



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:15 PM UTC

PDB ID : 2DU2 / pdb_00002du2
Title : Crystal Structure Analysis of the L-Lactate Oxidase
Authors : Morimoto, Y.
Deposited on : 2006-07-19
Resolution : 2.10 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

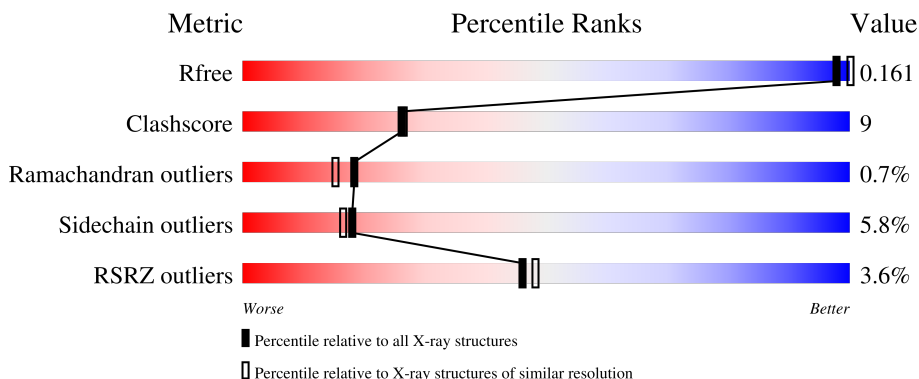
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	374	2% 85% 11% ..
1	B	374	4% 83% 13% ..
1	C	374	3% 81% 14% 5%
1	D	374	6% 80% 17% ..

2 Entry composition [i](#)

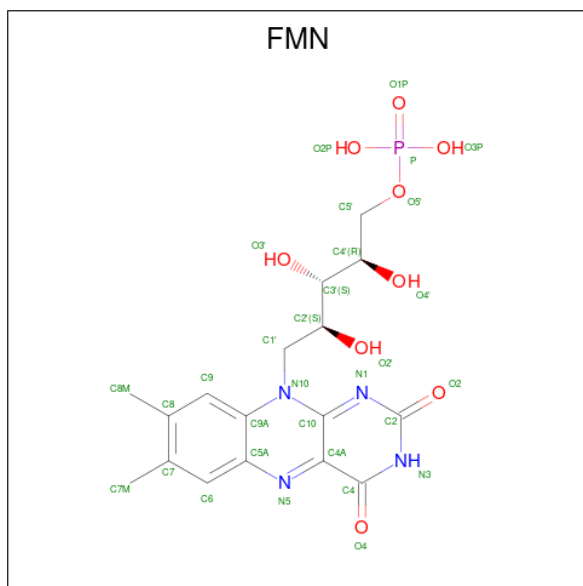
There are 3 unique types of molecules in this entry. The entry contains 12785 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			
1	B	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			
1	C	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			
1	D	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

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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		

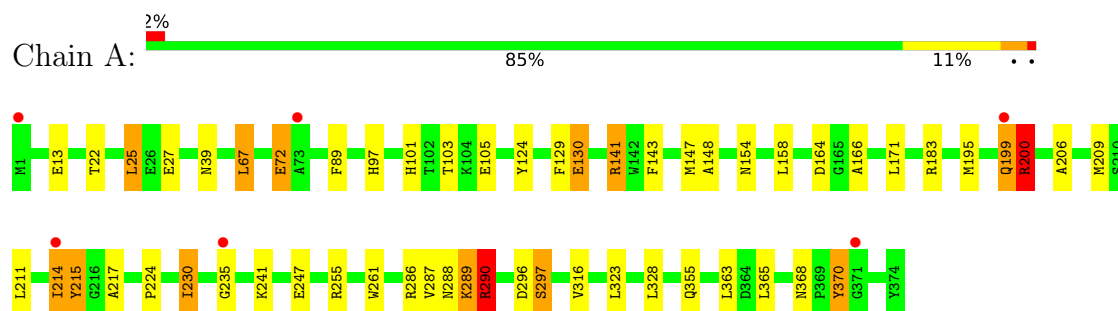
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	299	Total	O	0	0
			299	299		
3	B	266	Total	O	0	0
			266	266		
3	C	291	Total	O	0	0
			291	291		
3	D	253	Total	O	0	0
			253	253		

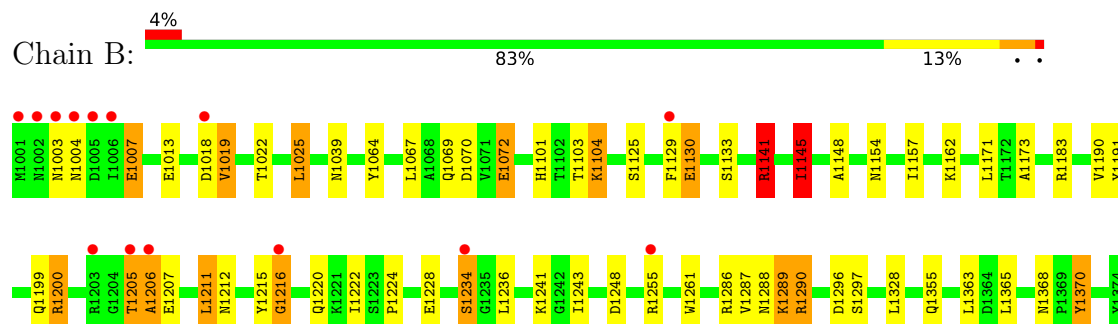
3 Residue-property plots [i](#)

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.

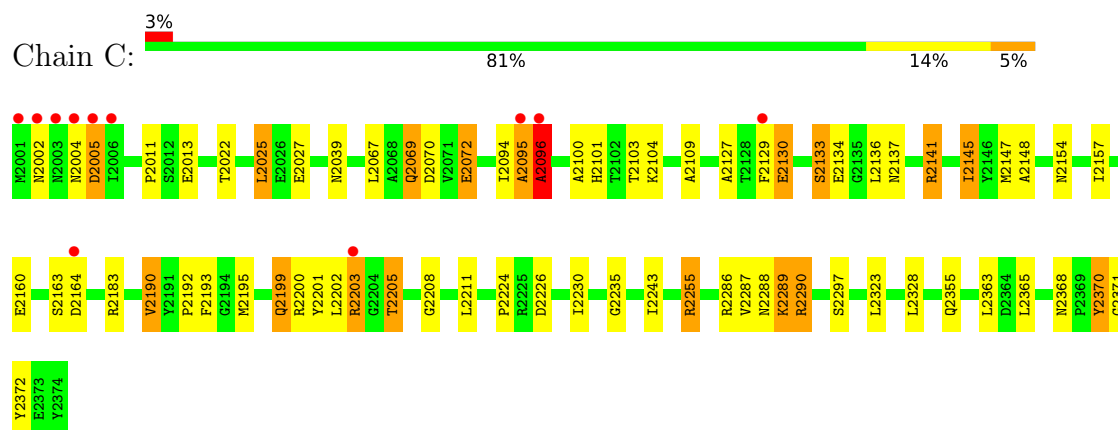
- Molecule 1: Lactate oxidase



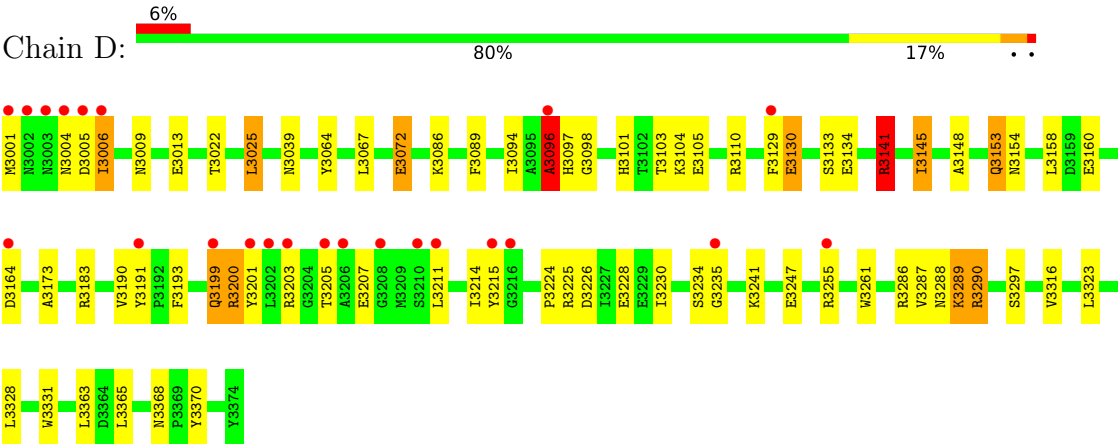
- Molecule 1: Lactate oxidase



- Molecule 1: Lactate oxidase



- Molecule 1: Lactate oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	191.10Å 191.10Å 194.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 99.8 (20.00-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.160 , 0.199 0.165 , 0.161	Depositor DCC
R_{free} test set	5455 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h 0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.01	1/2952 (0.0%)	1.10	10/4000 (0.2%)
1	B	1.03	2/2952 (0.1%)	1.22	27/4000 (0.7%)
1	C	1.01	4/2952 (0.1%)	1.20	16/4000 (0.4%)
1	D	1.04	2/2952 (0.1%)	1.12	14/4000 (0.3%)
All	All	1.02	9/11808 (0.1%)	1.16	67/16000 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2096	ALA	CA-CB	9.44	1.67	1.54
1	D	3096	ALA	CA-CB	8.61	1.67	1.53
1	C	2070	ASP	N-CA	6.67	1.56	1.46
1	B	1070	ASP	N-CA	5.77	1.55	1.46
1	A	230	ILE	CA-CB	5.69	1.61	1.54
1	C	2095	ALA	CA-C	-5.67	1.47	1.53
1	D	3096	ALA	C-O	-5.11	1.17	1.24
1	B	1205	THR	CA-CB	5.09	1.60	1.53
1	C	2372	TYR	N-CA	-5.06	1.40	1.46

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2069	GLN	CA-C-N	-17.00	99.74	123.20
1	C	2069	GLN	C-N-CA	-17.00	99.74	123.20
1	B	1069	GLN	CA-C-N	-16.56	100.60	122.79
1	B	1069	GLN	C-N-CA	-16.56	100.60	122.79
1	A	72	GLU	CA-C-N	-14.31	102.69	123.30
1	A	72	GLU	C-N-CA	-14.31	102.69	123.30
1	D	3072	GLU	CA-C-N	-12.43	105.95	122.98
1	D	3072	GLU	C-N-CA	-12.43	105.95	122.98
1	B	1215	TYR	CA-C-N	-11.13	104.83	122.86
1	B	1215	TYR	C-N-CA	-11.13	104.83	122.86
1	C	2072	GLU	CA-C-N	-10.73	107.84	123.30
1	C	2072	GLU	C-N-CA	-10.73	107.84	123.30
1	A	370	TYR	CA-C-N	-10.52	100.80	121.41
1	A	370	TYR	C-N-CA	-10.52	100.80	121.41
1	B	1370	TYR	CA-C-N	-9.96	101.90	121.41
1	B	1370	TYR	C-N-CA	-9.96	101.90	121.41
1	A	214	ILE	N-CA-C	-9.50	99.48	110.21
1	A	141	ARG	NE-CZ-NH1	-9.34	112.16	121.50
1	C	2145	ILE	CB-CA-C	-9.34	97.81	110.98
1	B	1145	ILE	CB-CA-C	-9.34	97.81	110.98
1	C	2370	TYR	CA-C-N	-9.23	103.32	121.41
1	C	2370	TYR	C-N-CA	-9.23	103.32	121.41
1	B	1018	ASP	N-CA-C	8.99	121.16	111.36
1	D	3145	ILE	CB-CA-C	-8.95	97.21	110.81
1	D	3096	ALA	N-CA-C	8.32	121.28	111.71
1	B	1069	GLN	N-CA-C	-8.04	98.93	110.59
1	A	141	ARG	NE-CZ-NH2	7.76	126.19	119.20
1	D	3215	TYR	N-CA-C	-7.62	100.45	110.43
1	C	2069	GLN	N-CA-C	-7.46	98.80	110.36
1	C	2095	ALA	CA-C-N	-7.33	110.73	122.24
1	C	2095	ALA	C-N-CA	-7.33	110.73	122.24
1	D	3290	ARG	NE-CZ-NH2	-7.28	112.65	119.20
1	C	2205	THR	CB-CA-C	-7.19	97.22	109.51
1	B	1072	GLU	CA-C-N	-7.15	113.18	122.98
1	B	1072	GLU	C-N-CA	-7.15	113.18	122.98
1	A	290	ARG	NE-CZ-NH2	-7.14	112.77	119.20
1	C	2370	TYR	O-C-N	-7.14	114.72	122.85
1	A	370	TYR	O-C-N	-7.12	114.97	122.94
1	C	2290	ARG	NE-CZ-NH2	-6.95	112.94	119.20
1	B	1215	TYR	N-CA-C	-6.91	100.96	110.35
1	B	1070	ASP	CB-CA-C	6.85	122.20	111.72
1	B	1370	TYR	O-C-N	-6.72	115.19	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3234	SER	CA-C-N	-6.70	108.28	121.41
1	D	3234	SER	C-N-CA	-6.70	108.28	121.41
1	D	3064	TYR	CA-C-N	-6.60	113.19	119.85
1	D	3064	TYR	C-N-CA	-6.60	113.19	119.85
1	D	3141	ARG	NE-CZ-NH1	-6.48	115.02	121.50
1	C	2070	ASP	CB-CA-C	6.48	121.29	111.70
1	B	1069	GLN	O-C-N	-6.46	115.12	122.68
1	C	2069	GLN	O-C-N	-6.40	114.26	122.20
1	B	1064	TYR	CA-C-N	-6.34	113.42	120.14
1	B	1064	TYR	C-N-CA	-6.34	113.42	120.14
1	B	1286	ARG	CG-CD-NE	-6.11	98.56	112.00
1	B	1205	THR	CA-C-N	5.63	132.29	121.54
1	B	1205	THR	C-N-CA	5.63	132.29	121.54
1	B	1234	SER	CB-CA-C	-5.50	102.05	111.41
1	B	1206	ALA	N-CA-C	5.47	122.45	110.80
1	B	1141	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	B	1286	ARG	NE-CZ-NH2	-5.37	114.36	119.20
1	C	2095	ALA	CB-CA-C	-5.36	104.33	111.88
1	B	1003	ASN	N-CA-C	5.35	118.91	112.38
1	B	1215	TYR	O-C-N	-5.24	116.36	122.81
1	D	3141	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	199	GLN	N-CA-C	-5.10	102.50	110.10
1	D	3215	TYR	CA-C-N	-5.08	111.17	122.00
1	D	3215	TYR	C-N-CA	-5.08	111.17	122.00
1	B	1290	ARG	NE-CZ-NH2	-5.07	114.64	119.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	GLY	Peptide
1	B	1216	GLY	Peptide
1	C	2096	ALA	Peptide
1	C	2235	GLY	Peptide
1	D	3096	ALA	Peptide
1	D	3235	GLY	Peptide

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	2888	0	2815	52	0
1	B	2888	0	2812	51	0
1	C	2888	0	2812	58	0
1	D	2888	0	2812	58	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	1	0
3	A	299	0	0	4	1
3	B	266	0	0	10	0
3	C	291	0	0	6	0
3	D	253	0	0	0	0
All	All	12785	0	11327	216	1

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 (216) 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:3129:PHE:CD2	1:D:3164:ASP:HB3	1.83	1.11
1:D:3224:PRO:HB3	1:D:3255:ARG:HG3	1.33	1.11
1:C:2224:PRO:HB3	1:C:2255:ARG:HG3	1.34	1.07
1:A:199:GLN:O	1:A:200:ARG:HB3	1.26	1.03
1:A:209:MET:HE2	1:A:217:ALA:HB3	1.37	1.01
1:A:148:ALA:H	1:A:154:ASN:HD21	1.08	0.99
1:D:3129:PHE:CE2	1:D:3164:ASP:HB3	1.98	0.98
1:B:1224:PRO:HB3	1:B:1255:ARG:HG3	1.45	0.98
1:C:2095:ALA:C	3:C:5650:HOH:O	2.06	0.97
1:A:224:PRO:HB3	1:A:255:ARG:HG3	1.47	0.96
1:D:3148:ALA:H	1:D:3154:ASN:HD21	1.02	0.96
1:B:1191:TYR:O	1:B:1207:GLU:O	1.84	0.96
1:A:209:MET:HE2	1:A:217:ALA:CB	1.97	0.94
1:C:2005:ASP:HA	1:C:2192:PRO:O	1.68	0.94
1:C:2129:PHE:CE2	1:C:2164:ASP:HB3	2.02	0.93
1:B:1216:GLY:HA2	1:B:1220:GLN:NE2	1.83	0.93
1:B:1148:ALA:H	1:B:1154:ASN:HD21	1.11	0.92
1:C:2129:PHE:CD2	1:C:2164:ASP:HB3	2.05	0.91
1:B:1234:SER:O	1:B:1234:SER:OG	1.67	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:VAL:O	1:B:1290:ARG:HD3	1.68	0.91
1:A:147:MET:HA	1:A:147:MET:HE2	1.52	0.90
1:A:199:GLN:O	1:A:200:ARG:CB	2.13	0.88
1:C:2255:ARG:HG2	3:C:5124:HOH:O	1.74	0.88
1:A:255:ARG:HG2	3:A:5122:HOH:O	1.75	0.86
1:C:2287:VAL:O	1:C:2290:ARG:HD3	1.77	0.84
1:D:3191:TYR:O	1:D:3207:GLU:O	1.96	0.84
1:D:3191:TYR:HE2	1:D:3193:PHE:CE1	1.96	0.82
1:B:1129:PHE:HB3	3:B:5321:HOH:O	1.78	0.81
1:D:3191:TYR:CE2	1:D:3193:PHE:CE1	2.68	0.81
1:C:2096:ALA:N	3:C:5650:HOH:O	2.13	0.79
1:C:2148:ALA:H	1:C:2154:ASN:HD21	1.29	0.78
1:D:3148:ALA:N	1:D:3154:ASN:HD21	1.82	0.78
1:A:39:ASN:HD22	1:A:183:ARG:HH11	1.28	0.77
1:D:3205:THR:HG22	1:D:3207:GLU:H	1.48	0.77
1:D:3287:VAL:O	1:D:3290:ARG:HD3	1.84	0.77
1:C:2287:VAL:O	1:C:2290:ARG:CD	2.33	0.76
1:A:287:VAL:O	1:A:290:ARG:HD3	1.86	0.75
1:A:287:VAL:O	1:A:290:ARG:CD	2.35	0.74
1:B:1148:ALA:N	1:B:1154:ASN:HD21	1.83	0.74
1:C:2226:ASP:O	1:C:2230:ILE:HG12	1.87	0.74
1:B:1039:ASN:HD22	1:B:1183:ARG:HH11	1.33	0.74
1:D:3153:GLN:HG2	1:D:3200:ARG:HG3	1.68	0.74
1:B:1216:GLY:HA2	1:B:1220:GLN:HE22	1.51	0.73
1:B:1224:PRO:CB	1:B:1255:ARG:HG3	2.18	0.72
1:C:2096:ALA:HB3	1:C:2323:LEU:HD21	1.72	0.72
1:D:3199:GLN:NE2	1:D:3205:THR:HA	2.05	0.71
1:B:1255:ARG:HG2	3:B:5289:HOH:O	1.90	0.71
1:D:3191:TYR:HE2	1:D:3193:PHE:HE1	1.36	0.71
1:D:3129:PHE:CE2	1:D:3133:SER:OG	2.42	0.71
1:A:101:HIS:HD2	1:A:103:THR:H	1.37	0.70
1:A:147:MET:HE3	1:A:171:LEU:HD13	1.72	0.69
1:C:2004:ASN:HB3	1:C:2193:PHE:HA	1.74	0.69
1:B:1148:ALA:H	1:B:1154:ASN:ND2	1.89	0.69
1:D:3004:ASN:HB3	1:D:3193:PHE:CB	2.23	0.69
1:B:1287:VAL:O	1:B:1290:ARG:CD	2.39	0.68
1:D:3039:ASN:HD22	1:D:3183:ARG:HH11	1.41	0.67
1:D:3129:PHE:CD2	1:D:3164:ASP:CB	2.72	0.67
1:C:2072:GLU:H	1:C:2355:GLN:HE22	1.43	0.67
1:A:206:ALA:HA	1:A:209:MET:HE3	1.76	0.67
1:C:2039:ASN:HD22	1:C:2183:ARG:HH11	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2129:PHE:CD2	1:C:2164:ASP:CB	2.79	0.65
1:B:1234:SER:HB2	3:B:5923:HOH:O	1.98	0.64
1:D:3148:ALA:H	1:D:3154:ASN:ND2	1.85	0.64
1:B:1133:SER:OG	1:B:1141:ARG:NH1	2.32	0.63
1:C:2129:PHE:CE2	1:C:2133:SER:OG	2.50	0.62
1:C:2022:THR:HA	1:C:2025:LEU:HD22	1.81	0.62
1:B:1228:GLU:OE2	1:B:1255:ARG:HD3	2.00	0.61
1:B:1101:HIS:HD2	1:B:1103:THR:H	1.48	0.61
1:C:2157:ILE:HD11	1:C:2200:ARG:HD2	1.82	0.61
1:B:1234:SER:O	1:B:1236:LEU:N	2.27	0.61
1:C:2129:PHE:CE2	1:C:2164:ASP:CB	2.80	0.60
1:D:3287:VAL:O	1:D:3290:ARG:CD	2.48	0.60
1:B:1216:GLY:CA	1:B:1220:GLN:HE22	2.15	0.60
1:A:195:MET:HE2	1:A:211:LEU:HD23	1.83	0.59
1:D:3096:ALA:HA	1:D:3191:TYR:OH	2.03	0.59
1:A:101:HIS:CD2	1:A:103:THR:H	2.20	0.58
1:C:2195:MET:H	1:C:2199:GLN:HE22	1.50	0.58
1:C:2133:SER:OG	1:C:2141:ARG:NH1	2.37	0.58
1:D:3199:GLN:HE22	1:D:3205:THR:HA	1.66	0.58
1:A:224:PRO:CB	1:A:255:ARG:HG3	2.30	0.57
1:B:1013:GLU:O	1:B:1101:HIS:HE1	1.86	0.57
1:B:1072:GLU:H	1:B:1355:GLN:HE22	1.51	0.57
1:A:22:THR:HA	1:A:25:LEU:HD22	1.85	0.57
1:A:39:ASN:ND2	1:A:183:ARG:HH11	2.02	0.57
1:A:209:MET:CE	1:A:217:ALA:CB	2.80	0.57
1:D:3228:GLU:OE2	1:D:3255:ARG:HD2	2.05	0.56
1:D:3368:ASN:HD21	1:D:3370:TYR:HB2	1.70	0.56
1:C:2190:VAL:HG13	1:C:2208:GLY:HA2	1.87	0.56
1:B:1129:PHE:CG	1:B:1130:GLU:N	2.73	0.56
1:B:1072:GLU:O	3:B:5748:HOH:O	2.17	0.56
1:A:195:MET:CE	1:A:211:LEU:HD23	2.36	0.56
1:C:2095:ALA:CA	3:C:5650:HOH:O	2.50	0.55
1:B:1212:ASN:OD1	3:B:5956:HOH:O	2.17	0.55
1:A:130:GLU:H	1:A:130:GLU:CD	2.15	0.55
1:C:2371:GLY:HA3	3:C:5759:HOH:O	2.08	0.55
1:D:3160:GLU:O	1:D:3164:ASP:CG	2.50	0.54
1:C:2147:MET:HE3	1:C:2230:ILE:HD11	1.90	0.54
1:D:3224:PRO:HB3	1:D:3255:ARG:CG	2.23	0.54
1:A:72:GLU:O	3:A:5618:HOH:O	2.18	0.54
1:C:2129:PHE:CD2	1:C:2164:ASP:CG	2.85	0.54
1:C:2130:GLU:H	1:C:2130:GLU:CD	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3039:ASN:ND2	1:D:3183:ARG:HH11	2.06	0.54
1:A:124:TYR:HB3	1:A:195:MET:HE2	1.90	0.53
1:D:3130:GLU:H	1:D:3130:GLU:CD	2.17	0.53
1:B:1224:PRO:HB3	1:B:1255:ARG:CG	2.30	0.53
1:B:1368:ASN:HD21	1:B:1370:TYR:HB2	1.73	0.53
1:B:1039:ASN:ND2	1:B:1183:ARG:HH11	2.06	0.53
1:C:2002:ASN:HD21	1:C:2004:ASN:HD22	1.55	0.53
1:D:3096:ALA:HB3	1:D:3323:LEU:HD21	1.91	0.53
1:B:1200:ARG:HD2	3:B:5654:HOH:O	2.08	0.53
1:D:3013:GLU:O	1:D:3101:HIS:HE1	1.92	0.52
1:C:2134:GLU:HG3	3:C:5408:HOH:O	2.09	0.52
1:D:3001:MET:HG3	1:D:3005:ASP:HB2	1.90	0.52
1:A:147:MET:HE2	1:A:147:MET:CA	2.34	0.52
1:A:287:VAL:O	1:A:290:ARG:HD2	2.10	0.52
1:B:1228:GLU:OE2	1:B:1255:ARG:CD	2.58	0.52
1:C:2101:HIS:HD2	1:C:2103:THR:H	1.58	0.52
1:D:3129:PHE:CE2	1:D:3164:ASP:CB	2.85	0.51
1:A:147:MET:HA	1:A:147:MET:CE	2.35	0.51
1:B:1101:HIS:CD2	1:B:1103:THR:H	2.28	0.51
1:D:3129:PHE:HD1	1:D:3130:GLU:OE2	1.94	0.51
1:C:2002:ASN:ND2	1:C:2004:ASN:HD22	2.09	0.51
1:C:2129:PHE:CG	1:C:2164:ASP:CG	2.89	0.51
1:B:1216:GLY:CA	1:B:1220:GLN:NE2	2.65	0.50
1:C:2160:GLU:O	1:C:2164:ASP:OD1	2.30	0.50
1:D:3158:LEU:HD11	1:D:3230:ILE:HD12	1.94	0.50
1:A:214:ILE:O	1:A:215:TYR:CD1	2.65	0.49
1:B:1243:ILE:HD12	1:B:1248:ASP:HB3	1.95	0.49
1:C:2022:THR:O	1:C:2025:LEU:HB2	2.12	0.49
1:B:1162:LYS:HB2	3:B:5923:HOH:O	2.11	0.49
1:A:72:GLU:H	1:A:355:GLN:HE22	1.59	0.49
1:D:3129:PHE:CG	1:D:3164:ASP:CG	2.92	0.48
1:D:3022:THR:HA	1:D:3025:LEU:HD22	1.94	0.48
1:D:3224:PRO:CB	1:D:3255:ARG:HG3	2.23	0.48
1:B:1067:LEU:HD22	1:D:3173:ALA:HB3	1.95	0.48
1:C:2160:GLU:O	1:C:2164:ASP:CG	2.55	0.48
1:B:1222:ILE:O	1:C:2069:GLN:O	2.32	0.48
1:C:2094:ILE:HG21	1:C:2323:LEU:HD22	1.95	0.48
1:C:2101:HIS:CD2	1:C:2103:THR:H	2.31	0.48
1:A:158:LEU:HD11	1:A:230:ILE:HD12	1.96	0.47
1:B:1191:TYR:OH	1:B:1211:LEU:HG	2.14	0.47
1:C:2148:ALA:N	1:C:2154:ASN:HD21	2.05	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:HIS:CD2	1:A:105:GLU:HG3	2.49	0.47
1:C:2368:ASN:HD21	1:C:2370:TYR:HB2	1.79	0.47
1:D:3288:ASN:C	1:D:3289:LYS:HG3	2.39	0.47
1:C:2013:GLU:O	1:C:2101:HIS:HE1	1.97	0.47
1:C:2148:ALA:HB2	1:C:2201:TYR:CD2	2.49	0.47
1:D:3004:ASN:HB3	1:D:3193:PHE:HB3	1.95	0.47
1:B:1104:LYS:HE3	3:B:5435:HOH:O	2.15	0.47
1:B:1130:GLU:HG2	3:B:5414:HOH:O	2.13	0.47
1:D:3133:SER:OG	1:D:3141:ARG:NH1	2.48	0.47
1:A:241:LYS:HA	1:A:261:TRP:HB3	1.96	0.46
1:C:2101:HIS:CD2	1:C:2103:THR:OG1	2.69	0.46
1:B:1199:GLN:HG3	1:B:1205:THR:HG23	1.98	0.46
1:A:13:GLU:O	1:A:101:HIS:HE1	1.98	0.46
1:B:1022:THR:HA	1:B:1025:LEU:HD22	1.98	0.46
1:A:288:ASN:C	1:A:289:LYS:HG3	2.41	0.46
1:A:368:ASN:HD21	1:A:370:TYR:HB2	1.81	0.46
1:A:214:ILE:O	1:A:215:TYR:CB	2.63	0.46
1:B:1234:SER:C	1:B:1236:LEU:H	2.22	0.46
1:C:2101:HIS:HD2	1:C:2103:THR:OG1	1.98	0.46
1:A:67:LEU:HD11	1:C:2243:ILE:HG12	1.96	0.46
1:A:214:ILE:O	1:A:215:TYR:CG	2.69	0.45
1:A:195:MET:HE1	1:A:214:ILE:HD12	1.97	0.45
1:D:3101:HIS:HD2	1:D:3103:THR:H	1.65	0.45
1:C:2104:LYS:HE3	1:C:2127:ALA:HB2	1.97	0.45
1:D:3004:ASN:HB3	1:D:3193:PHE:HB2	1.99	0.45
1:B:1173:ALA:HB3	1:C:2067:LEU:HD22	1.99	0.45
1:A:296:ASP:OD1	1:A:296:ASP:C	2.60	0.45
1:B:1241:LYS:HA	1:B:1261:TRP:HB3	1.98	0.45
1:B:1288:ASN:C	1:B:1289:LYS:HG3	2.42	0.45
1:D:3226:ASP:O	1:D:3230:ILE:HG12	2.16	0.45
1:A:143:PHE:CD2	1:A:166:ALA:HB2	2.51	0.45
2:D:3512:FMN:HM83	2:D:3512:FMN:HM71	1.85	0.45
1:A:206:ALA:O	1:A:209:MET:HB2	2.18	0.44
1:C:2288:ASN:ND2	1:C:2289:LYS:HE3	2.33	0.44
1:D:3153:GLN:NE2	1:D:3201:TYR:HB3	2.32	0.44
1:C:2255:ARG:HD3	1:C:2255:ARG:HA	1.84	0.44
1:C:2004:ASN:HB3	1:C:2193:PHE:CA	2.46	0.44
1:C:2011:PRO:HD2	1:C:2100:ALA:O	2.17	0.44
1:C:2190:VAL:CG1	1:C:2208:GLY:HA2	2.47	0.44
1:B:1145:ILE:HD12	1:B:1171:LEU:HA	2.00	0.43
1:A:199:GLN:O	3:A:5718:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:OE2	1:A:286:ARG:NH2	2.51	0.43
1:A:206:ALA:CA	1:A:209:MET:HE3	2.47	0.43
1:B:1129:PHE:CD1	1:B:1130:GLU:N	2.87	0.43
1:C:2109:ALA:HB1	1:C:2136:LEU:HG	1.99	0.43
1:D:3098:GLY:CA	1:D:3104:LYS:HG2	2.49	0.43
1:C:2287:VAL:O	1:C:2290:ARG:HD2	2.16	0.43
1:A:296:ASP:O	1:A:297:SER:HB2	2.19	0.43
1:A:89:PHE:HA	1:A:316:VAL:O	2.19	0.42
1:D:3101:HIS:HD2	1:D:3103:THR:OG1	2.02	0.42
1:D:3255:ARG:HD3	1:D:3255:ARG:HA	1.85	0.42
1:D:3094:ILE:HG21	1:D:3323:LEU:HD22	2.02	0.42
1:D:3228:GLU:OE2	1:D:3255:ARG:CD	2.67	0.42
1:B:1129:PHE:CD1	1:B:1129:PHE:N	2.88	0.42
1:C:2202:LEU:O	1:C:2203:ARG:CB	2.68	0.42
1:D:3368:ASN:ND2	1:D:3368:ASN:C	2.78	0.42
1:B:1129:PHE:HE1	3:B:5800:HOH:O	2.03	0.41
1:B:1296:ASP:OD1	1:B:1296:ASP:C	2.62	0.41
1:C:2129:PHE:HE2	1:C:2141:ARG:HH11	1.68	0.41
1:C:2148:ALA:H	1:C:2154:ASN:ND2	2.07	0.41
1:D:3241:LYS:HA	1:D:3261:TRP:HB3	2.03	0.41
1:A:199:GLN:HG3	3:A:5723:HOH:O	2.21	0.41
1:D:3110:ARG:HG2	1:D:3331:TRP:CD2	2.56	0.41
1:A:143:PHE:HD2	1:A:166:ALA:HB2	1.85	0.41
1:D:3247:GLU:OE2	1:D:3286:ARG:NH2	2.51	0.41
1:A:129:PHE:CZ	1:A:164:ASP:HB3	2.55	0.41
1:A:209:MET:HE2	1:A:217:ALA:HB1	1.96	0.41
1:A:255:ARG:HD3	1:A:255:ARG:HA	1.73	0.40
1:D:3101:HIS:CD2	1:D:3103:THR:H	2.38	0.40
1:D:3089:PHE:HA	1:D:3316:VAL:O	2.21	0.40
1:D:3129:PHE:HE2	1:D:3141:ARG:HH11	1.68	0.40
1:D:3148:ALA:HB2	1:D:3201:TYR:CD1	2.57	0.40
1:B:1157:ILE:HD11	1:B:1200:ARG:HD3	2.03	0.40
1:D:3097:HIS:CG	1:D:3105:GLU:HG3	2.56	0.40

All (1) 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:A:5545:HOH:O	3:A:5873:HOH:O[16_444]	2.19	0.01

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	372/374 (100%)	361 (97%)	8 (2%)	3 (1%)	16	12
1	B	372/374 (100%)	355 (95%)	13 (4%)	4 (1%)	11	8
1	C	372/374 (100%)	358 (96%)	12 (3%)	2 (0%)	24	22
1	D	372/374 (100%)	358 (96%)	12 (3%)	2 (0%)	24	22
All	All	1488/1496 (100%)	1432 (96%)	45 (3%)	11 (1%)	18	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	TYR
1	A	297	SER
1	B	1206	ALA
1	B	1297	SER
1	C	2297	SER
1	D	3297	SER
1	A	200	ARG
1	B	1019	VAL
1	C	2005	ASP
1	B	1007	GLU
1	D	3006	ILE

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	298/298 (100%)	286 (96%)	12 (4%)	28	29
1	B	298/298 (100%)	282 (95%)	16 (5%)	20	18
1	C	298/298 (100%)	279 (94%)	19 (6%)	16	14
1	D	298/298 (100%)	276 (93%)	22 (7%)	13	10
All	All	1192/1192 (100%)	1123 (94%)	69 (6%)	18	16

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	27	GLU
1	A	67	LEU
1	A	130	GLU
1	A	141	ARG
1	A	200	ARG
1	A	289	LYS
1	A	290	ARG
1	A	323	LEU
1	A	328	LEU
1	A	363	LEU
1	A	365	LEU
1	B	1004	ASN
1	B	1007	GLU
1	B	1019	VAL
1	B	1025	LEU
1	B	1104	LYS
1	B	1125	SER
1	B	1130	GLU
1	B	1141	ARG
1	B	1145	ILE
1	B	1190	VAL
1	B	1200	ARG
1	B	1211	LEU
1	B	1289	LYS
1	B	1328	LEU
1	B	1363	LEU
1	B	1365	LEU
1	C	2025	LEU
1	C	2027	GLU
1	C	2130	GLU
1	C	2133	SER
1	C	2137	ASN

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Mol	Chain	Res	Type
1	C	2141	ARG
1	C	2145	ILE
1	C	2163	SER
1	C	2190	VAL
1	C	2199	GLN
1	C	2203	ARG
1	C	2205	THR
1	C	2211	LEU
1	C	2255	ARG
1	C	2286	ARG
1	C	2289	LYS
1	C	2328	LEU
1	C	2363	LEU
1	C	2365	LEU
1	D	3006	ILE
1	D	3009	ASN
1	D	3025	LEU
1	D	3067	LEU
1	D	3072	GLU
1	D	3086	LYS
1	D	3130	GLU
1	D	3134	GLU
1	D	3141	ARG
1	D	3145	ILE
1	D	3153	GLN
1	D	3190	VAL
1	D	3199	GLN
1	D	3200	ARG
1	D	3203	ARG
1	D	3211	LEU
1	D	3214	ILE
1	D	3225	ARG
1	D	3289	LYS
1	D	3328	LEU
1	D	3363	LEU
1	D	3365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	ASN

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Mol	Chain	Res	Type
1	A	101	HIS
1	A	137	ASN
1	A	154	ASN
1	A	187	ASN
1	A	288	ASN
1	A	355	GLN
1	A	368	ASN
1	B	1003	ASN
1	B	1039	ASN
1	B	1083	HIS
1	B	1101	HIS
1	B	1137	ASN
1	B	1154	ASN
1	B	1187	ASN
1	B	1212	ASN
1	B	1288	ASN
1	B	1350	GLN
1	B	1355	GLN
1	B	1368	ASN
1	C	2002	ASN
1	C	2004	ASN
1	C	2035	HIS
1	C	2039	ASN
1	C	2083	HIS
1	C	2101	HIS
1	C	2153	GLN
1	C	2154	ASN
1	C	2187	ASN
1	C	2199	GLN
1	C	2288	ASN
1	C	2350	GLN
1	C	2355	GLN
1	C	2368	ASN
1	D	3009	ASN
1	D	3035	HIS
1	D	3039	ASN
1	D	3069	GLN
1	D	3101	HIS
1	D	3137	ASN
1	D	3153	GLN
1	D	3154	ASN
1	D	3187	ASN

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Mol	Chain	Res	Type
1	D	3199	GLN
1	D	3355	GLN
1	D	3368	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	3512	-	33,33,33	1.27	4 (12%)	48,50,50	1.29	6 (12%)
2	FMN	C	2512	-	33,33,33	1.04	1 (3%)	48,50,50	1.41	7 (14%)
2	FMN	A	512	-	33,33,33	1.17	2 (6%)	48,50,50	1.26	5 (10%)
2	FMN	B	1512	-	33,33,33	1.10	3 (9%)	48,50,50	1.38	8 (16%)

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	D	3512	-	-	2/18/18/18	0/3/3/3
2	FMN	C	2512	-	-	1/18/18/18	0/3/3/3
2	FMN	A	512	-	-	1/18/18/18	0/3/3/3
2	FMN	B	1512	-	-	1/18/18/18	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3512	FMN	C4A-N5	4.21	1.39	1.30
2	A	512	FMN	C4A-N5	4.14	1.39	1.30
2	B	1512	FMN	C4A-N5	3.77	1.38	1.30
2	C	2512	FMN	C4A-N5	3.29	1.37	1.30
2	D	3512	FMN	C10-N1	2.97	1.39	1.33
2	A	512	FMN	C10-N1	2.68	1.38	1.33
2	D	3512	FMN	C1'-C2'	2.15	1.55	1.52
2	B	1512	FMN	O4-C4	2.11	1.27	1.23
2	D	3512	FMN	C1'-N10	2.10	1.52	1.47
2	B	1512	FMN	C10-N1	2.05	1.37	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1512	FMN	C10-C4A-N5	-3.77	117.10	124.81
2	B	1512	FMN	C4A-C10-N10	3.63	121.68	116.48
2	B	1512	FMN	C4-C4A-N5	3.52	123.07	118.21
2	A	512	FMN	O4-C4-C4A	-3.28	117.87	126.53
2	A	512	FMN	C8M-C8-C9	-3.14	114.05	119.57
2	C	2512	FMN	C4A-C10-N10	3.13	120.96	116.48
2	A	512	FMN	C5A-C9A-N10	3.07	120.75	117.97
2	D	3512	FMN	C4A-C10-N10	2.90	120.64	116.48
2	C	2512	FMN	C10-C4A-N5	-2.64	119.42	124.81
2	D	3512	FMN	C5A-C9A-N10	2.60	120.32	117.97
2	B	1512	FMN	O2-C2-N1	-2.60	117.49	121.80
2	C	2512	FMN	C9A-C5A-N5	-2.52	119.78	122.45
2	A	512	FMN	C9A-C5A-N5	-2.50	119.80	122.45
2	C	2512	FMN	C4-N3-C2	-2.42	121.35	125.64
2	D	3512	FMN	C10-C4A-N5	-2.35	120.02	124.81
2	C	2512	FMN	O3P-P-O5'	2.31	112.70	106.67
2	D	3512	FMN	C9A-C5A-N5	-2.27	120.05	122.45
2	B	1512	FMN	C4-N3-C2	-2.26	121.63	125.64
2	A	512	FMN	C4-N3-C2	-2.23	121.69	125.64
2	D	3512	FMN	C4A-C4-N3	2.14	118.69	113.25
2	C	2512	FMN	O2P-P-O5'	2.13	112.23	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3512	FMN	C4-C4A-N5	2.13	121.15	118.21
2	C	2512	FMN	C4-C4A-C10	2.13	120.58	116.93
2	B	1512	FMN	C5A-N5-C4A	2.11	121.49	118.09
2	B	1512	FMN	O2-C2-N3	2.09	122.59	118.58
2	B	1512	FMN	C4A-C10-N1	-2.06	119.55	124.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

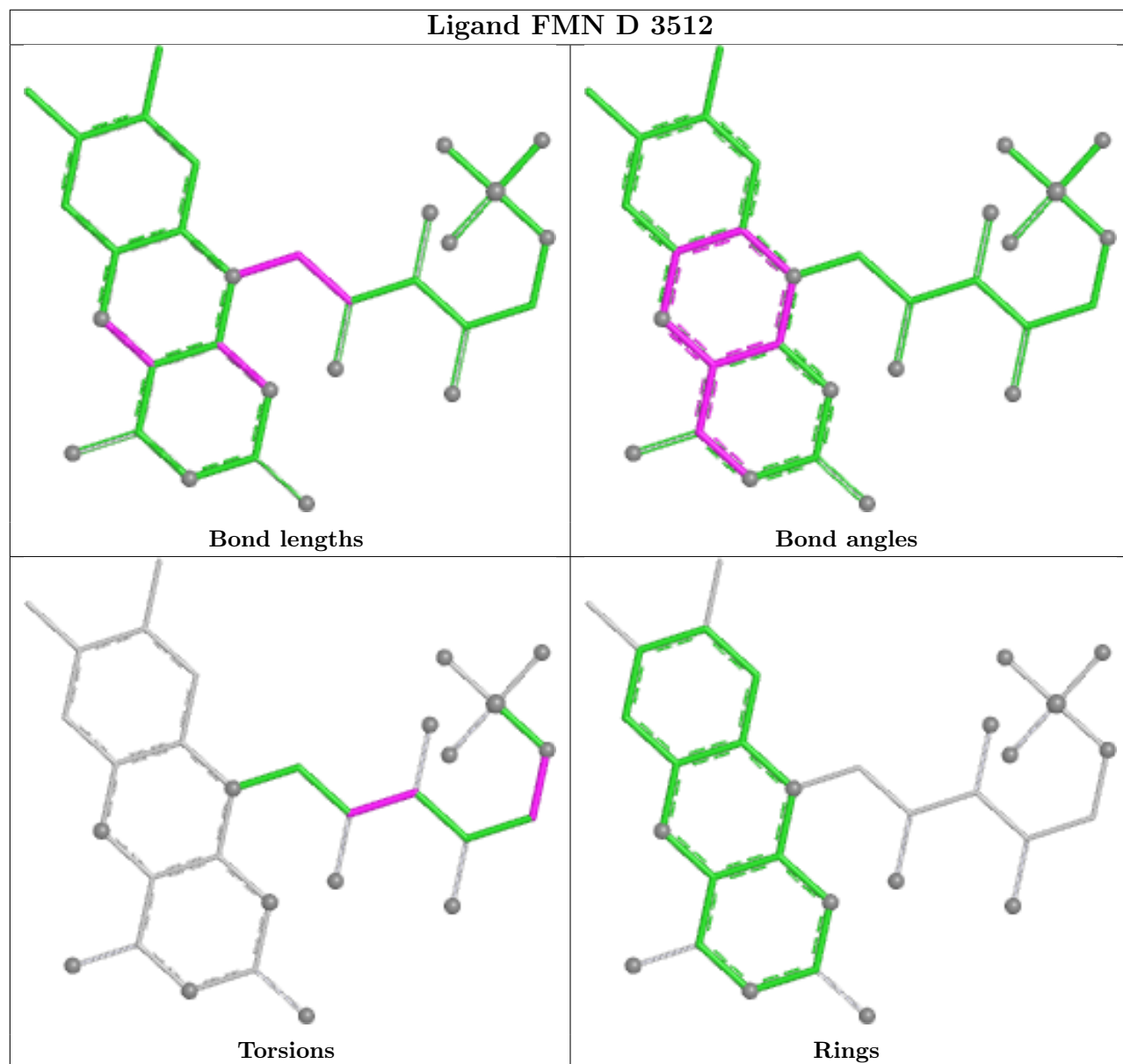
Mol	Chain	Res	Type	Atoms
2	B	1512	FMN	C4'-C5'-O5'-P
2	C	2512	FMN	C4'-C5'-O5'-P
2	A	512	FMN	C4'-C5'-O5'-P
2	D	3512	FMN	C4'-C5'-O5'-P
2	D	3512	FMN	O2'-C2'-C3'-C4'

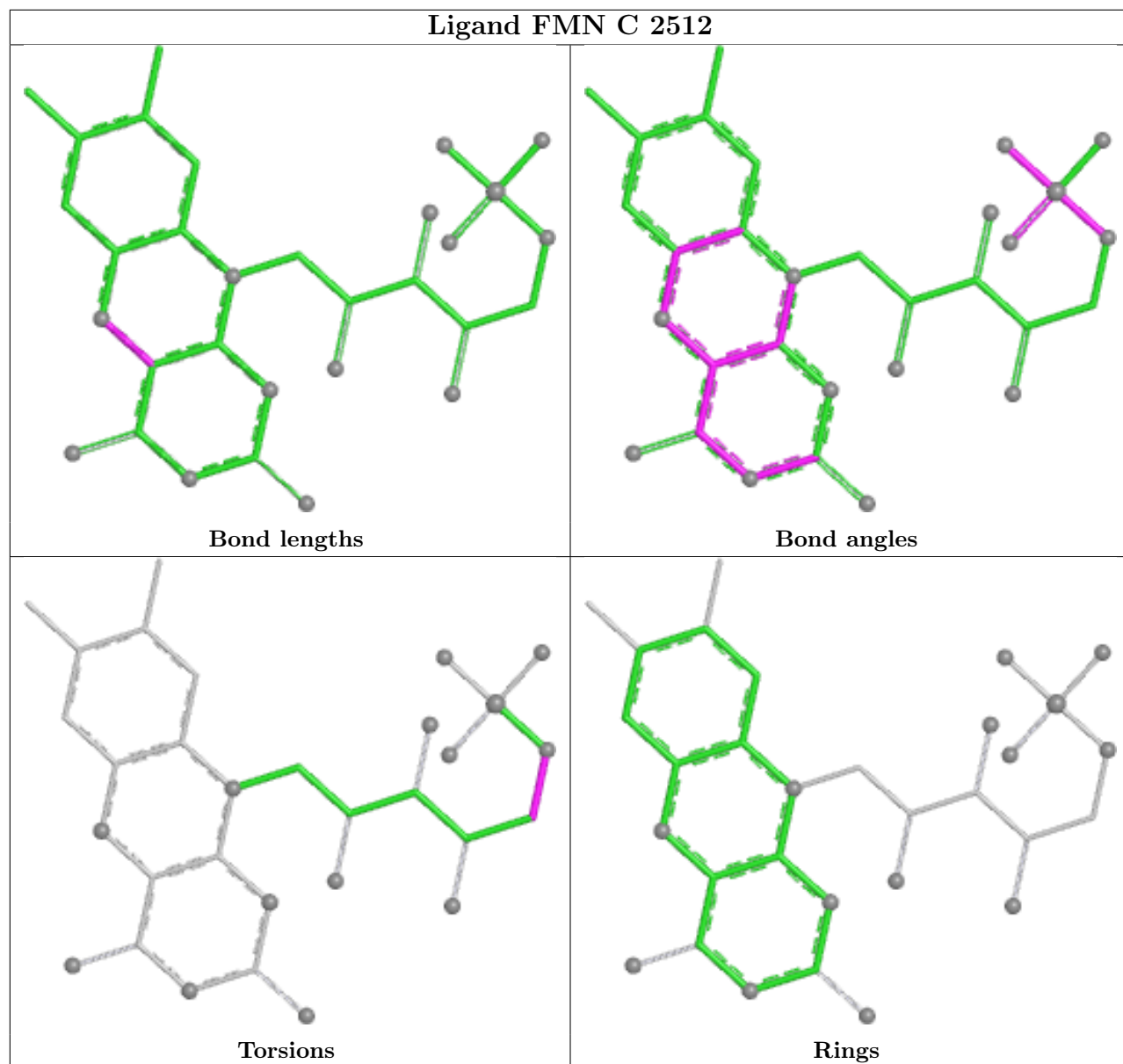
There are no ring outliers.

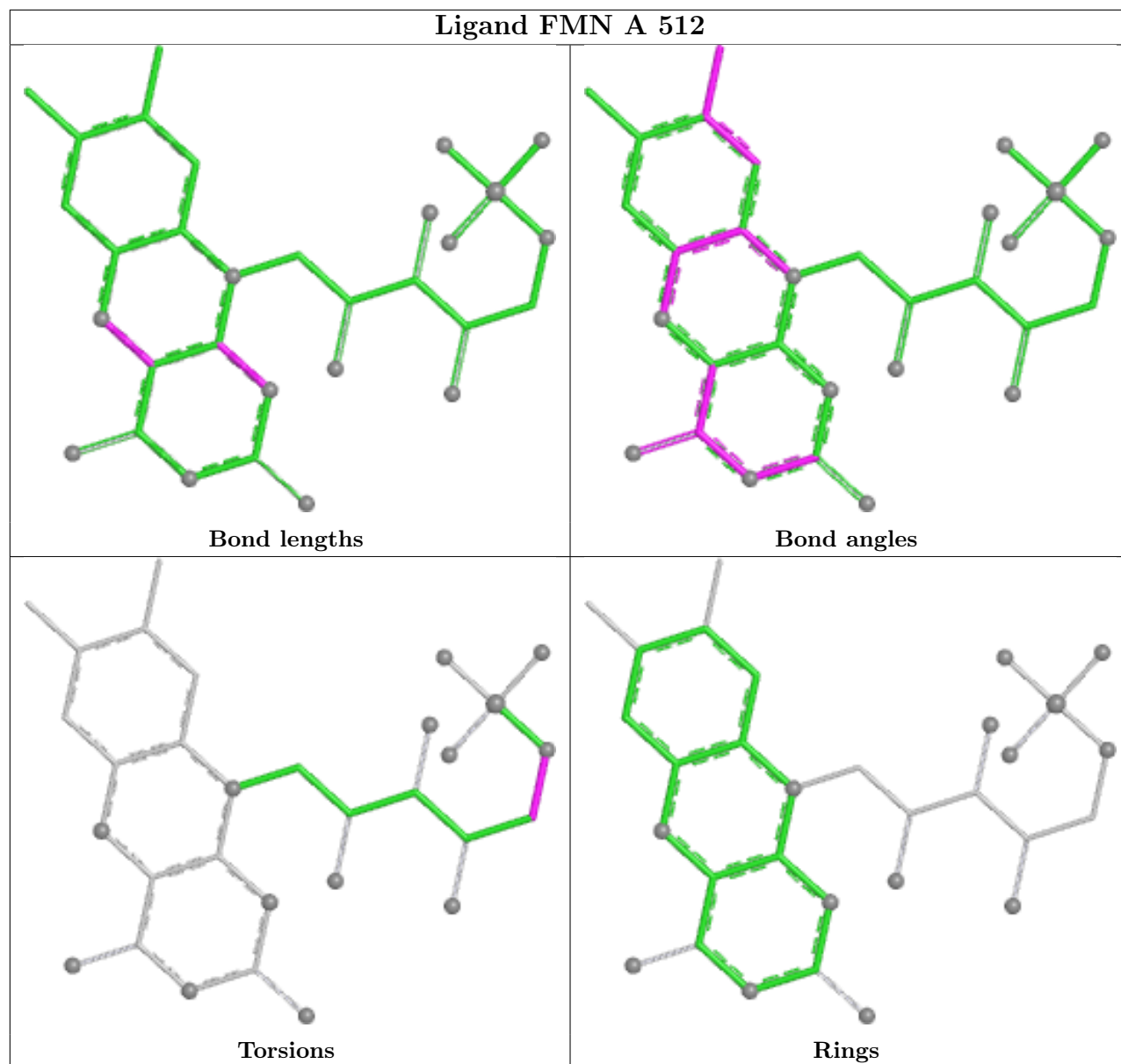
1 monomer is involved in 1 short contact:

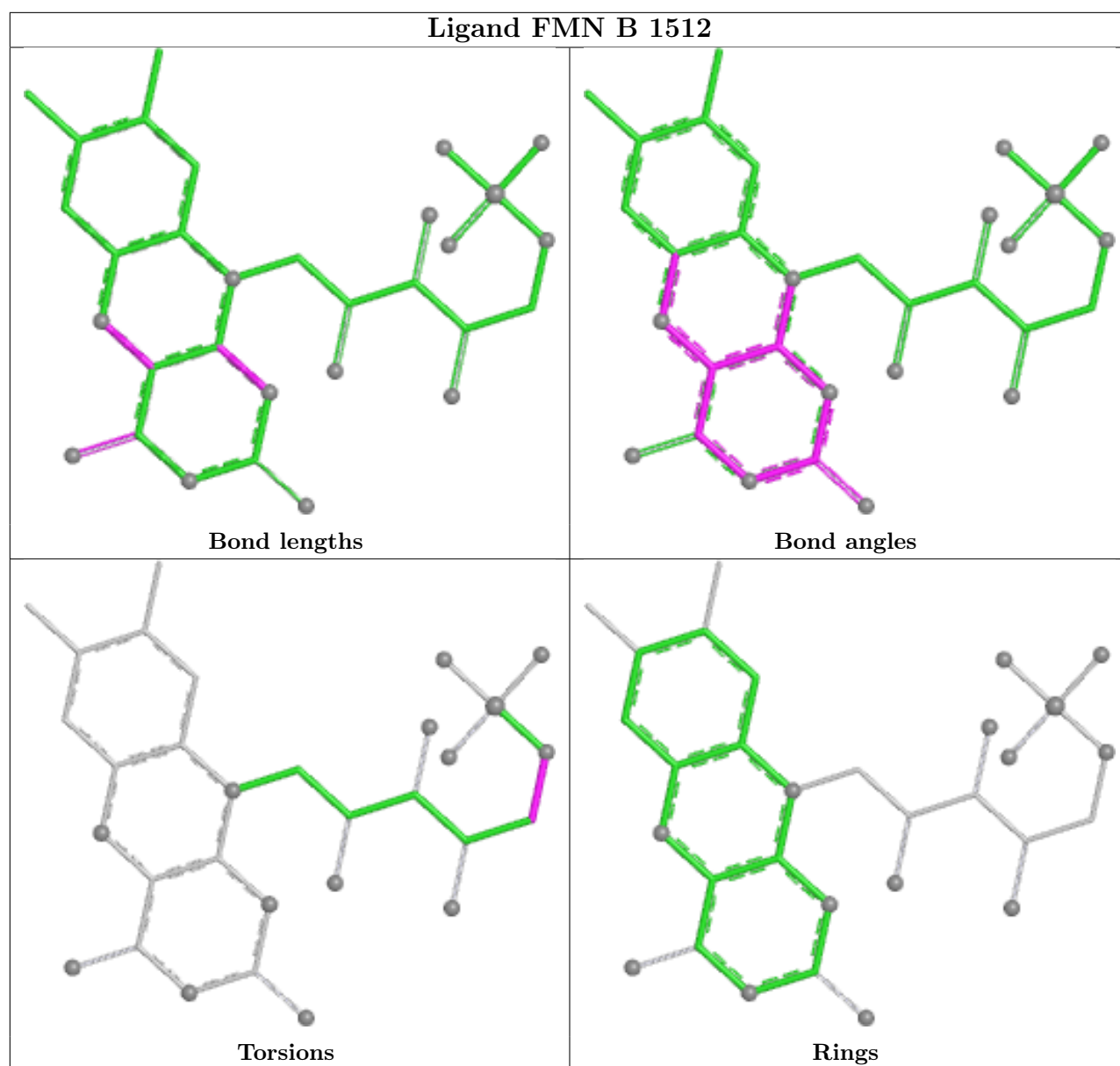
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3512	FMN	1	0

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	374/374 (100%)	-0.59	6 (1%) 70 73	8, 14, 31, 47	0
1	B	374/374 (100%)	-0.40	14 (3%) 45 47	9, 17, 31, 91	0
1	C	374/374 (100%)	-0.41	11 (2%) 53 56	9, 17, 30, 89	0
1	D	374/374 (100%)	-0.31	23 (6%) 27 29	9, 16, 41, 91	0
All	All	1496/1496 (100%)	-0.42	54 (3%) 46 48	8, 16, 33, 91	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1006	ILE	10.7
1	C	2005	ASP	7.9
1	D	3006	ILE	7.7
1	B	1003	ASN	7.2
1	C	2006	ILE	6.3
1	B	1205	THR	6.1
1	D	3004	ASN	5.6
1	B	1129	PHE	5.5
1	C	2002	ASN	5.5
1	C	2001	MET	5.5
1	C	2004	ASN	5.1
1	C	2164	ASP	5.1
1	D	3005	ASP	5.0
1	D	3191	TYR	5.0
1	C	2129	PHE	4.8
1	D	3003	ASN	4.6
1	B	1005	ASP	4.2
1	D	3216	GLY	4.1
1	D	3129	PHE	4.0
1	B	1203	ARG	4.0
1	D	3201	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	3001	MET	3.7
1	C	2095	ALA	3.7
1	A	214	ILE	3.6
1	A	1	MET	3.5
1	D	3164	ASP	3.4
1	D	3205	THR	3.4
1	B	1001	MET	3.3
1	C	2096	ALA	3.3
1	D	3202	LEU	3.3
1	B	1002	ASN	3.1
1	B	1004	ASN	3.0
1	D	3206	ALA	2.9
1	D	3203	ARG	2.9
1	C	2003	ASN	2.8
1	D	3096	ALA	2.7
1	B	1255	ARG	2.7
1	D	3255	ARG	2.6
1	A	371	GLY	2.6
1	A	199	GLN	2.6
1	A	235	GLY	2.5
1	D	3210	SER	2.5
1	D	3208	GLY	2.5
1	B	1216	GLY	2.4
1	D	3199	GLN	2.4
1	B	1234	SER	2.4
1	D	3215	TYR	2.3
1	D	3002	ASN	2.3
1	D	3211	LEU	2.3
1	A	73	ALA	2.2
1	D	3235	GLY	2.2
1	C	2203	ARG	2.1
1	B	1206	ALA	2.1
1	B	1018	ASP	2.1

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 ⓘ

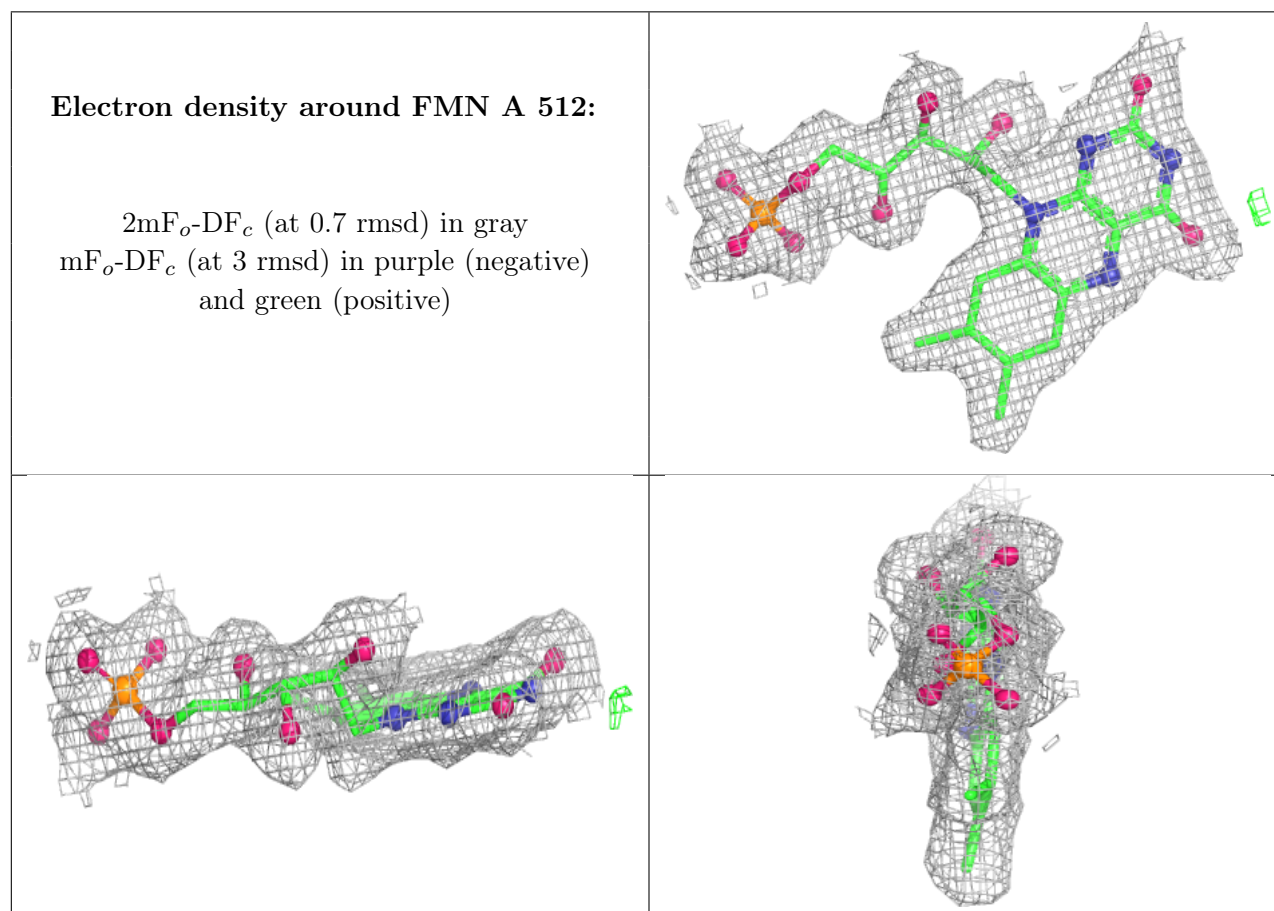
There are no oligosaccharides in this entry.

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.

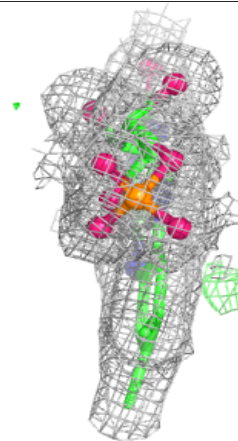
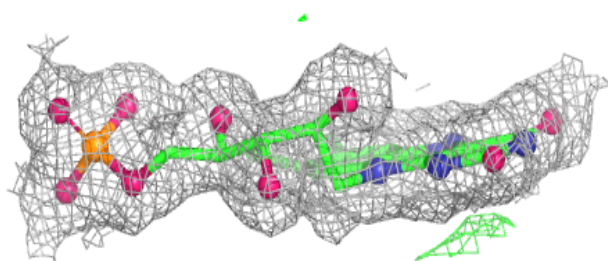
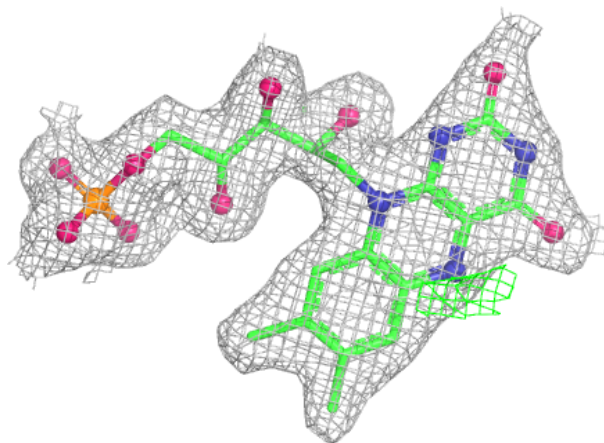
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	A	512	31/31	0.98	0.04	7,11,14,15	0
2	FMN	B	1512	31/31	0.98	0.05	11,13,15,15	0
2	FMN	C	2512	31/31	0.98	0.05	11,13,14,17	0
2	FMN	D	3512	31/31	0.98	0.05	10,14,15,16	0

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.



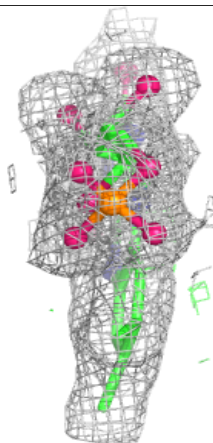
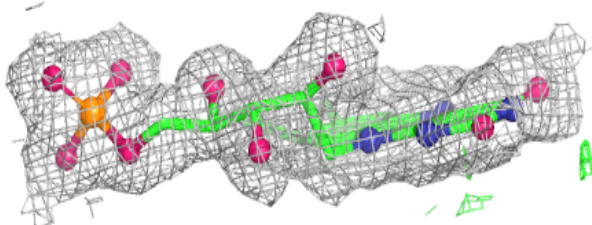
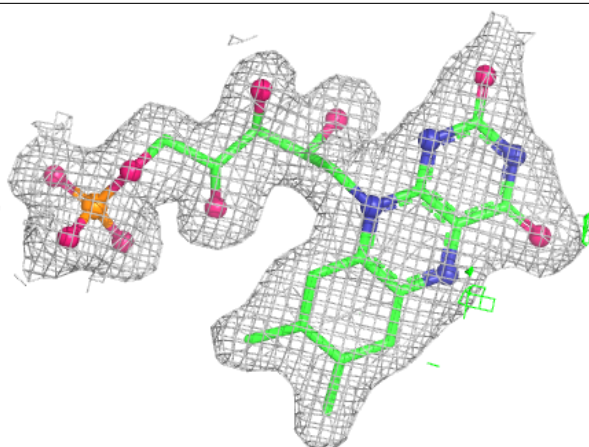
Electron density around FMN B 1512:

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



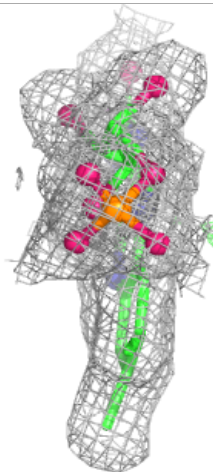
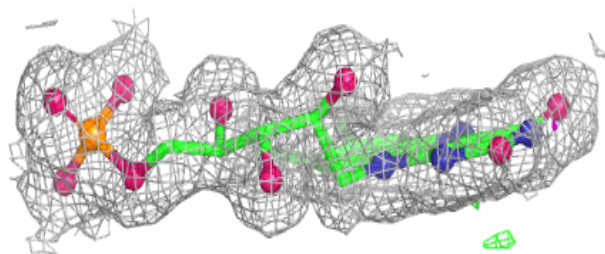
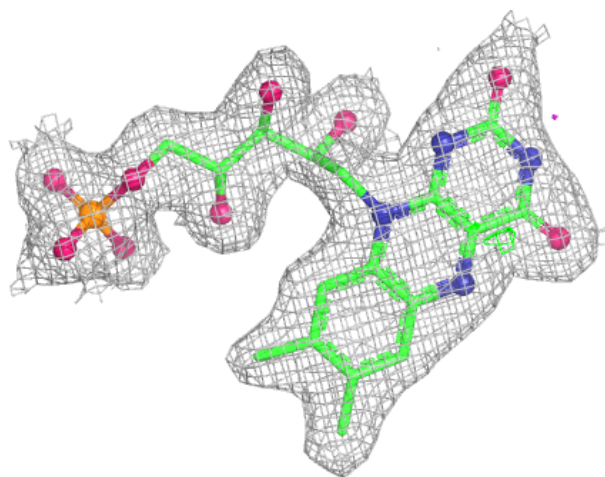
Electron density around FMN C 2512:

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



Electron density around FMN D 3512:

$2mF_o-DF_c$ (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.