP:C	2.54	0.51
1:D:337:LEU:N	1:D:337:LEU:CD1	2.72	0.51
1:C:61:LEU:HD23	1:D:119:ARG:NH2	2.26	0.50
1:D:66:SER:O	1:D:68:GLY:HA2	2.11	0.50
1:D:344:THR:O	1:D:347:GLN:N	2.44	0.50
1:B:65:ASP:O	1:B:69:ASP:HA	2.10	0.50
1:D:363:GLU:OE1	1:D:366:ARG:NH1	2.44	0.50
1:C:68:GLY:O	1:C:70:ASN:OD1	2.30	0.50
1:B:151:ASP:O	1:B:151:ASP:OD2	2.30	0.50
1:C:320:ASN:OD1	1:C:320:ASN:O	2.30	0.50
1:D:346:LEU:CD2	1:D:347:GLN:CA	2.79	0.50
1:A:246:PHE:CE1	2:A:500:FMN:H6	2.47	0.50
1:C:65:ASP:OD2	1:D:210:ARG:NH2	2.45	0.50
1:D:372:VAL:O	1:D:372:VAL:HG12	2.12	0.50
1:A:227:GLN:C	1:A:227:GLN:OE1	2.55	0.49
1:B:67:TYR:CD2	1:B:311:SER:CB	2.94	0.49
1:B:250:PRO:HG2	1:B:254:ILE:HD12	1.94	0.49
1:D:272:ASP:O	3:D:601:HOH:O	2.20	0.49
1:B:277:LYS:HE3	1:B:442:LEU:O	2.12	0.49
1:D:199:TYR:HB3	1:D:201:ASN:HD21	1.77	0.49
1:D:361:LEU:HD23	1:D:364:LEU:HD12	1.93	0.49
1:C:354:GLY:C	1:C:356:GLY:N	2.68	0.49
1:A:146:ARG:HD3	1:B:210:ARG:HD2	1.93	0.49
1:D:17:ASN:ND2	1:D:18:VAL:HG12	2.28	0.49
1:C:100:ARG:CZ	1:C:436:THR:HG22	2.43	0.49
1:C:67:TYR:CD2	1:C:322:SER:CB	2.86	0.49
1:C:150:VAL:HG12	1:C:152:GLU:HG2	1.94	0.49
1:A:154:LEU:HB3	1:A:159:ARG:HG2	1.95	0.48
1:D:277:LYS:HE3	1:D:442:LEU:O	2.13	0.48
1:C:178:SER:HB2	1:C:196:LYS:HB3	1.94	0.48
1:A:235:ARG:NH1	1:A:261:ASP:OD2	2.46	0.48
1:B:67:TYR:CE1	1:B:322:SER:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASP:O	1:B:153:HIS:N	2.46	0.48
1:A:65:ASP:O	1:A:69:ASP:CA	2.61	0.48
1:B:70:ASN:OD1	1:B:70:ASN:O	2.31	0.48
1:B:246:PHE:CE1	2:B:500:FMN:H6	2.48	0.48
1:D:282:VAL:HG12	1:D:376:PRO:HG2	1.95	0.48
1:A:140:LEU:O	1:A:140:LEU:HG	2.14	0.48
1:B:333:ILE:HD13	1:B:361:LEU:HD21	1.96	0.48
1:D:343:PRO:O	1:D:347:GLN:HG3	2.14	0.48
1:A:115:TYR:OH	1:A:214:GLN:NE2	2.42	0.48
1:D:259:TYR:CZ	1:D:263:LYS:HE3	2.48	0.48
1:C:212:PRO:HG2	1:D:63:ILE:HD12	1.95	0.48
1:D:104:GLY:HA2	1:D:133:SER:O	2.14	0.47
1:D:227:GLN:HG2	1:D:242:ALA:HB2	1.96	0.47
1:C:134:TRP:CE2	1:C:136:VAL:HG22	2.49	0.47
1:C:145:ALA:O	1:C:150:VAL:HG23	2.14	0.47
1:A:259:TYR:CZ	1:A:263:LYS:HE3	2.50	0.47
1:A:305:HIS:HB3	1:A:308:VAL:HG22	1.96	0.47
1:C:319:LEU:HD23	1:C:319:LEU:N	2.29	0.47
1:B:67:TYR:CG	1:B:311:SER:HA	2.49	0.47
1:C:146:ARG:CB	1:D:210:ARG:HD3	2.45	0.47
1:A:173:LEU:HD11	1:A:209:VAL:HG21	1.95	0.47
1:C:277:LYS:NZ	3:C:608:HOH:O	2.48	0.46
1:B:154:LEU:HD21	1:B:206:TRP:CH2	2.50	0.46
1:D:199:TYR:HB3	1:D:201:ASN:ND2	2.31	0.46
1:B:178:SER:HB2	1:B:196:LYS:HB3	1.96	0.46
1:D:349:PHE:O	1:D:349:PHE:CD1	2.69	0.46
1:A:198:GLN:O	1:A:212:PRO:HB3	2.16	0.46
1:B:67:TYR:CD2	1:B:311:SER:HB2	2.51	0.46
1:D:337:LEU:HD23	1:D:341:HIS:O	2.16	0.46
1:D:342:VAL:CG1	1:D:347:GLN:CD	2.89	0.46
1:A:232:PRO:O	1:A:236:ARG:HG3	2.16	0.45
1:B:309:GLY:HA3	1:B:365:GLY:O	2.15	0.45
1:D:64:GLU:OE1	1:D:80:GLN:HB3	2.16	0.45
1:B:267:ALA:HB2	1:B:273:PRO:HG3	1.97	0.45
1:B:139:SER:OG	2:B:500:FMN:H3'	2.15	0.45
1:D:359:LEU:HD11	1:D:367:ARG:NH1	2.31	0.45
1:D:274:GLU:OE2	1:D:275:GLN:NE2	2.33	0.45
1:D:314:SER:HA	1:D:321:LEU:CD1	2.13	0.45
1:D:328:THR:HG22	1:D:333:ILE:HG22	1.97	0.45
1:B:142:ASP:HA	1:B:145:ALA:CB	2.46	0.45
1:D:70:ASN:OD1	1:D:70:ASN:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:NZ	3:A:602:HOH:O	2.23	0.45
1:C:305:HIS:O	1:C:308:VAL:HG22	2.17	0.45
1:A:67:TYR:CD2	1:A:67:TYR:C	2.94	0.44
1:B:65:ASP:O	1:B:69:ASP:CA	2.65	0.44
1:B:142:ASP:CA	1:B:145:ALA:HB3	2.47	0.44
1:A:277:LYS:HE3	1:A:442:LEU:O	2.17	0.44
1:B:195:LYS:HE2	1:B:195:LYS:HB2	1.70	0.44
1:D:338:GLY:C	1:D:340:ARG:N	2.75	0.44
1:D:346:LEU:HD22	1:D:347:GLN:HG2	2.00	0.44
1:A:288:GLU:OE1	1:A:288:GLU:N	2.42	0.44
1:B:67:TYR:CD1	1:B:322:SER:HB3	2.53	0.44
1:A:76:GLY:HA2	1:B:192:ALA:O	2.18	0.44
1:B:67:TYR:HA	1:B:68:GLY:HA2	1.14	0.44
1:B:292:VAL:O	1:B:296:ARG:HG3	2.17	0.44
1:C:67:TYR:HA	1:C:68:GLY:HA2	1.44	0.44
1:A:66:SER:C	1:A:68:GLY:HA2	2.30	0.44
1:A:67:TYR:HA	1:A:68:GLY:HA2	1.52	0.44
1:A:409:PRO:HD2	3:C:615:HOH:O	2.17	0.44
1:B:47:LEU:HD12	1:B:55:LEU:HD12	2.00	0.44
1:B:152:GLU:O	1:B:152:GLU:HG3	2.17	0.44
1:C:334:VAL:HG12	1:C:342:VAL:HG11	1.99	0.44
1:D:274:GLU:O	1:D:277:LYS:HE2	2.17	0.44
1:B:137:VAL:HG11	2:B:500:FMN:C2	2.48	0.44
1:D:348:MET:O	1:D:352:VAL:N	2.49	0.44
1:C:145:ALA:HA	1:C:150:VAL:HG23	2.00	0.43
1:C:334:VAL:O	1:C:338:GLY:N	2.49	0.43
1:D:67:TYR:HB3	1:D:311:SER:HA	2.00	0.43
1:D:331:SER:O	1:D:334:VAL:CB	2.66	0.43
1:D:337:LEU:N	1:D:337:LEU:HD12	2.25	0.43
1:B:40:TYR:HB3	1:B:94:MET:HE3	2.01	0.43
1:B:61:LEU:HD22	1:B:148:PHE:CE1	2.49	0.43
1:D:337:LEU:HD12	1:D:337:LEU:HA	1.46	0.43
1:C:259:TYR:CZ	1:C:263:LYS:HE3	2.53	0.43
1:A:333:ILE:HD13	1:A:361:LEU:HD21	2.00	0.43
1:C:41:LYS:HD3	1:C:97:VAL:HG11	2.00	0.43
1:C:286:LEU:O	1:C:296:ARG:NH1	2.46	0.43
1:A:63:ILE:HG13	1:B:214:GLN:HG2	2.00	0.43
1:D:67:TYR:HA	1:D:68:GLY:HA2	1.71	0.43
1:D:346:LEU:O	1:D:349:PHE:HB3	2.19	0.43
2:D:500:FMN:H9	2:D:500:FMN:H1'1	1.52	0.43
1:C:309:GLY:HA3	1:C:365:GLY:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LYS:HD2	1:D:195:LYS:HA	1.56	0.42
1:D:202:HIS:HB3	1:D:209:VAL:HG13	2.00	0.42
1:A:47:LEU:HD12	1:A:55:LEU:HD12	2.00	0.42
1:B:65:ASP:O	1:B:70:ASN:N	2.52	0.42
1:C:173:LEU:HD11	1:C:209:VAL:HG21	2.00	0.42
1:D:246:PHE:CE2	2:D:500:FMN:H6	2.54	0.42
1:A:40:TYR:HB3	1:A:94:MET:HE3	2.01	0.42
1:A:135:ASN:HA	1:A:226:LEU:HB2	2.01	0.42
1:D:345:MET:SD	1:D:346:LEU:N	2.92	0.42
1:B:119:ARG:HB2	1:B:213:LEU:HD11	2.02	0.42
1:D:319:LEU:HD23	1:D:320:ASN:C	2.44	0.42
1:A:250:PRO:HG2	1:A:254:ILE:HD12	2.00	0.42
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.70	0.42
1:D:352:VAL:O	1:D:352:VAL:HG12	2.17	0.42
1:D:139:SER:OG	2:D:500:FMN:O2	2.24	0.42
1:A:64:GLU:O	1:A:64:GLU:HG2	2.20	0.42
1:C:227:GLN:HG2	1:C:242:ALA:HB2	2.02	0.42
1:A:227:GLN:HG3	1:A:242:ALA:HB2	2.02	0.42
1:C:146:ARG:HB3	1:D:210:ARG:HD3	2.01	0.41
1:D:40:TYR:HB3	1:D:94:MET:HE3	2.01	0.41
1:D:274:GLU:OE2	1:D:274:GLU:O	2.38	0.41
1:D:368:TYR:CE1	1:D:372:VAL:HA	2.55	0.41
1:B:279:PHE:HA	1:B:400:GLY:O	2.20	0.41
1:C:291:GLN:HG3	1:C:295:GLU:OE2	2.20	0.41
1:C:326:LEU:HA	1:C:361:LEU:CD1	2.50	0.41
1:D:61:LEU:HD12	1:D:111:TYR:CD2	2.55	0.41
1:D:405:PRO:HA	1:D:411:ILE:HG21	2.01	0.41
1:B:110:THR:OG1	1:B:139:SER:O	2.37	0.41
1:A:418:GLN:HG2	1:C:29:GLY:HA2	2.02	0.41
1:D:367:ARG:O	1:D:370:THR:HB	2.21	0.41
1:A:14:SER:HA	1:A:58:PRO:HD2	2.01	0.41
1:A:337:LEU:O	1:A:341:HIS:HB2	2.21	0.41
1:C:277:LYS:HE3	1:C:442:LEU:O	2.19	0.41
1:C:288:GLU:OE1	1:C:288:GLU:N	2.50	0.41
1:D:63:ILE:HG23	1:D:82:ALA:HA	2.03	0.41
1:C:61:LEU:HB2	1:C:144:GLU:HG2	2.03	0.41
1:D:7:LEU:HD12	1:D:7:LEU:C	2.46	0.41
1:B:65:ASP:HA	1:B:70:ASN:O	2.21	0.41
1:C:346:LEU:HD23	1:C:346:LEU:O	2.20	0.41
1:D:309:GLY:HA3	1:D:365:GLY:O	2.21	0.41
1:B:259:TYR:CZ	1:B:263:LYS:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:LEU:HB3	1:C:362:ALA:HB2	2.03	0.41
1:D:67:TYR:CD2	1:D:67:TYR:C	3.00	0.40
1:D:226:LEU:HD23	1:D:244:ALA:O	2.22	0.40
1:C:292:VAL:O	1:C:296:ARG:HG3	2.22	0.40
1:A:210:ARG:HD3	1:A:210:ARG:HH11	1.75	0.40
1:A:323:LYS:HB3	1:A:323:LYS:HE3	1.58	0.40
1:C:324:TYR:HA	1:C:325:PRO:HD3	1.86	0.40
1:D:73:THR:HG21	1:D:311:SER:HB2	2.02	0.40
1:D:272:ASP:HA	1:D:273:PRO:HD3	1.89	0.40
1:D:313:LEU:HD13	1:D:368:TYR:CD2	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:648:HOH:O	3:B:648:HOH:O[2_555]	1.39	0.81
1:A:153:HIS:NE2	1:C:340:ARG:NH1[3_455]	2.15	0.05
1:A:153:HIS:CD2	1:C:340:ARG:CZ[3_455]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	443/453 (98%)	432 (98%)	11 (2%)	0	100	100
1	B	443/453 (98%)	436 (98%)	7 (2%)	0	100	100
1	C	443/453 (98%)	431 (97%)	11 (2%)	1 (0%)	43	58
1	D	443/453 (98%)	427 (96%)	16 (4%)	0	100	100
All	All	1772/1812 (98%)	1726 (97%)	45 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	356	GLY

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	357/363 (98%)	340 (95%)	17 (5%)	23	40
1	B	357/363 (98%)	346 (97%)	11 (3%)	35	57
1	C	357/363 (98%)	338 (95%)	19 (5%)	20	36
1	D	357/363 (98%)	334 (94%)	23 (6%)	16	28
All	All	1428/1452 (98%)	1358 (95%)	70 (5%)	22	39

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	64	GLU
1	A	66	SER
1	A	67	TYR
1	A	69	ASP
1	A	71	LEU
1	A	132	ILE
1	A	137	VAL
1	A	140	LEU
1	A	150	VAL
1	A	154	LEU
1	A	227	GLN
1	A	298	GLU
1	A	323	LYS
1	A	345	MET
1	A	372	VAL
1	A	426	ARG
1	B	64	GLU
1	B	67	TYR
1	B	132	ILE
1	B	137	VAL

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Mol	Chain	Res	Type
1	B	143	SER
1	B	151	ASP
1	B	152	GLU
1	B	209	VAL
1	B	333	ILE
1	B	345	MET
1	B	372	VAL
1	C	64	GLU
1	C	67	TYR
1	C	69	ASP
1	C	132	ILE
1	C	137	VAL
1	C	144	GLU
1	C	146	ARG
1	C	150	VAL
1	C	151	ASP
1	C	187	VAL
1	C	235	ARG
1	C	320	ASN
1	C	324	TYR
1	C	329	LYS
1	C	341	HIS
1	C	342	VAL
1	C	347	GLN
1	C	352	VAL
1	C	372	VAL
1	D	54	LEU
1	D	132	ILE
1	D	137	VAL
1	D	198	GLN
1	D	201	ASN
1	D	209	VAL
1	D	274	GLU
1	D	315	SER
1	D	320	ASN
1	D	321	LEU
1	D	322	SER
1	D	323	LYS
1	D	326	LEU
1	D	331	SER
1	D	333	ILE
1	D	334	VAL

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Mol	Chain	Res	Type
1	D	340	ARG
1	D	343	PRO
1	D	346	LEU
1	D	352	VAL
1	D	359	LEU
1	D	370	THR
1	D	426	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	214	GLN
1	B	135	ASN
1	B	147	ASN
1	B	201	ASN
1	B	341	HIS
1	C	42	GLN
1	C	135	ASN
1	C	341	HIS
1	D	135	ASN
1	D	153	HIS
1	D	201	ASN
1	D	320	ASN

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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	B	500	-	33,33,33	1.15	3 (9%)	48,50,50	1.85	13 (27%)
2	FMN	C	500	-	33,33,33	1.15	3 (9%)	48,50,50	1.93	14 (29%)
2	FMN	D	500	-	33,33,33	1.16	2 (6%)	48,50,50	1.75	12 (25%)
2	FMN	A	500	-	33,33,33	1.09	2 (6%)	48,50,50	1.65	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	500	-	-	9/18/18/18	0/3/3/3
2	FMN	C	500	-	-	10/18/18/18	0/3/3/3
2	FMN	D	500	-	-	13/18/18/18	0/3/3/3
2	FMN	A	500	-	-	10/18/18/18	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FMN	C4A-N5	3.81	1.39	1.30
2	C	500	FMN	C4A-N5	3.72	1.38	1.30
2	A	500	FMN	C4A-N5	3.57	1.38	1.30
2	D	500	FMN	C4A-N5	3.35	1.38	1.30
2	A	500	FMN	C10-N1	2.69	1.38	1.33
2	D	500	FMN	C10-N1	2.62	1.38	1.33
2	C	500	FMN	C2'-C3'	2.50	1.57	1.53
2	B	500	FMN	C10-N1	2.27	1.37	1.33
2	B	500	FMN	C2'-C3'	2.15	1.57	1.53
2	C	500	FMN	C10-N1	2.09	1.37	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FMN	C4'-C3'-C2'	6.25	123.96	113.57
2	D	500	FMN	C4'-C3'-C2'	5.78	123.18	113.57
2	C	500	FMN	O2'-C2'-C3'	5.40	121.89	109.25
2	A	500	FMN	C4'-C3'-C2'	4.91	121.75	113.57
2	B	500	FMN	C4'-C3'-C2'	4.85	121.64	113.57
2	B	500	FMN	O2'-C2'-C3'	4.18	119.03	109.25
2	C	500	FMN	C4-N3-C2	-3.77	118.95	125.64
2	D	500	FMN	C4-N3-C2	-3.64	119.17	125.64
2	B	500	FMN	C9A-C5A-N5	-3.43	118.81	122.45
2	A	500	FMN	O4'-C4'-C5'	-3.33	102.64	109.99
2	B	500	FMN	C5A-C9A-N10	3.33	120.98	117.97
2	B	500	FMN	C4-N3-C2	-3.32	119.74	125.64
2	D	500	FMN	O2'-C2'-C3'	3.30	116.97	109.25
2	A	500	FMN	C4-N3-C2	-3.28	119.82	125.64
2	C	500	FMN	C4A-C10-N10	3.20	121.06	116.48
2	B	500	FMN	C4A-C10-N10	3.06	120.86	116.48
2	A	500	FMN	C4A-C10-N10	3.01	120.79	116.48
2	A	500	FMN	O2'-C2'-C3'	2.92	116.08	109.25
2	C	500	FMN	C4A-C4-N3	2.91	120.66	113.25
2	B	500	FMN	C10-C4A-N5	-2.85	119.00	124.81
2	C	500	FMN	O5'-C5'-C4'	-2.75	102.03	109.36
2	D	500	FMN	C4A-C4-N3	2.73	120.20	113.25
2	B	500	FMN	C4A-C4-N3	2.64	119.98	113.25
2	A	500	FMN	C4A-C4-N3	2.60	119.88	113.25
2	A	500	FMN	C5A-C9A-N10	2.59	120.31	117.97
2	B	500	FMN	C4-C4A-N5	2.57	121.76	118.21
2	D	500	FMN	C5A-C9A-N10	2.57	120.29	117.97
2	C	500	FMN	C10-C4A-N5	-2.55	119.60	124.81
2	D	500	FMN	C10-C4A-N5	-2.53	119.64	124.81
2	A	500	FMN	C10-C4A-N5	-2.52	119.65	124.81
2	B	500	FMN	O4'-C4'-C5'	-2.45	104.59	109.99
2	D	500	FMN	C1'-N10-C9A	-2.43	115.92	120.63
2	C	500	FMN	O4'-C4'-C3'	2.42	114.92	109.25
2	D	500	FMN	C4A-C10-N1	-2.39	118.73	124.59
2	D	500	FMN	C9A-C5A-N5	-2.36	119.95	122.45
2	B	500	FMN	C9-C9A-N10	-2.35	118.70	121.85
2	C	500	FMN	O4-C4-C4A	-2.33	120.38	126.53
2	D	500	FMN	C4A-C10-N10	2.33	119.81	116.48
2	A	500	FMN	C9A-C5A-N5	-2.26	120.05	122.45
2	B	500	FMN	C5'-C4'-C3'	-2.24	108.00	112.22
2	A	500	FMN	C4A-C10-N1	-2.22	119.14	124.59
2	C	500	FMN	C4-C4A-N5	2.22	121.27	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FMN	O2'-C2'-C1'	-2.18	101.22	110.20
2	C	500	FMN	O3'-C3'-C2'	2.14	113.79	108.93
2	A	500	FMN	O3P-P-O2P	2.09	115.62	107.80
2	B	500	FMN	O3P-P-O2P	2.04	115.46	107.80
2	C	500	FMN	C5A-C9A-N10	2.03	119.81	117.97
2	D	500	FMN	O4'-C4'-C5'	-2.03	105.51	109.99
2	D	500	FMN	C4-C4A-C10	2.02	120.40	116.93
2	C	500	FMN	C9A-C5A-N5	-2.01	120.32	122.45

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FMN	N10-C1'-C2'-O2'
2	A	500	FMN	N10-C1'-C2'-C3'
2	A	500	FMN	O3'-C3'-C4'-O4'
2	A	500	FMN	C5'-O5'-P-O1P
2	A	500	FMN	C5'-O5'-P-O2P
2	A	500	FMN	C5'-O5'-P-O3P
2	B	500	FMN	N10-C1'-C2'-O2'
2	B	500	FMN	N10-C1'-C2'-C3'
2	B	500	FMN	C5'-O5'-P-O1P
2	B	500	FMN	C5'-O5'-P-O2P
2	B	500	FMN	C5'-O5'-P-O3P
2	C	500	FMN	N10-C1'-C2'-O2'
2	C	500	FMN	N10-C1'-C2'-C3'
2	C	500	FMN	C1'-C2'-C3'-O3'
2	C	500	FMN	C5'-O5'-P-O1P
2	C	500	FMN	C5'-O5'-P-O2P
2	C	500	FMN	C5'-O5'-P-O3P
2	D	500	FMN	N10-C1'-C2'-O2'
2	D	500	FMN	N10-C1'-C2'-C3'
2	D	500	FMN	C1'-C2'-C3'-O3'
2	D	500	FMN	C2'-C3'-C4'-C5'
2	D	500	FMN	O3'-C3'-C4'-O4'
2	D	500	FMN	O3'-C3'-C4'-C5'
2	D	500	FMN	C5'-O5'-P-O1P
2	D	500	FMN	C5'-O5'-P-O2P
2	D	500	FMN	C5'-O5'-P-O3P
2	C	500	FMN	O3'-C3'-C4'-C5'
2	A	500	FMN	O3'-C3'-C4'-C5'
2	C	500	FMN	O3'-C3'-C4'-O4'

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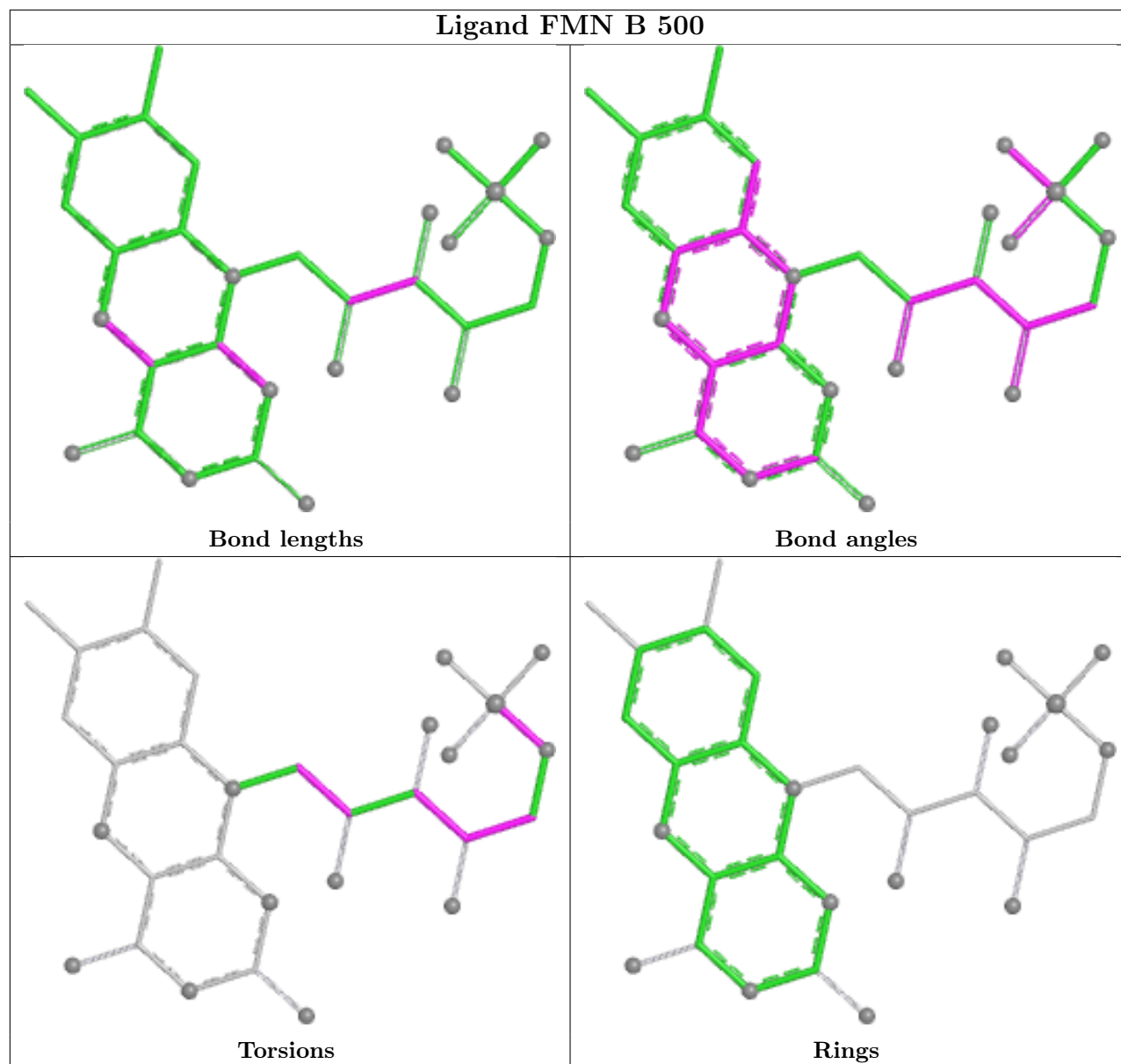
Mol	Chain	Res	Type	Atoms
2	B	500	FMN	O3'-C3'-C4'-O4'
2	D	500	FMN	O2'-C2'-C3'-O3'
2	D	500	FMN	C2'-C3'-C4'-O4'
2	B	500	FMN	C3'-C4'-C5'-O5'
2	C	500	FMN	O2'-C2'-C3'-O3'
2	A	500	FMN	C2'-C3'-C4'-C5'
2	C	500	FMN	C2'-C3'-C4'-C5'
2	A	500	FMN	C2'-C3'-C4'-O4'
2	B	500	FMN	C2'-C3'-C4'-C5'
2	A	500	FMN	C3'-C4'-C5'-O5'
2	D	500	FMN	C2'-C1'-N10-C10
2	B	500	FMN	O3'-C3'-C4'-C5'
2	D	500	FMN	C1'-C2'-C3'-C4'

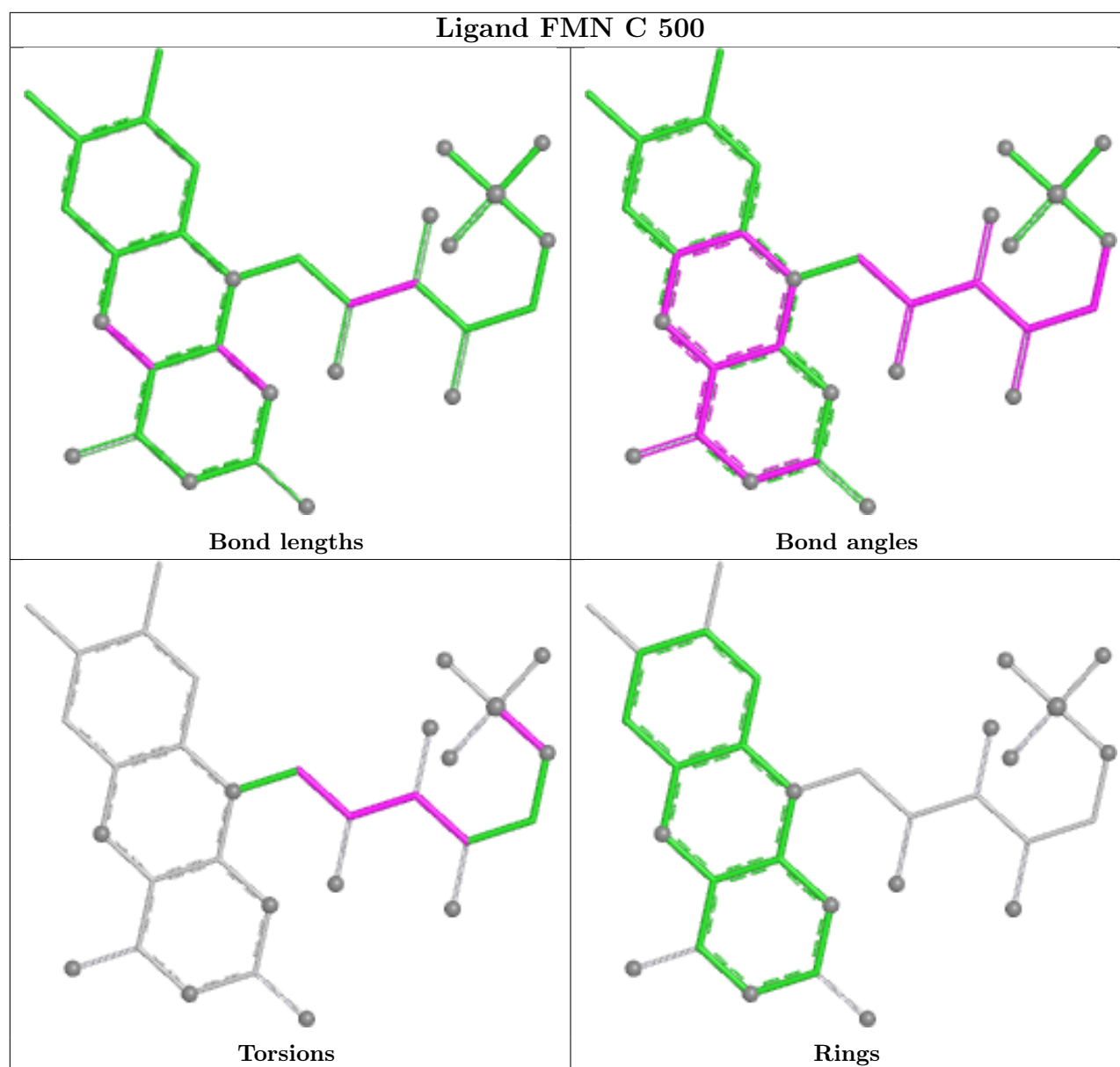
There are no ring outliers.

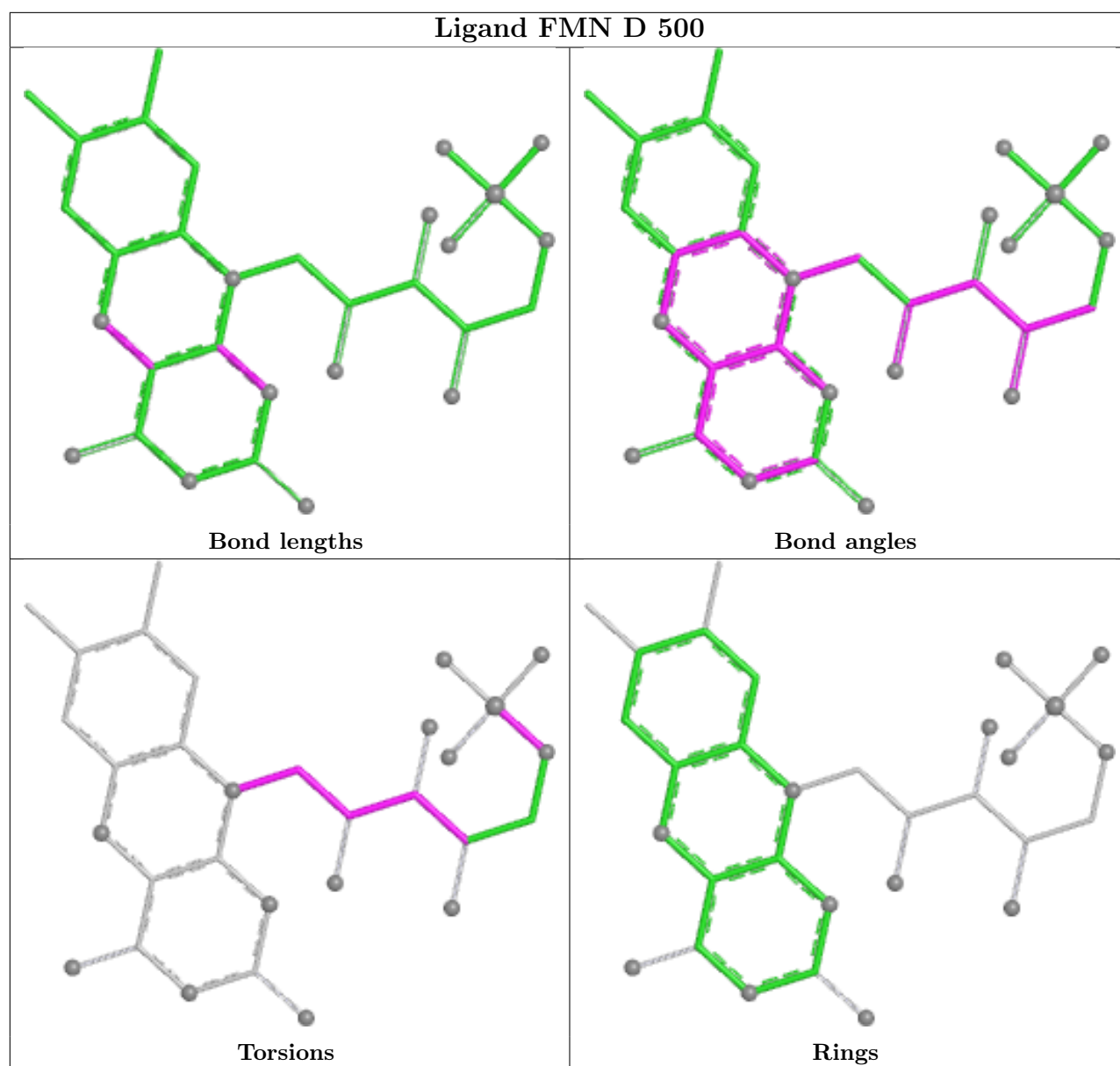
3 monomers are involved in 7 short contacts:

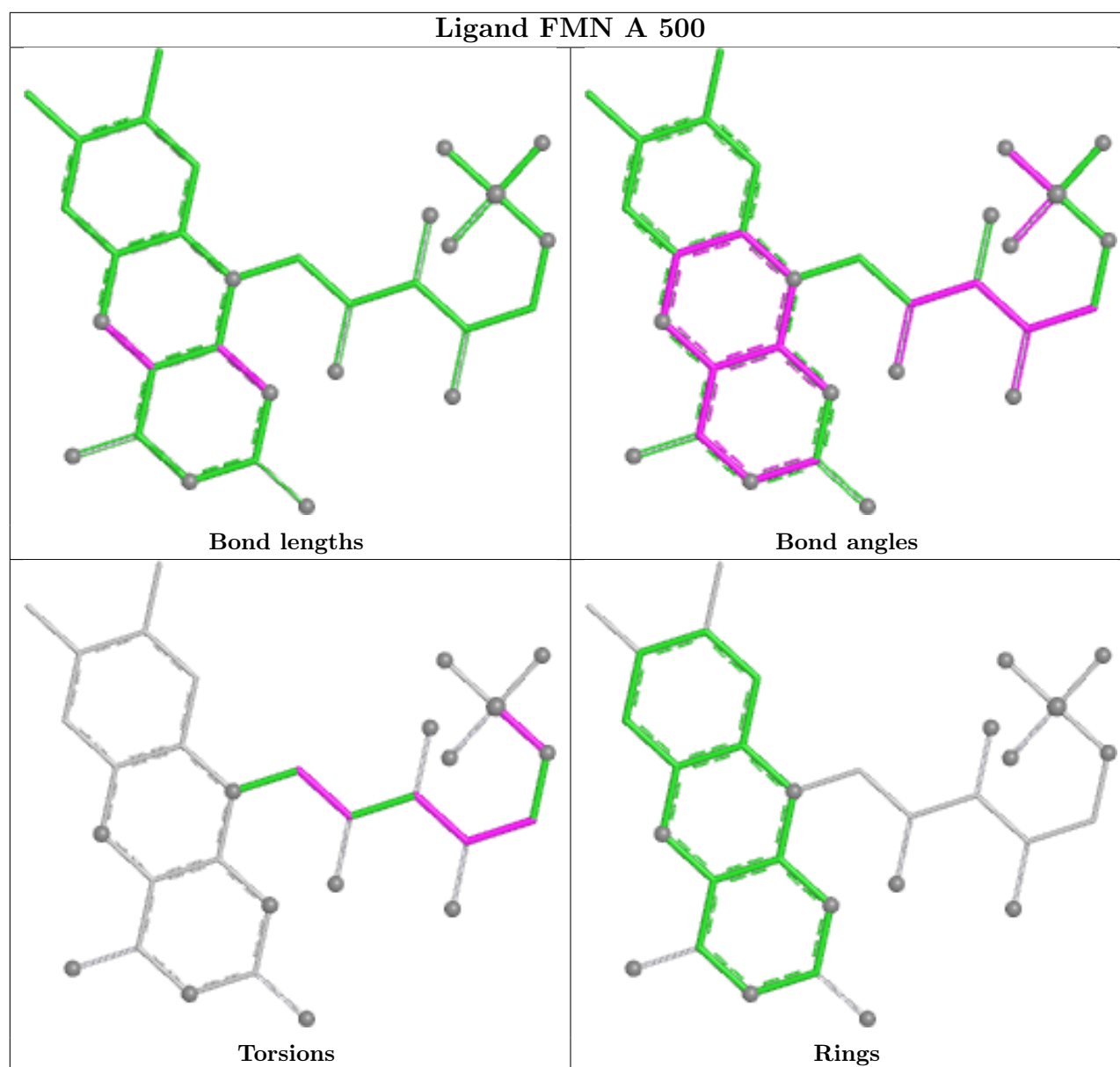
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	FMN	3	0
2	D	500	FMN	3	0
2	A	500	FMN	1	0

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 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	445/453 (98%)	0.12	19 (4%)	40	36	26, 39, 72, 108	0
1	B	445/453 (98%)	0.15	21 (4%)	36	32	28, 40, 73, 104	0
1	C	445/453 (98%)	0.31	40 (8%)	15	12	28, 42, 92, 114	0
1	D	445/453 (98%)	0.61	53 (11%)	9	6	33, 53, 112, 127	0
All	All	1780/1812 (98%)	0.30	133 (7%)	20	17	26, 43, 90, 127	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	VAL	9.8
1	A	150	VAL	6.5
1	D	150	VAL	5.9
1	D	333	ILE	5.3
1	D	343	PRO	5.2
1	D	319	LEU	5.1
1	B	67	TYR	5.0
1	C	150	VAL	4.9
1	A	67	TYR	4.8
1	B	147	ASN	4.7
1	A	71	LEU	4.4
1	D	344	THR	4.4
1	D	352	VAL	4.4
1	D	353	ALA	4.3
1	A	61	LEU	4.3
1	B	68	GLY	4.2
1	C	333	ILE	4.2
1	B	149	GLY	4.2
1	B	71	LEU	4.0
1	D	335	ALA	4.0
1	B	66	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	337	LEU	3.9
1	D	153	HIS	3.9
1	B	63	ILE	3.8
1	C	337	LEU	3.8
1	C	352	VAL	3.7
1	D	357	ALA	3.7
1	D	320	ASN	3.6
1	A	68	GLY	3.6
1	B	146	ARG	3.6
1	D	349	PHE	3.6
1	D	342	VAL	3.6
1	A	64	GLU	3.6
1	D	317	SER	3.6
1	A	65	ASP	3.6
1	C	67	TYR	3.5
1	C	355	GLY	3.5
1	B	145	ALA	3.4
1	C	66	SER	3.4
1	C	330	PHE	3.4
1	D	330	PHE	3.3
1	B	61	LEU	3.3
1	C	357	ALA	3.3
1	D	354	GLY	3.3
1	D	356	GLY	3.3
1	C	344	THR	3.3
1	D	321	LEU	3.2
1	D	351	ALA	3.2
1	B	65	ASP	3.2
1	C	354	GLY	3.2
1	D	345	MET	3.2
1	D	449	VAL	3.1
1	D	312	THR	3.1
1	C	61	LEU	3.1
1	D	334	VAL	3.1
1	C	361	LEU	3.1
1	D	359	LEU	3.1
1	A	66	SER	3.0
1	D	149	GLY	3.0
1	C	319	LEU	3.0
1	D	316	HIS	3.0
1	C	339	ASP	3.0
1	B	201	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	151	ASP	3.0
1	C	335	ALA	2.9
1	D	360	THR	2.9
1	A	199	TYR	2.9
1	A	70	ASN	2.9
1	C	351	ALA	2.9
1	C	341	HIS	2.9
1	D	341	HIS	2.9
1	C	324	TYR	2.9
1	B	148	PHE	2.8
1	C	338	GLY	2.8
1	A	345	MET	2.8
1	D	348	MET	2.8
1	A	63	ILE	2.7
1	D	346	LEU	2.7
1	C	328	THR	2.7
1	C	60	GLY	2.7
1	C	347	GLN	2.7
1	B	70	ASN	2.7
1	C	334	VAL	2.7
1	C	71	LEU	2.7
1	D	355	GLY	2.6
1	D	314	SER	2.6
1	D	350	SER	2.6
1	C	62	ALA	2.6
1	D	361	LEU	2.6
1	B	62	ALA	2.6
1	A	69	ASP	2.6
1	B	269	ALA	2.5
1	C	346	LEU	2.5
1	D	326	LEU	2.5
1	D	62	ALA	2.5
1	D	327	ASP	2.5
1	C	323	LYS	2.5
1	D	325	PRO	2.5
1	C	359	LEU	2.5
1	C	68	GLY	2.5
1	C	148	PHE	2.5
1	A	323	LYS	2.5
1	D	339	ASP	2.5
1	C	342	VAL	2.4
1	A	206	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	324	TYR	2.4
1	A	145	ALA	2.4
1	D	67	TYR	2.4
1	D	318	GLY	2.4
1	C	145	ALA	2.3
1	B	64	GLU	2.3
1	C	345	MET	2.3
1	C	340	ARG	2.3
1	D	338	GLY	2.3
1	D	313	LEU	2.2
1	A	147	ASN	2.2
1	C	348	MET	2.2
1	D	5	ARG	2.1
1	D	323	LYS	2.1
1	C	353	ALA	2.1
1	D	315	SER	2.1
1	D	358	ASP	2.1
1	B	153	HIS	2.1
1	A	62	ALA	2.1
1	B	345	MET	2.1
1	D	154	LEU	2.1
1	D	274	GLU	2.1
1	C	142	ASP	2.1
1	C	322	SER	2.1
1	A	200	VAL	2.1
1	B	60	GLY	2.1
1	C	208	SER	2.0
1	D	336	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

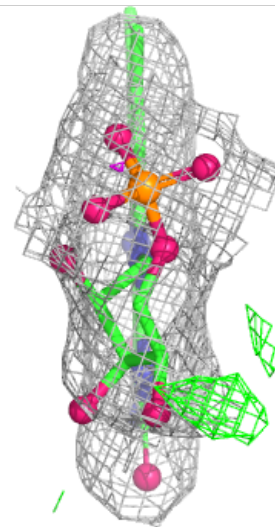
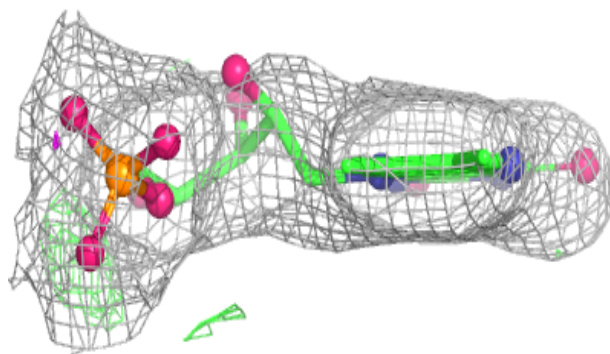
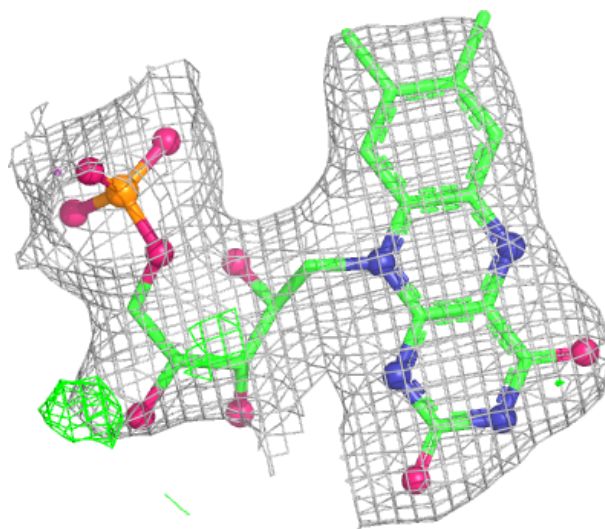
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	D	500	31/31	0.90	0.10	48,56,66,75	0
2	FMN	C	500	31/31	0.92	0.09	34,40,46,55	0
2	FMN	A	500	31/31	0.92	0.09	32,45,55,59	0
2	FMN	B	500	31/31	0.94	0.08	34,43,51,56	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.

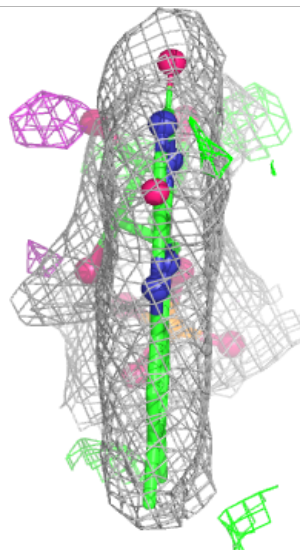
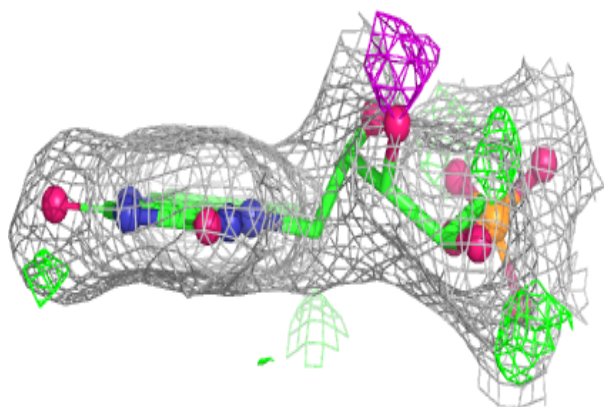
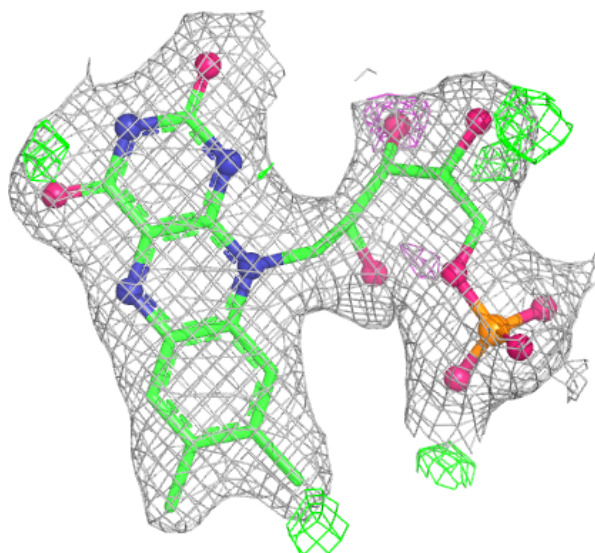
Electron density around FMN D 500:

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



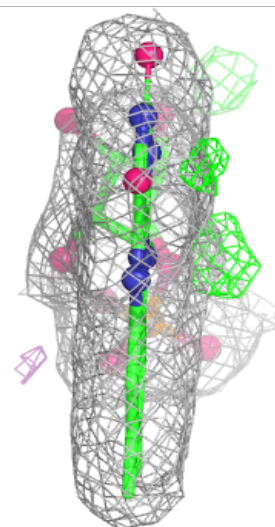
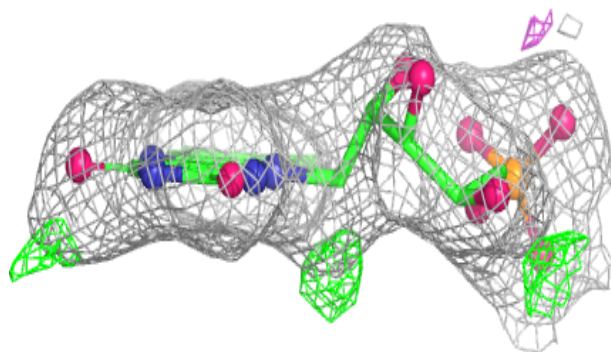
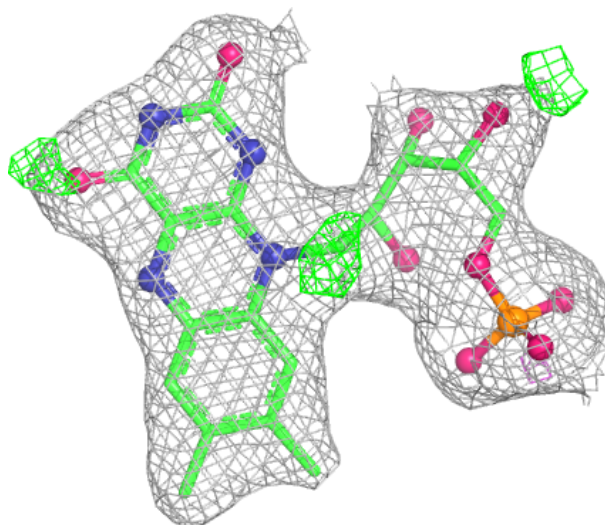
Electron density around FMN C 500:

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



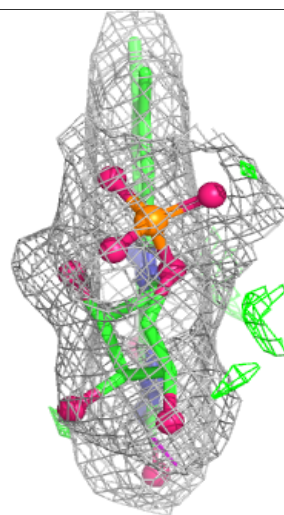
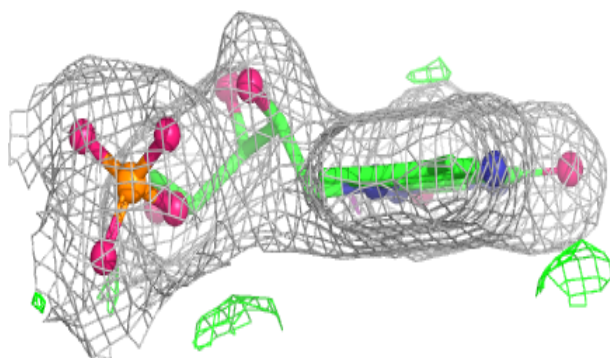
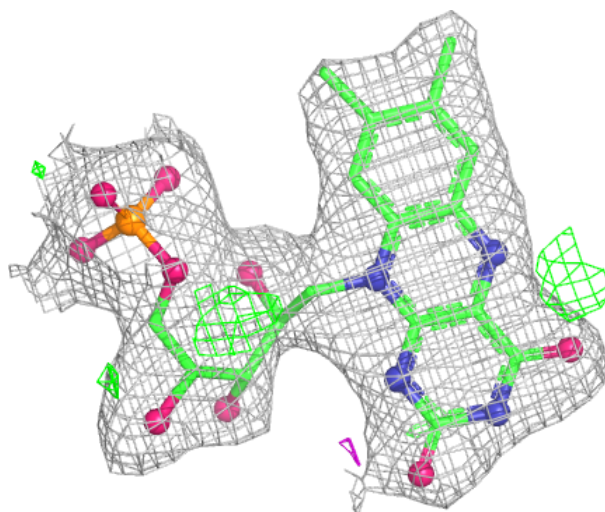
Electron density around FMN A 500:

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



Electron density around FMN B 500:

$2mF_o-DF_c$ (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.