



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:07 PM UTC

PDB ID : 1UM0 / pdb_00001um0
Title : Crystal structure of chorismate synthase complexed with FMN
Authors : Ahn, H.J.; Yoon, H.J.; Lee, B.; Suh, S.W.
Deposited on : 2003-09-18
Resolution : 1.95 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

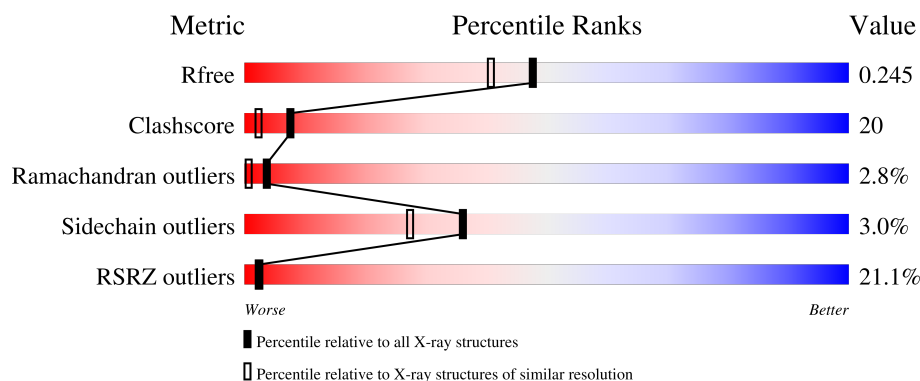
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	365	15% 75% 21% .
1	B	365	25% 69% 27% .
1	C	365	30% 65% 30% 5%
1	D	365	15% 68% 28% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	B	2400	-	-	X	-

2 Entry composition [i](#)

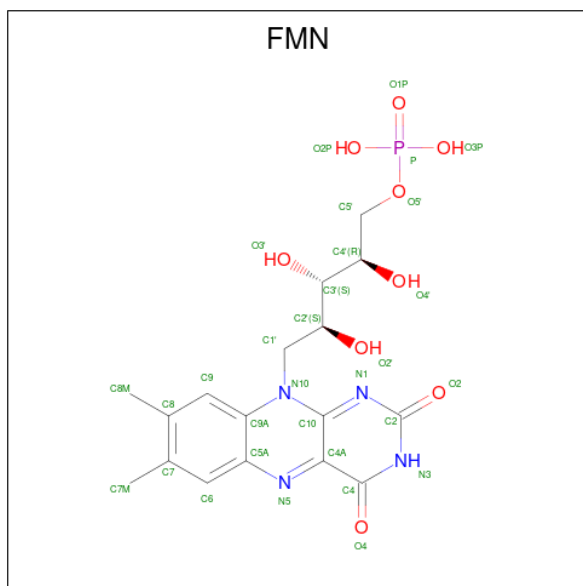
There are 3 unique types of molecules in this entry. The entry contains 11843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	B	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	C	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	D	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			

- 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		

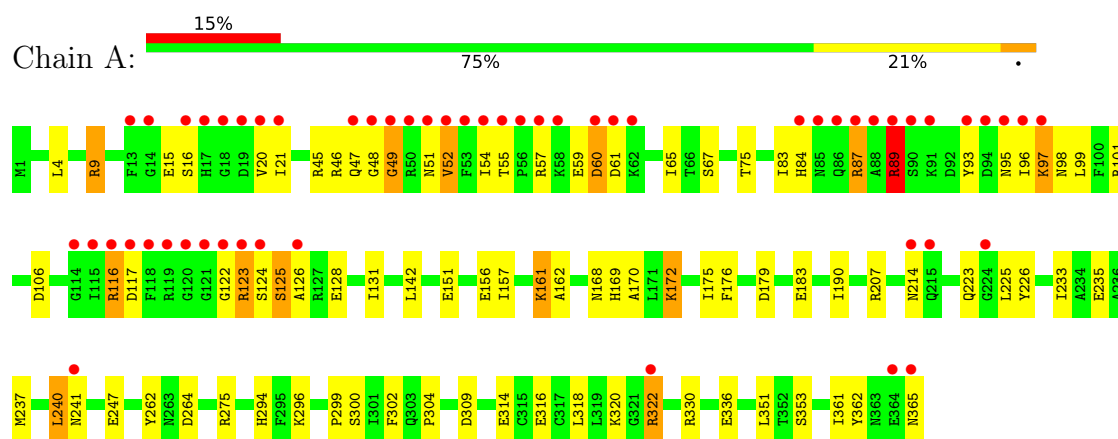
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total	O	0	0
			158	158		
3	B	84	Total	O	0	0
			84	84		
3	C	76	Total	O	0	0
			76	76		
3	D	137	Total	O	0	0
			137	137		

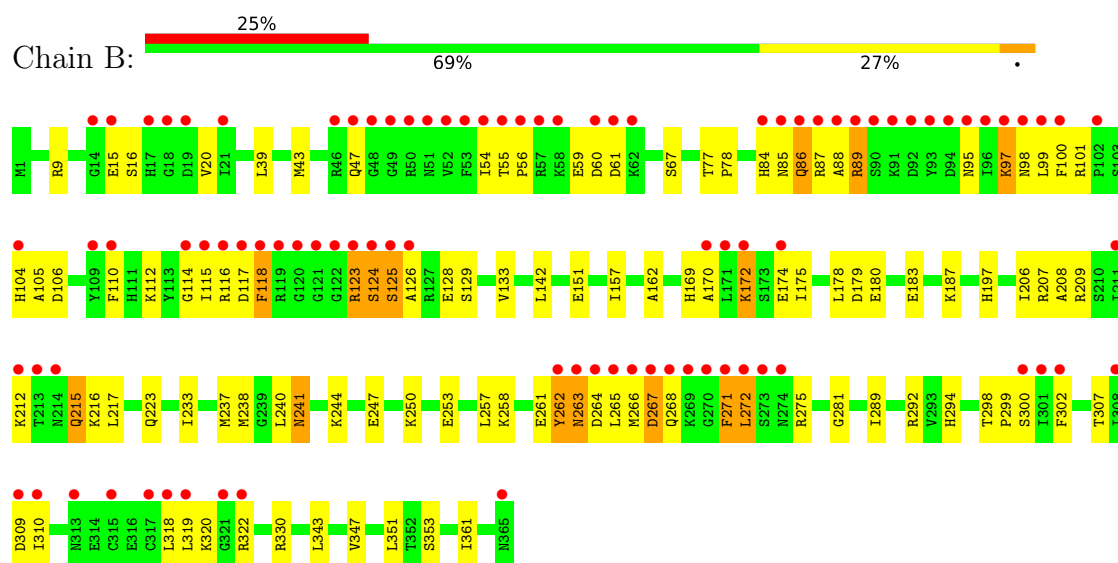
3 Residue-property plots [i](#)

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: Chorismate synthase

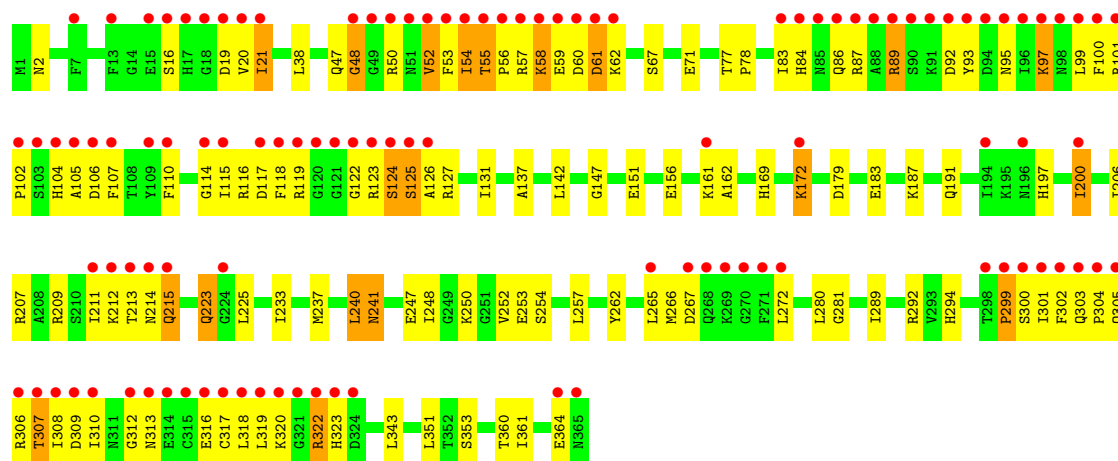


• Molecule 1: Chorismate synthase

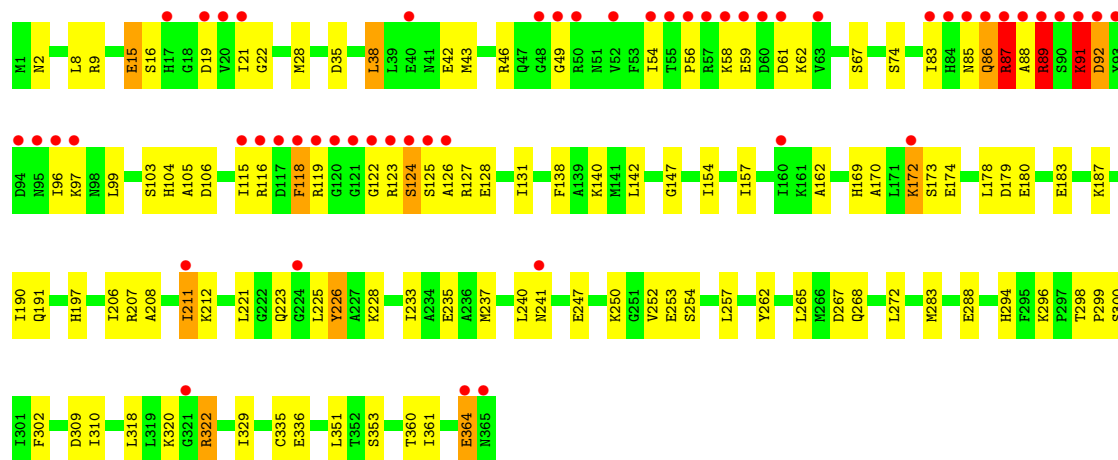


• Molecule 1: Chorismate synthase





• Molecule 1: Chorismate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.69Å 146.69Å 132.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 1.95 29.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.90-1.95) 99.5 (29.90-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.243 0.216 , 0.245	Depositor DCC
R_{free} test set	10100 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11843	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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	0.39	0/2857	0.88	8/3833 (0.2%)
1	B	0.35	0/2857	0.84	5/3833 (0.1%)
1	C	0.36	0/2857	0.85	6/3833 (0.2%)
1	D	0.38	0/2857	0.87	9/3833 (0.2%)
All	All	0.37	0/11428	0.86	28/15332 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	SER	N-CA-C	10.22	122.00	111.07
1	C	353	SER	N-CA-C	9.74	121.49	111.07
1	A	353	SER	N-CA-C	8.70	120.77	111.28
1	D	353	SER	N-CA-C	8.19	119.83	111.07
1	D	223	GLN	N-CA-C	7.36	120.40	108.41
1	D	211	ILE	N-CA-C	-7.17	106.02	112.90
1	A	223	GLN	N-CA-C	6.75	119.42	108.41
1	A	161	LYS	N-CA-C	6.49	120.62	110.17
1	C	223	GLN	N-CA-C	6.26	118.61	108.41
1	A	60	ASP	N-CA-C	5.84	116.13	108.07
1	D	8	LEU	N-CA-C	-5.59	98.62	108.23
1	B	123	ARG	CB-CA-C	-5.58	109.15	115.79
1	D	226	TYR	N-CA-C	5.43	119.60	112.92
1	B	223	GLN	N-CA-C	5.34	117.36	108.02
1	D	89	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	89	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	87	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	87	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	C	89	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	B	87	ARG	NE-CZ-NH2	5.25	123.93	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	C	87	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	A	226	TYR	N-CA-C	5.16	119.53	112.88
1	D	119	ARG	CB-CA-C	-5.08	109.76	117.07
1	D	364	GLU	N-CA-C	-5.07	107.60	112.97
1	A	9	ARG	N-CA-C	5.06	116.98	108.73
1	C	313	ASN	CB-CA-C	-5.05	109.80	117.07
1	C	92	ASP	CB-CA-C	-5.01	109.23	116.54

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	2816	0	2852	99	0
1	B	2816	0	2852	122	1
1	C	2816	0	2852	158	4
1	D	2816	0	2852	120	3
2	A	31	0	19	6	0
2	B	31	0	19	9	0
2	C	31	0	19	3	0
2	D	31	0	19	7	0
3	A	158	0	0	3	0
3	B	84	0	0	2	0
3	C	76	0	0	0	0
3	D	137	0	0	7	0
All	All	11843	0	11484	456	5

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 20.

All (456) 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:307:THR:HG23	1:C:308:ILE:H	1.25	0.97
1:D:105:ALA:H	1:D:123:ARG:HH12	1.07	0.94
1:A:322:ARG:H	1:A:322:ARG:NH1	1.70	0.90
1:B:281:GLY:HA3	1:C:105:ALA:HB2	1.54	0.89
1:A:322:ARG:HH11	1:A:322:ARG:N	1.71	0.89
1:C:267:ASP:HB2	1:C:272:LEU:HD21	1.54	0.88
1:B:105:ALA:H	1:B:123:ARG:HH12	0.94	0.87
1:C:322:ARG:HH11	1:C:322:ARG:H	1.23	0.86
1:D:105:ALA:H	1:D:123:ARG:NH1	1.74	0.86
1:B:105:ALA:N	1:B:123:ARG:HH12	1.72	0.85
1:A:318:LEU:HD12	1:A:320:LYS:HE3	1.59	0.85
1:D:21:ILE:HG13	1:D:131:ILE:HD11	1.60	0.84
1:D:318:LEU:HD12	1:D:320:LYS:HE3	1.57	0.83
1:C:21:ILE:HG13	1:C:131:ILE:HD11	1.60	0.83
1:B:105:ALA:H	1:B:123:ARG:NH1	1.77	0.83
1:A:302:PHE:HE2	1:A:318:LEU:HD11	1.43	0.82
1:C:197:HIS:HB3	1:C:302:PHE:HB3	1.61	0.82
1:D:322:ARG:H	1:D:322:ARG:HH11	1.29	0.79
1:D:105:ALA:N	1:D:123:ARG:HH22	1.81	0.78
1:A:361:ILE:O	1:A:365:ASN:OXT	2.03	0.77
1:C:102:PRO:HG2	1:C:305:GLN:HB3	1.66	0.77
1:C:117:ASP:CG	1:C:118:PHE:H	1.93	0.77
1:A:169:HIS:O	1:A:172:LYS:HD3	1.86	0.76
1:C:122:GLY:O	1:C:123:ARG:HG2	1.85	0.76
1:A:123:ARG:HG3	1:A:124:SER:H	1.52	0.75
1:B:318:LEU:HD12	1:B:320:LYS:HE3	1.67	0.74
1:C:300:SER:HA	1:C:305:GLN:HE22	1.52	0.73
1:A:322:ARG:H	1:A:322:ARG:HH11	0.86	0.73
1:C:212:LYS:HD3	1:C:215:GLN:HG2	1.71	0.73
1:C:322:ARG:HH11	1:C:322:ARG:N	1.86	0.72
1:B:302:PHE:HE2	1:B:318:LEU:HD11	1.54	0.72
1:D:302:PHE:HE2	1:D:318:LEU:HD11	1.54	0.72
1:B:169:HIS:HA	1:B:172:LYS:HE3	1.72	0.72
1:B:238:MET:HE1	1:B:244:LYS:HA	1.72	0.71
1:A:351:LEU:HD22	1:B:361:ILE:HD12	1.73	0.71
1:B:128:GLU:HG3	1:C:225:LEU:HD13	1.72	0.70
1:B:105:ALA:HB3	1:B:123:ARG:HH22	1.56	0.70
1:C:61:ASP:HA	1:C:84:HIS:O	1.91	0.70
1:A:75:THR:HA	1:C:115:ILE:HD12	1.74	0.70
1:A:45:ARG:HD2	3:A:1524:HOH:O	1.91	0.70
1:B:183:GLU:HG2	1:B:187:LYS:HE3	1.74	0.69
1:C:322:ARG:H	1:C:322:ARG:HD3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:HIS:CD2	1:D:172:LYS:HE3	2.27	0.69
1:C:197:HIS:HB2	1:C:303:GLN:HG3	1.74	0.69
1:B:56:PRO:HA	1:B:59:GLU:HB2	1.74	0.69
1:C:307:THR:HG23	1:C:308:ILE:N	2.06	0.68
1:A:128:GLU:HG3	1:D:225:LEU:HD13	1.73	0.68
1:C:169:HIS:HA	1:C:172:LYS:NZ	2.09	0.68
1:B:104:HIS:HD2	1:B:123:ARG:HD2	1.59	0.68
1:A:302:PHE:CE2	1:A:318:LEU:HD11	2.26	0.67
1:A:169:HIS:CD2	1:A:172:LYS:HE3	2.29	0.67
1:D:253:GLU:O	1:D:257:LEU:HD13	1.94	0.67
1:C:102:PRO:HG2	1:C:305:GLN:CB	2.25	0.67
1:D:49:GLY:O	1:D:174:GLU:HA	1.95	0.67
1:D:322:ARG:NH1	1:D:322:ARG:HB2	2.10	0.67
1:D:105:ALA:N	1:D:123:ARG:HH12	1.87	0.66
1:A:225:LEU:HD13	1:D:128:GLU:HG3	1.77	0.66
1:B:264:ASP:C	1:B:265:LEU:HD12	2.21	0.66
1:B:101:ARG:HG3	1:B:101:ARG:HH11	1.61	0.65
1:C:322:ARG:N	1:C:322:ARG:HD3	2.11	0.65
1:D:85:ASN:ND2	1:D:86:GLN:HG3	2.11	0.65
2:B:2400:FMN:O3P	1:C:280:LEU:HD12	1.96	0.65
1:D:169:HIS:O	1:D:172:LYS:HD3	1.95	0.65
1:C:55:THR:H	1:C:56:PRO:CD	2.09	0.65
1:A:51:ASN:OD1	1:A:52:VAL:HG23	1.97	0.65
1:A:241:ASN:HB3	2:A:1400:FMN:H3'	1.79	0.65
1:D:169:HIS:NE2	1:D:172:LYS:HE3	2.12	0.64
1:C:97:LYS:HZ2	1:C:97:LYS:HB2	1.63	0.64
1:C:322:ARG:HB2	1:C:322:ARG:NH1	2.13	0.64
1:B:100:PHE:HB2	1:C:266:MET:HE1	1.80	0.63
1:D:115:ILE:HD12	1:D:115:ILE:O	1.98	0.63
1:A:157:ILE:HD13	1:A:190:ILE:HD11	1.80	0.63
1:C:305:GLN:HB2	1:C:317:CYS:SG	2.39	0.63
1:B:247:GLU:OE1	1:B:294:HIS:HE1	1.82	0.63
1:C:97:LYS:HB2	1:C:97:LYS:NZ	2.14	0.62
1:A:241:ASN:ND2	1:D:228:LYS:NZ	2.47	0.62
1:C:247:GLU:OE2	1:C:252:VAL:HG22	1.99	0.62
1:C:52:VAL:HB	1:C:56:PRO:HB3	1.82	0.62
1:A:318:LEU:HD12	1:A:320:LYS:CE	2.29	0.62
1:B:320:LYS:H	1:B:320:LYS:HD2	1.63	0.62
1:C:301:ILE:H	1:C:305:GLN:NE2	1.98	0.61
1:D:300:SER:H	2:D:4400:FMN:HM82	1.64	0.61
1:C:247:GLU:HB2	1:C:292:ARG:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:GLU:HG2	3:D:4505:HOH:O	2.00	0.61
1:D:241:ASN:ND2	3:D:4433:HOH:O	2.34	0.60
1:B:253:GLU:O	1:B:257:LEU:HD13	2.01	0.60
1:C:318:LEU:HD12	1:C:320:LYS:HE3	1.81	0.60
1:A:330:ARG:HH21	1:A:330:ARG:HB3	1.65	0.60
1:D:322:ARG:HH11	1:D:322:ARG:N	1.99	0.60
1:A:54:ILE:HG22	1:A:55:THR:N	2.15	0.60
1:A:262:TYR:O	1:A:275:ARG:HD3	2.03	0.59
1:A:247:GLU:OE1	1:A:294:HIS:HE1	1.86	0.59
1:C:308:ILE:HG12	1:C:309:ASP:N	2.17	0.59
1:A:21:ILE:HG13	1:A:131:ILE:HD11	1.82	0.59
1:A:361:ILE:HD11	1:B:361:ILE:HD11	1.84	0.59
1:C:38:LEU:C	1:C:38:LEU:HD23	2.27	0.59
1:B:266:MET:H	1:C:307:THR:HA	1.68	0.58
1:A:161:LYS:HE2	3:A:1441:HOH:O	2.02	0.58
1:B:238:MET:HE2	1:C:248:ILE:HG13	1.85	0.58
1:A:55:THR:O	1:A:59:GLU:HG2	2.02	0.58
1:B:116:ARG:HD3	1:B:310:ILE:HD13	1.86	0.58
1:D:21:ILE:HG23	1:D:83:ILE:HB	1.86	0.58
1:D:162:ALA:HB1	1:D:179:ASP:HB2	1.85	0.58
1:A:241:ASN:ND2	1:D:228:LYS:HZ3	2.01	0.57
1:A:320:LYS:HD2	1:A:320:LYS:H	1.67	0.57
1:B:265:LEU:HG	1:C:306:ARG:O	2.04	0.57
1:A:361:ILE:HD12	1:B:351:LEU:HD22	1.87	0.57
1:A:300:SER:H	2:A:1400:FMN:C8M	2.17	0.57
1:A:330:ARG:HB3	1:A:330:ARG:NH2	2.20	0.57
1:D:116:ARG:H	1:D:116:ARG:HD2	1.69	0.57
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.20	0.57
1:B:241:ASN:HD21	2:B:2400:FMN:H5'2	1.68	0.57
1:C:302:PHE:N	1:C:323:HIS:HD2	2.03	0.57
1:C:351:LEU:HD22	1:D:361:ILE:HD12	1.86	0.57
1:C:308:ILE:HD11	1:C:312:GLY:HA2	1.86	0.56
1:D:247:GLU:OE1	1:D:294:HIS:HE1	1.88	0.56
1:C:322:ARG:H	1:C:322:ARG:NH1	1.99	0.56
1:D:122:GLY:O	1:D:123:ARG:HG2	2.06	0.56
1:A:241:ASN:HD21	1:D:228:LYS:NZ	2.03	0.56
1:D:174:GLU:CD	1:D:174:GLU:H	2.14	0.56
1:B:67:SER:HB3	1:D:16:SER:HB3	1.87	0.56
1:C:116:ARG:HD3	1:C:310:ILE:HG21	1.88	0.56
1:C:54:ILE:O	1:C:55:THR:HG23	2.06	0.56
1:A:296:LYS:HD2	1:D:262:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:HB2	2:A:1400:FMN:HM81	1.87	0.56
1:B:271:PHE:HD1	1:B:271:PHE:H	1.54	0.56
1:C:253:GLU:O	1:C:257:LEU:HD13	2.04	0.56
1:C:316:GLU:HG2	1:C:318:LEU:H	1.71	0.56
1:C:106:ASP:HA	1:C:118:PHE:CZ	2.41	0.56
1:A:48:GLY:O	1:A:49:GLY:C	2.48	0.56
1:C:19:ASP:HA	1:C:86:GLN:OE1	2.06	0.56
1:D:104:HIS:HB3	1:D:123:ARG:NH2	2.20	0.56
1:A:122:GLY:O	1:A:124:SER:N	2.39	0.56
1:B:99:LEU:HA	1:B:309:ASP:HA	1.88	0.56
1:C:55:THR:H	1:C:56:PRO:HD3	1.71	0.56
1:C:124:SER:O	1:C:126:ALA:N	2.39	0.56
1:A:20:VAL:HG22	1:A:84:HIS:ND1	2.21	0.55
1:B:322:ARG:HD3	1:B:322:ARG:N	2.21	0.55
1:C:99:LEU:HD12	1:C:99:LEU:O	2.05	0.55
1:C:172:LYS:H	1:C:172:LYS:HD3	1.69	0.55
1:D:28:MET:HE2	1:D:138:PHE:HB3	1.88	0.55
1:D:124:SER:HA	1:D:127:ARG:HD2	1.88	0.55
1:C:117:ASP:CG	1:C:118:PHE:N	2.64	0.55
1:A:123:ARG:CG	1:A:124:SER:H	2.20	0.55
1:B:300:SER:H	2:B:2400:FMN:HM82	1.72	0.55
1:D:207:ARG:HG2	1:D:208:ALA:N	2.21	0.55
1:B:16:SER:HB3	1:D:67:SER:HB3	1.87	0.55
1:C:267:ASP:HB2	1:C:272:LEU:CD2	2.32	0.55
1:C:100:PHE:CE2	1:C:310:ILE:HA	2.42	0.55
1:C:250:LYS:HE3	1:C:253:GLU:HB3	1.88	0.54
1:D:21:ILE:HD12	1:D:22:GLY:H	1.71	0.54
1:B:263:ASN:HD21	1:C:299:PRO:HA	1.72	0.54
1:B:197:HIS:HB3	1:B:302:PHE:HB3	1.89	0.54
1:C:197:HIS:O	1:C:303:GLN:HG3	2.08	0.54
1:A:54:ILE:HG22	1:A:55:THR:H	1.72	0.54
1:C:58:LYS:N	1:C:58:LYS:HD3	2.21	0.54
1:D:106:ASP:H	1:D:123:ARG:HH22	1.56	0.54
1:C:320:LYS:H	1:C:320:LYS:HD2	1.72	0.53
1:C:95:ASN:HB2	1:C:319:LEU:HD23	1.90	0.53
1:D:105:ALA:H	1:D:123:ARG:CZ	2.20	0.53
1:A:75:THR:HA	1:C:115:ILE:CD1	2.38	0.53
1:B:105:ALA:HB3	1:B:123:ARG:NH2	2.23	0.53
1:B:241:ASN:CG	2:B:2400:FMN:H3'	2.34	0.53
1:B:54:ILE:HB	1:B:59:GLU:OE2	2.09	0.53
1:C:212:LYS:HD3	1:C:215:GLN:CG	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LYS:HB3	1:C:254:SER:OG	2.08	0.53
1:C:320:LYS:HD2	1:C:320:LYS:N	2.24	0.53
1:C:322:ARG:HH11	1:C:322:ARG:HB2	1.74	0.53
1:A:264:ASP:OD1	1:A:275:ARG:HD2	2.09	0.53
1:A:318:LEU:O	1:A:320:LYS:HD2	2.09	0.53
1:C:104:HIS:HB3	1:C:123:ARG:HH21	1.74	0.53
1:C:151:GLU:OE1	1:C:209:ARG:NH1	2.42	0.53
1:C:142:LEU:C	1:C:142:LEU:HD23	2.34	0.53
1:C:307:THR:CG2	1:C:308:ILE:H	2.08	0.53
1:D:105:ALA:N	1:D:123:ARG:NH2	2.55	0.53
1:B:206:ILE:HD12	1:B:206:ILE:N	2.25	0.52
1:D:97:LYS:HB2	1:D:97:LYS:NZ	2.24	0.52
1:A:330:ARG:HH21	1:A:330:ARG:CB	2.22	0.52
1:C:101:ARG:HD2	1:C:319:LEU:HD11	1.90	0.52
1:D:106:ASP:N	1:D:123:ARG:HH22	2.08	0.52
1:D:169:HIS:NE2	1:D:180:GLU:HB3	2.24	0.52
1:B:142:LEU:C	1:B:142:LEU:HD23	2.34	0.52
1:D:54:ILE:HG22	1:D:58:LYS:HD2	1.92	0.52
1:D:206:ILE:HD12	1:D:206:ILE:N	2.24	0.52
1:B:169:HIS:HE1	1:B:183:GLU:OE2	1.92	0.52
1:D:302:PHE:CE2	1:D:318:LEU:HD11	2.41	0.52
1:C:187:LYS:O	1:C:191:GLN:HG3	2.09	0.52
1:C:265:LEU:HD22	1:C:265:LEU:N	2.25	0.52
1:D:58:LYS:HG3	1:D:59:GLU:HG2	1.91	0.52
1:B:151:GLU:OE1	1:B:209:ARG:NH1	2.41	0.52
1:B:123:ARG:HE	1:B:124:SER:H	1.58	0.51
1:D:250:LYS:HB3	1:D:254:SER:OG	2.10	0.51
1:B:266:MET:HE3	1:C:307:THR:OG1	2.11	0.51
1:C:48:GLY:HA2	1:C:52:VAL:HG21	1.93	0.51
1:D:169:HIS:HE1	1:D:183:GLU:OE2	1.93	0.51
1:B:20:VAL:HG22	1:B:84:HIS:ND1	2.25	0.51
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.43	0.51
1:C:233:ILE:O	1:C:237:MET:HG2	2.10	0.51
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.26	0.51
1:D:322:ARG:N	1:D:322:ARG:HD3	2.26	0.51
1:A:169:HIS:HE1	1:A:183:GLU:OE2	1.94	0.51
1:C:50:ARG:NH2	1:C:323:HIS:HA	2.26	0.50
1:C:183:GLU:HG2	1:C:187:LYS:HE3	1.92	0.50
1:C:147:GLY:HA2	1:C:211:ILE:HD12	1.92	0.50
1:B:183:GLU:CG	1:B:187:LYS:HE3	2.40	0.50
1:B:307:THR:OG1	1:C:266:MET:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:HIS:HA	1:C:172:LYS:HZ2	1.76	0.50
1:A:162:ALA:HB1	1:A:179:ASP:HB2	1.93	0.50
1:B:98:ASN:O	1:B:310:ILE:HG13	2.10	0.50
1:B:267:ASP:OD2	1:B:268:GLN:HG3	2.11	0.50
1:C:162:ALA:HB1	1:C:179:ASP:HB2	1.92	0.50
1:B:162:ALA:HB1	1:B:179:ASP:HB2	1.94	0.50
1:B:250:LYS:HE2	1:B:257:LEU:HD21	1.94	0.50
1:B:266:MET:HE1	1:C:107:PHE:HB2	1.92	0.50
1:A:128:GLU:HG3	1:D:225:LEU:CD1	2.40	0.50
1:B:9:ARG:HD2	3:B:2423:HOH:O	2.11	0.50
1:D:105:ALA:H	1:D:123:ARG:NH2	2.10	0.50
1:A:304:PRO:HB3	1:A:316:GLU:OE1	2.11	0.50
1:B:258:LYS:HG2	1:C:200:ILE:HG22	1.93	0.50
3:B:2470:HOH:O	1:D:115:ILE:HD11	2.12	0.50
1:B:298:THR:HG22	2:B:2400:FMN:HM82	1.93	0.49
1:C:52:VAL:HB	1:C:56:PRO:CB	2.42	0.49
1:D:211:ILE:HG22	1:D:211:ILE:O	2.12	0.49
1:A:320:LYS:HD2	1:A:320:LYS:N	2.28	0.49
1:C:156:GLU:OE1	1:C:161:LYS:HG2	2.12	0.49
1:D:298:THR:HG22	2:D:4400:FMN:HM82	1.94	0.49
1:A:9:ARG:HD2	3:A:1447:HOH:O	2.12	0.49
1:A:67:SER:HB3	1:C:16:SER:HB3	1.94	0.49
1:A:318:LEU:HD13	1:A:318:LEU:C	2.37	0.49
1:C:100:PHE:CD1	1:C:106:ASP:HB3	2.47	0.49
1:D:123:ARG:NH2	3:D:4478:HOH:O	2.45	0.49
1:D:237:MET:HE1	1:D:335:CYS:O	2.11	0.49
1:D:116:ARG:HD2	1:D:116:ARG:N	2.27	0.49
1:D:169:HIS:CE1	1:D:172:LYS:HE3	2.48	0.49
1:B:47:GLN:HE22	1:B:60:ASP:HB2	1.78	0.49
1:D:104:HIS:CE1	1:D:299:PRO:HB2	2.47	0.49
1:C:100:PHE:HB3	1:C:106:ASP:HB2	1.95	0.49
1:D:296:LYS:HE3	1:D:299:PRO:HG3	1.95	0.49
1:B:172:LYS:HD3	1:B:172:LYS:H	1.77	0.49
1:B:262:TYR:HD1	1:B:263:ASN:N	2.11	0.49
1:A:16:SER:HB3	1:C:67:SER:HB3	1.95	0.48
1:B:115:ILE:HD12	1:D:74:SER:O	2.12	0.48
1:B:101:ARG:HD2	1:B:319:LEU:HD21	1.94	0.48
1:D:187:LYS:O	1:D:191:GLN:HG3	2.13	0.48
1:D:140:LYS:NZ	1:D:336:GLU:OE2	2.44	0.48
1:A:262:TYR:CE1	1:D:296:LYS:HD2	2.48	0.48
1:B:169:HIS:O	1:B:172:LYS:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:HIS:HD2	1:C:123:ARG:HE	1.61	0.48
1:D:9:ARG:HD2	3:D:4468:HOH:O	2.12	0.48
1:C:247:GLU:OE1	1:C:294:HIS:HE1	1.96	0.48
1:C:100:PHE:CE1	1:C:310:ILE:HG12	2.48	0.48
1:A:125:SER:O	1:A:126:ALA:C	2.57	0.48
1:A:314:GLU:HG3	1:D:268:GLN:HG3	1.95	0.48
1:A:169:HIS:NE2	1:A:172:LYS:HE3	2.29	0.48
1:B:100:PHE:CB	1:C:266:MET:HE1	2.44	0.48
1:D:87:ARG:HB2	1:D:88:ALA:H	1.47	0.48
1:A:21:ILE:HG23	1:A:83:ILE:HB	1.96	0.48
1:B:258:LYS:HZ3	1:B:261:GLU:CD	2.22	0.48
1:A:46:ARG:NH1	1:A:330:ARG:HH12	2.11	0.47
1:D:320:LYS:H	1:D:320:LYS:HD2	1.79	0.47
1:D:124:SER:O	1:D:126:ALA:N	2.46	0.47
1:B:54:ILE:HG22	1:B:55:THR:N	2.27	0.47
1:C:48:GLY:HA2	1:C:52:VAL:CG2	2.44	0.47
1:C:200:ILE:O	1:C:200:ILE:HD12	2.14	0.47
1:D:322:ARG:H	1:D:322:ARG:HD3	1.78	0.47
1:D:360:THR:HG23	1:D:364:GLU:OE1	2.14	0.47
1:C:322:ARG:HH11	1:C:322:ARG:CB	2.28	0.47
1:A:45:ARG:HH22	1:A:336:GLU:CD	2.22	0.47
1:B:299:PRO:HD2	2:B:2400:FMN:H9	1.96	0.47
1:C:302:PHE:CE2	1:C:320:LYS:HA	2.49	0.47
1:C:304:PRO:HG3	1:C:318:LEU:CD2	2.45	0.47
1:C:47:GLN:HE22	1:C:60:ASP:CG	2.23	0.47
1:C:100:PHE:HD1	1:C:106:ASP:HB3	1.79	0.47
1:C:305:GLN:O	1:C:317:CYS:HB3	2.15	0.47
1:D:97:LYS:HA	3:D:4500:HOH:O	2.13	0.47
1:D:154:ILE:HG21	1:D:157:ILE:HD11	1.97	0.47
1:D:35:ASP:CG	1:D:38:LEU:HB2	2.40	0.47
1:C:104:HIS:CD2	1:C:123:ARG:HE	2.33	0.47
1:B:157:ILE:HD12	1:B:175:ILE:HD12	1.96	0.47
1:D:170:ALA:HB2	1:D:178:LEU:HD23	1.97	0.47
1:B:112:LYS:HZ3	1:C:223:GLN:NE2	2.14	0.46
1:B:207:ARG:HA	1:B:289:ILE:O	2.15	0.46
1:A:322:ARG:N	1:A:322:ARG:HD3	2.31	0.46
1:C:58:LYS:N	1:C:58:LYS:CD	2.79	0.46
1:C:123:ARG:O	1:C:124:SER:HB2	2.15	0.46
1:A:142:LEU:HD23	1:A:142:LEU:C	2.39	0.46
1:C:38:LEU:HD22	1:C:137:ALA:HB1	1.96	0.46
1:B:104:HIS:CD2	1:B:123:ARG:HD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:O	1:B:114:GLY:HA2	2.15	0.46
1:B:241:ASN:ND2	2:B:2400:FMN:H3'	2.30	0.46
1:C:213:THR:O	1:C:214:ASN:HB2	2.14	0.46
1:D:241:ASN:HB3	2:D:4400:FMN:H3'	1.98	0.46
1:B:247:GLU:OE1	1:B:294:HIS:CE1	2.66	0.46
1:B:258:LYS:NZ	1:B:261:GLU:OE1	2.48	0.46
1:B:265:LEU:HD23	1:C:306:ARG:HB2	1.97	0.46
1:B:330:ARG:HB3	1:B:330:ARG:NH2	2.31	0.46
1:D:91:LYS:HB2	1:D:92:ASP:H	1.57	0.46
1:B:101:ARG:HG3	1:B:101:ARG:NH1	2.29	0.45
1:C:206:ILE:N	1:C:206:ILE:HD12	2.30	0.45
1:D:123:ARG:NH1	2:D:4400:FMN:O4'	2.50	0.45
1:B:101:ARG:HD2	1:B:319:LEU:HD11	1.98	0.45
1:C:54:ILE:O	1:C:54:ILE:HG22	2.15	0.45
1:D:116:ARG:HG2	1:D:310:ILE:HD13	1.97	0.45
1:D:99:LEU:HA	1:D:309:ASP:HA	1.97	0.45
1:D:265:LEU:HB2	1:D:272:LEU:HD12	1.97	0.45
1:B:320:LYS:HD2	1:B:320:LYS:N	2.30	0.45
1:B:85:ASN:O	1:B:86:GLN:HB2	2.17	0.45
1:B:233:ILE:O	1:B:237:MET:HG2	2.17	0.45
1:C:53:PHE:O	1:C:54:ILE:C	2.58	0.45
1:C:318:LEU:HD12	1:C:320:LYS:CE	2.47	0.45
1:D:267:ASP:HA	3:D:4515:HOH:O	2.15	0.45
1:D:318:LEU:O	1:D:320:LYS:HD2	2.16	0.45
1:B:9:ARG:NH1	1:D:2:ASN:OD1	2.49	0.45
1:C:102:PRO:HG3	1:C:307:THR:HG22	1.98	0.45
1:C:241:ASN:CG	2:C:3400:FMN:O3'	2.60	0.45
1:A:9:ARG:NH1	1:C:2:ASN:OD1	2.49	0.45
1:D:142:LEU:HD23	1:D:142:LEU:C	2.42	0.45
1:A:168:ASN:HD22	1:A:168:ASN:C	2.25	0.44
1:B:101:ARG:O	1:B:104:HIS:HB2	2.17	0.44
1:B:170:ALA:HB2	1:B:178:LEU:HD23	1.99	0.44
1:B:212:LYS:HB2	1:B:215:GLN:CB	2.47	0.44
1:B:215:GLN:OE1	1:B:216:LYS:N	2.50	0.44
1:C:93:TYR:HA	1:C:320:LYS:O	2.17	0.44
1:C:99:LEU:HD12	1:C:99:LEU:C	2.41	0.44
1:C:102:PRO:N	1:C:307:THR:HG21	2.32	0.44
1:A:99:LEU:HA	1:A:309:ASP:HA	1.99	0.44
1:C:124:SER:O	1:C:125:SER:C	2.60	0.44
1:D:147:GLY:HA3	1:D:212:LYS:HD3	1.98	0.44
1:A:122:GLY:C	1:A:123:ARG:HG2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ALA:HB2	1:C:281:GLY:HA3	1.99	0.44
1:D:247:GLU:OE2	1:D:252:VAL:HG22	2.17	0.44
1:A:151:GLU:OE2	1:A:207:ARG:NH1	2.39	0.44
1:D:61:ASP:O	1:D:62:LYS:HB2	2.18	0.44
1:C:127:ARG:NH1	1:C:127:ARG:HG2	2.32	0.44
1:D:38:LEU:HD22	1:D:42:GLU:HG2	1.99	0.44
1:A:101:ARG:NH1	1:A:106:ASP:OD2	2.50	0.44
1:B:47:GLN:HE22	1:B:60:ASP:CB	2.30	0.44
1:B:101:ARG:NH1	1:B:118:PHE:CZ	2.85	0.44
1:B:112:LYS:NZ	1:C:223:GLN:NE2	2.66	0.44
1:C:117:ASP:O	1:C:118:PHE:HB2	2.17	0.44
1:A:296:LYS:HE3	1:A:299:PRO:HG3	1.99	0.44
1:A:300:SER:H	2:A:1400:FMN:HM83	1.83	0.43
1:B:262:TYR:CD1	1:B:263:ASN:N	2.86	0.43
1:B:263:ASN:ND2	1:C:299:PRO:HA	2.33	0.43
1:C:169:HIS:HA	1:C:172:LYS:CE	2.47	0.43
1:C:207:ARG:HA	1:C:289:ILE:O	2.18	0.43
1:D:54:ILE:CG2	1:D:58:LYS:HD2	2.48	0.43
1:D:123:ARG:CG	1:D:124:SER:N	2.81	0.43
2:D:4400:FMN:H2'	2:D:4400:FMN:H9	2.00	0.43
1:C:93:TYR:HA	1:C:320:LYS:C	2.43	0.43
1:C:102:PRO:HA	1:C:307:THR:HB	2.00	0.43
1:A:96:ILE:C	1:A:98:ASN:H	2.26	0.43
1:B:330:ARG:CB	1:B:330:ARG:HH21	2.32	0.43
1:A:123:ARG:HG3	1:A:124:SER:N	2.27	0.43
1:B:272:LEU:N	1:B:272:LEU:HD23	2.33	0.43
1:C:77:THR:HB	1:C:78:PRO:CD	2.49	0.43
1:D:172:LYS:NZ	1:D:173:SER:HA	2.34	0.43
1:A:47:GLN:HE22	1:A:60:ASP:CG	2.26	0.43
1:A:59:GLU:HA	1:A:59:GLU:OE1	2.18	0.43
1:B:169:HIS:CD2	1:B:180:GLU:HB3	2.53	0.43
1:C:127:ARG:HG2	1:C:127:ARG:HH11	1.84	0.43
1:C:308:ILE:HG12	1:C:309:ASP:H	1.84	0.43
1:A:235:GLU:HB2	1:D:235:GLU:HB2	2.00	0.43
1:A:300:SER:H	2:A:1400:FMN:HM81	1.84	0.43
1:B:261:GLU:O	1:B:275:ARG:NH1	2.52	0.43
2:B:2400:FMN:P	1:C:281:GLY:H	2.41	0.43
1:C:265:LEU:HD22	1:C:265:LEU:H	1.84	0.43
1:D:106:ASP:H	1:D:123:ARG:NH2	2.17	0.43
1:D:221:LEU:O	1:D:283:MET:HA	2.18	0.43
1:D:318:LEU:HD12	1:D:320:LYS:CE	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:SER:O	1:B:133:VAL:HG23	2.19	0.43
1:C:47:GLN:HE22	1:C:60:ASP:CB	2.31	0.43
1:C:262:TYR:CD1	1:C:262:TYR:C	2.96	0.43
1:B:262:TYR:O	1:B:263:ASN:O	2.37	0.42
1:A:240:LEU:HD22	2:A:1400:FMN:O2	2.18	0.42
1:C:172:LYS:H	1:C:172:LYS:CD	2.32	0.42
1:A:124:SER:O	1:A:126:ALA:N	2.53	0.42
1:B:117:ASP:OD1	1:B:118:PHE:N	2.52	0.42
1:D:15:GLU:H	1:D:15:GLU:CD	2.18	0.42
1:D:21:ILE:CG2	1:D:83:ILE:HB	2.47	0.42
1:C:110:PHE:O	1:C:114:GLY:N	2.52	0.42
1:D:299:PRO:HG2	2:D:4400:FMN:H4'	2.02	0.42
1:B:209:ARG:C	1:B:217:LEU:HD21	2.45	0.42
1:C:21:ILE:HG23	1:C:83:ILE:HB	2.02	0.42
1:D:233:ILE:O	1:D:237:MET:HG2	2.20	0.42
1:B:300:SER:H	2:B:2400:FMN:C8M	2.32	0.42
1:C:169:HIS:HE1	1:C:183:GLU:OE2	2.02	0.42
1:C:320:LYS:H	1:C:320:LYS:CD	2.32	0.42
1:D:106:ASP:OD1	1:D:123:ARG:NH2	2.50	0.42
1:A:4:LEU:HB2	1:D:226:TYR:CD1	2.54	0.42
1:B:117:ASP:O	1:B:118:PHE:O	2.38	0.42
1:B:123:ARG:HG3	1:B:124:SER:N	2.34	0.42
1:B:125:SER:O	1:B:126:ALA:HB3	2.19	0.42
1:C:59:GLU:O	1:C:59:GLU:HG2	2.20	0.42
1:D:19:ASP:HB2	1:D:85:ASN:O	2.20	0.42
1:D:190:ILE:HD11	1:D:329:ILE:HD11	2.02	0.42
1:D:322:ARG:HB2	1:D:322:ARG:CZ	2.49	0.42
1:C:38:LEU:C	1:C:38:LEU:CD2	2.93	0.42
1:A:47:GLN:HE22	1:A:60:ASP:CB	2.32	0.42
1:A:170:ALA:O	1:A:176:PHE:HA	2.20	0.42
1:B:318:LEU:C	1:B:318:LEU:HD13	2.44	0.42
1:A:101:ARG:NH2	1:A:123:ARG:HE	2.18	0.42
1:B:99:LEU:C	1:B:99:LEU:HD12	2.45	0.42
1:B:265:LEU:HD12	1:B:265:LEU:N	2.35	0.42
1:C:317:CYS:SG	1:C:317:CYS:O	2.77	0.42
1:B:250:LYS:HE3	1:B:253:GLU:HB3	2.02	0.41
1:D:106:ASP:N	1:D:123:ARG:NH2	2.68	0.41
1:A:96:ILE:O	1:A:99:LEU:HG	2.19	0.41
1:D:43:MET:O	1:D:46:ARG:HG2	2.19	0.41
1:A:21:ILE:CG2	1:A:83:ILE:HB	2.50	0.41
1:A:225:LEU:HD13	1:D:128:GLU:CG	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:HD22	2:C:3400:FMN:O2	2.19	0.41
1:D:197:HIS:HB3	1:D:302:PHE:HB3	2.03	0.41
1:D:300:SER:H	2:D:4400:FMN:C8M	2.30	0.41
1:A:15:GLU:H	1:A:15:GLU:CD	2.21	0.41
1:A:169:HIS:CE1	1:A:172:LYS:HE3	2.56	0.41
1:B:39:LEU:O	1:B:43:MET:HG2	2.20	0.41
1:C:20:VAL:HG22	1:C:84:HIS:ND1	2.35	0.41
1:C:99:LEU:HA	1:C:309:ASP:HA	2.01	0.41
1:C:361:ILE:HD12	1:D:351:LEU:HD22	2.02	0.41
1:A:169:HIS:CG	1:A:172:LYS:HE3	2.56	0.41
1:C:54:ILE:O	1:C:55:THR:CB	2.67	0.41
1:A:54:ILE:CG2	1:A:55:THR:N	2.82	0.41
1:D:318:LEU:C	1:D:318:LEU:HD13	2.45	0.41
1:B:104:HIS:HB3	1:B:123:ARG:NH1	2.34	0.41
1:B:208:ALA:HB3	1:B:289:ILE:HB	2.02	0.41
1:B:322:ARG:N	1:B:322:ARG:CD	2.84	0.41
1:B:169:HIS:NE2	1:B:180:GLU:HB3	2.36	0.41
1:B:15:GLU:H	1:B:15:GLU:CD	2.28	0.41
1:B:123:ARG:CG	1:B:124:SER:N	2.84	0.41
1:C:300:SER:HB3	2:C:3400:FMN:C8M	2.51	0.41
1:D:115:ILE:HD12	1:D:115:ILE:C	2.45	0.41
1:A:124:SER:O	1:A:125:SER:C	2.64	0.41
1:A:233:ILE:O	1:A:237:MET:HG2	2.20	0.41
1:A:247:GLU:OE1	1:A:294:HIS:CE1	2.71	0.41
1:B:250:LYS:HE3	1:B:253:GLU:CB	2.51	0.41
1:C:54:ILE:O	1:C:55:THR:OG1	2.27	0.41
1:C:57:ARG:HH11	1:C:57:ARG:HG3	1.86	0.41
1:A:156:GLU:CD	1:A:161:LYS:HG2	2.45	0.40
1:D:267:ASP:OD2	1:D:267:ASP:C	2.63	0.40
1:D:288:GLU:HG3	3:D:4520:HOH:O	2.20	0.40
1:A:65:ILE:HD13	1:A:65:ILE:HG21	1.88	0.40
1:A:175:ILE:HG21	1:A:190:ILE:HD12	2.04	0.40
1:A:362:TYR:CE2	1:B:347:VAL:HG13	2.56	0.40
1:B:77:THR:HB	1:B:78:PRO:CD	2.52	0.40
1:C:360:THR:HG23	1:C:364:GLU:OE1	2.21	0.40
1:D:122:GLY:C	1:D:124:SER:H	2.29	0.40
1:B:174:GLU:H	1:B:174:GLU:CD	2.29	0.40
1:B:330:ARG:HB3	1:B:330:ARG:HH21	1.86	0.40
1:C:38:LEU:HD23	1:C:38:LEU:O	2.20	0.40
1:C:60:ASP:O	1:C:62:LYS:HD2	2.22	0.40
1:A:116:ARG:HH11	1:A:116:ARG:HG3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:HB2	1:B:292:ARG:HB2	2.04	0.40
1:C:47:GLN:O	1:C:48:GLY:C	2.65	0.40
1:C:53:PHE:N	1:C:53:PHE:CD1	2.89	0.40
1:C:318:LEU:O	1:C:320:LYS:HD2	2.21	0.40

All (5) 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)
1:C:71:GLU:OE1	1:D:89:ARG:NE[6_555]	1.85	0.35
1:B:272:LEU:CD2	1:B:272:LEU:CD2[2_655]	1.87	0.33
1:C:71:GLU:CB	1:D:89:ARG:NH2[6_555]	1.91	0.29
1:C:316:GLU:OE1	1:C:316:GLU:OE1[2_655]	1.98	0.22
1:C:71:GLU:OE1	1:D:89:ARG:CZ[6_555]	2.09	0.11

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	363/365 (100%)	327 (90%)	25 (7%)	11 (3%)	3	0
1	B	363/365 (100%)	323 (89%)	29 (8%)	11 (3%)	3	0
1	C	363/365 (100%)	321 (88%)	32 (9%)	10 (3%)	4	1
1	D	363/365 (100%)	336 (93%)	18 (5%)	9 (2%)	4	1
All	All	1452/1460 (100%)	1307 (90%)	104 (7%)	41 (3%)	4	1

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	95	ASN

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Mol	Chain	Res	Type
1	A	116	ARG
1	A	123	ARG
1	A	125	SER
1	B	61	ASP
1	B	95	ASN
1	B	118	PHE
1	B	125	SER
1	B	262	TYR
1	B	263	ASN
1	B	271	PHE
1	C	54	ILE
1	C	55	THR
1	C	124	SER
1	C	125	SER
1	C	307	THR
1	D	124	SER
1	A	49	GLY
1	A	52	VAL
1	B	124	SER
1	C	61	ASP
1	D	56	PRO
1	D	92	ASP
1	D	118	PHE
1	D	125	SER
1	B	88	ALA
1	A	87	ARG
1	A	89	ARG
1	A	97	LYS
1	A	117	ASP
1	C	119	ARG
1	D	86	GLN
1	D	89	ARG
1	B	86	GLN
1	B	267	ASP
1	D	91	LYS
1	C	299	PRO
1	C	48	GLY
1	C	52	VAL
1	D	96	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	300/300 (100%)	293 (98%)	7 (2%)	44	38
1	B	300/300 (100%)	292 (97%)	8 (3%)	39	32
1	C	300/300 (100%)	289 (96%)	11 (4%)	30	20
1	D	300/300 (100%)	290 (97%)	10 (3%)	33	24
All	All	1200/1200 (100%)	1164 (97%)	36 (3%)	36	27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	89	ARG
1	A	93	TYR
1	A	172	LYS
1	A	214	ASN
1	A	240	LEU
1	A	322	ARG
1	B	89	ARG
1	B	97	LYS
1	B	172	LYS
1	B	215	GLN
1	B	240	LEU
1	B	241	ASN
1	B	272	LEU
1	B	343	LEU
1	C	21	ILE
1	C	58	LYS
1	C	89	ARG
1	C	97	LYS
1	C	172	LYS
1	C	200	ILE
1	C	215	GLN
1	C	240	LEU
1	C	241	ASN

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Mol	Chain	Res	Type
1	C	322	ARG
1	C	343	LEU
1	D	15	GLU
1	D	38	LEU
1	D	87	ARG
1	D	89	ARG
1	D	91	LYS
1	D	103	SER
1	D	118	PHE
1	D	172	LYS
1	D	240	LEU
1	D	322	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	85	ASN
1	A	111	HIS
1	A	168	ASN
1	A	182	GLN
1	A	186	GLN
1	A	191	GLN
1	A	215	GLN
1	A	223	GLN
1	A	241	ASN
1	A	294	HIS
1	A	305	GLN
1	A	313	ASN
1	B	47	GLN
1	B	51	ASN
1	B	85	ASN
1	B	111	HIS
1	B	168	ASN
1	B	186	GLN
1	B	191	GLN
1	B	214	ASN
1	B	223	GLN
1	B	241	ASN
1	B	263	ASN
1	B	294	HIS
1	B	313	ASN

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Mol	Chain	Res	Type
1	B	323	HIS
1	C	47	GLN
1	C	51	ASN
1	C	168	ASN
1	C	182	GLN
1	C	186	GLN
1	C	191	GLN
1	C	192	ASN
1	C	196	ASN
1	C	214	ASN
1	C	223	GLN
1	C	241	ASN
1	C	294	HIS
1	C	303	GLN
1	C	305	GLN
1	C	313	ASN
1	C	323	HIS
1	D	85	ASN
1	D	104	HIS
1	D	111	HIS
1	D	168	ASN
1	D	186	GLN
1	D	191	GLN
1	D	196	ASN
1	D	215	GLN
1	D	223	GLN
1	D	241	ASN
1	D	263	ASN
1	D	294	HIS

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	D	4400	-	33,33,33	1.94	11 (33%)	48,50,50	1.72	7 (14%)
2	FMN	B	2400	-	33,33,33	1.99	11 (33%)	48,50,50	1.72	7 (14%)
2	FMN	A	1400	-	33,33,33	1.94	10 (30%)	48,50,50	1.74	9 (18%)
2	FMN	C	3400	-	33,33,33	1.97	11 (33%)	48,50,50	1.69	7 (14%)

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	4400	-	-	15/18/18/18	0/3/3/3
2	FMN	B	2400	-	-	6/18/18/18	0/3/3/3
2	FMN	A	1400	-	-	5/18/18/18	0/3/3/3
2	FMN	C	3400	-	-	6/18/18/18	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3400	FMN	C9A-N10	-4.44	1.33	1.41
2	A	1400	FMN	C1'-C2'	4.11	1.58	1.52
2	B	2400	FMN	C9A-N10	-4.02	1.34	1.41
2	D	4400	FMN	C1'-C2'	3.92	1.58	1.52
2	D	4400	FMN	C9A-N10	-3.85	1.34	1.41
2	A	1400	FMN	C9A-N10	-3.84	1.34	1.41
2	A	1400	FMN	C9A-C5A	3.74	1.47	1.41
2	B	2400	FMN	C1'-C2'	3.66	1.57	1.52
2	D	4400	FMN	C9A-C5A	3.64	1.47	1.41
2	C	3400	FMN	C1'-C2'	3.62	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2400	FMN	C5'-C4'	3.52	1.56	1.51
2	B	2400	FMN	C9A-C5A	3.48	1.46	1.41
2	C	3400	FMN	C9A-C5A	3.29	1.46	1.41
2	C	3400	FMN	C4A-N5	3.12	1.37	1.30
2	B	2400	FMN	C4A-N5	3.09	1.37	1.30
2	D	4400	FMN	C4A-N5	2.84	1.36	1.30
2	C	3400	FMN	C4-N3	2.83	1.44	1.38
2	C	3400	FMN	C6-C7	2.82	1.43	1.39
2	A	1400	FMN	C4A-N5	2.80	1.36	1.30
2	A	1400	FMN	C8-C7	2.77	1.47	1.40
2	A	1400	FMN	C5'-C4'	2.76	1.55	1.51
2	B	2400	FMN	C8-C7	2.72	1.47	1.40
2	A	1400	FMN	C4-N3	2.70	1.43	1.38
2	D	4400	FMN	C8-C7	2.70	1.47	1.40
2	C	3400	FMN	C8-C7	2.68	1.47	1.40
2	B	2400	FMN	C4-N3	2.68	1.43	1.38
2	D	4400	FMN	C4-N3	2.68	1.43	1.38
2	B	2400	FMN	C6-C7	2.67	1.43	1.39
2	C	3400	FMN	C5'-C4'	2.53	1.55	1.51
2	D	4400	FMN	C2'-C3'	2.45	1.57	1.53
2	D	4400	FMN	C6-C7	2.42	1.42	1.39
2	C	3400	FMN	C10-N1	2.39	1.38	1.33
2	D	4400	FMN	C1'-N10	2.32	1.53	1.47
2	C	3400	FMN	C9-C9A	2.31	1.43	1.39
2	A	1400	FMN	C1'-N10	2.31	1.53	1.47
2	B	2400	FMN	C10-N1	2.25	1.37	1.33
2	D	4400	FMN	C10-N1	2.23	1.37	1.33
2	C	3400	FMN	P-O3P	2.23	1.63	1.54
2	A	1400	FMN	C6-C7	2.23	1.42	1.39
2	B	2400	FMN	C2'-C3'	2.21	1.57	1.53
2	D	4400	FMN	C9-C9A	2.14	1.43	1.39
2	B	2400	FMN	C1'-N10	2.07	1.52	1.47
2	A	1400	FMN	C10-N1	2.01	1.37	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3400	FMN	C9A-C5A-N5	-5.54	116.57	122.45
2	B	2400	FMN	C9A-C5A-N5	-5.33	116.80	122.45
2	B	2400	FMN	C5A-C9A-N10	5.30	122.76	117.97
2	A	1400	FMN	C9A-C5A-N5	-5.27	116.86	122.45
2	D	4400	FMN	C9A-C5A-N5	-5.24	116.89	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1400	FMN	C5A-C9A-N10	5.18	122.65	117.97
2	D	4400	FMN	C5A-C9A-N10	5.06	122.55	117.97
2	C	3400	FMN	C5A-C9A-N10	4.84	122.35	117.97
2	A	1400	FMN	C6-C5A-C9A	3.54	123.91	119.05
2	D	4400	FMN	C6-C5A-C9A	3.48	123.83	119.05
2	B	2400	FMN	C6-C5A-C9A	3.33	123.62	119.05
2	C	3400	FMN	C6-C5A-C9A	3.26	123.53	119.05
2	B	2400	FMN	C8M-C8-C9	-2.87	114.51	119.57
2	A	1400	FMN	C8M-C8-C9	-2.83	114.58	119.57
2	D	4400	FMN	O4'-C4'-C3'	2.77	115.73	109.25
2	D	4400	FMN	C8M-C8-C9	-2.69	114.84	119.57
2	C	3400	FMN	O4'-C4'-C3'	2.67	115.49	109.25
2	A	1400	FMN	O4'-C4'-C3'	2.65	115.44	109.25
2	D	4400	FMN	C9-C9A-C5A	-2.51	115.59	120.03
2	C	3400	FMN	C8M-C8-C9	-2.49	115.18	119.57
2	B	2400	FMN	O4'-C4'-C3'	2.46	115.01	109.25
2	A	1400	FMN	C9-C9A-C5A	-2.43	115.73	120.03
2	B	2400	FMN	C9-C9A-C5A	-2.36	115.86	120.03
2	A	1400	FMN	O3P-P-O5'	-2.18	100.98	106.67
2	C	3400	FMN	C9-C9A-C5A	-2.13	116.26	120.03
2	A	1400	FMN	O4-C4-C4A	-2.08	121.04	126.53
2	D	4400	FMN	O4-C4-C4A	-2.05	121.13	126.53
2	A	1400	FMN	O4-C4-N3	2.05	123.96	120.11
2	B	2400	FMN	O4-C4-C4A	-2.04	121.14	126.53
2	C	3400	FMN	C10-C4A-N5	-2.03	120.67	124.81

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1400	FMN	C5'-O5'-P-O2P
2	A	1400	FMN	C5'-O5'-P-O3P
2	B	2400	FMN	C3'-C4'-C5'-O5'
2	C	3400	FMN	C3'-C4'-C5'-O5'
2	C	3400	FMN	O4'-C4'-C5'-O5'
2	C	3400	FMN	C5'-O5'-P-O1P
2	C	3400	FMN	C5'-O5'-P-O2P
2	C	3400	FMN	C5'-O5'-P-O3P
2	D	4400	FMN	C2'-C1'-N10-C10
2	D	4400	FMN	C1'-C2'-C3'-O3'
2	D	4400	FMN	C1'-C2'-C3'-C4'
2	D	4400	FMN	C2'-C3'-C4'-O4'

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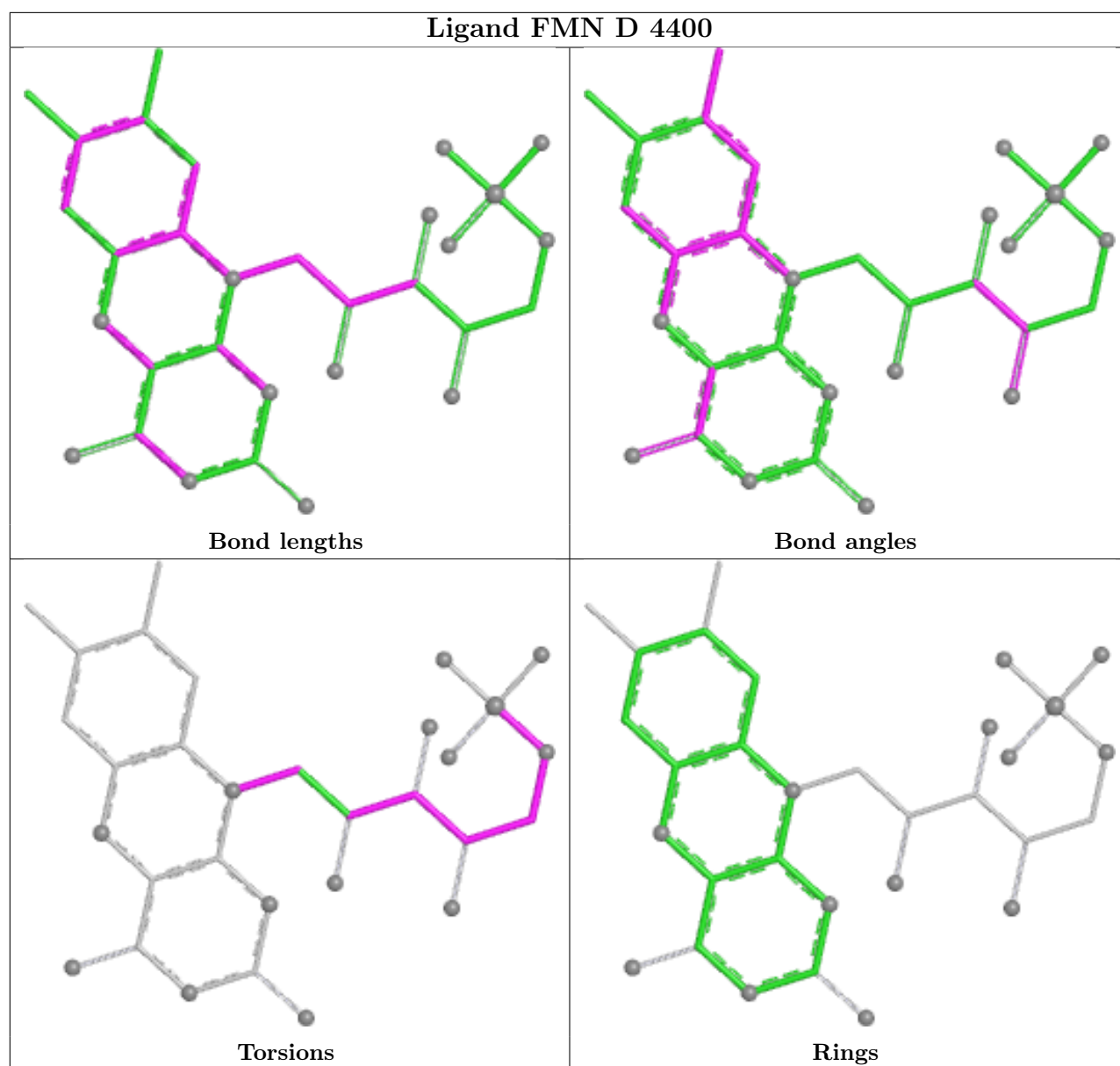
Mol	Chain	Res	Type	Atoms
2	D	4400	FMN	O3'-C3'-C4'-O4'
2	D	4400	FMN	C3'-C4'-C5'-O5'
2	D	4400	FMN	O4'-C4'-C5'-O5'
2	D	4400	FMN	C5'-O5'-P-O2P
2	D	4400	FMN	C5'-O5'-P-O3P
2	D	4400	FMN	O3'-C3'-C4'-C5'
2	D	4400	FMN	C2'-C3'-C4'-C5'
2	D	4400	FMN	O2'-C2'-C3'-C4'
2	D	4400	FMN	O2'-C2'-C3'-O3'
2	D	4400	FMN	C5'-O5'-P-O1P
2	A	1400	FMN	C5'-O5'-P-O1P
2	D	4400	FMN	C4'-C5'-O5'-P
2	B	2400	FMN	O3'-C3'-C4'-C5'
2	B	2400	FMN	O2'-C2'-C3'-C4'
2	B	2400	FMN	C1'-C2'-C3'-O3'
2	C	3400	FMN	C4'-C5'-O5'-P
2	B	2400	FMN	O3'-C3'-C4'-O4'
2	B	2400	FMN	C2'-C3'-C4'-O4'
2	A	1400	FMN	O3'-C3'-C4'-C5'
2	A	1400	FMN	O3'-C3'-C4'-O4'

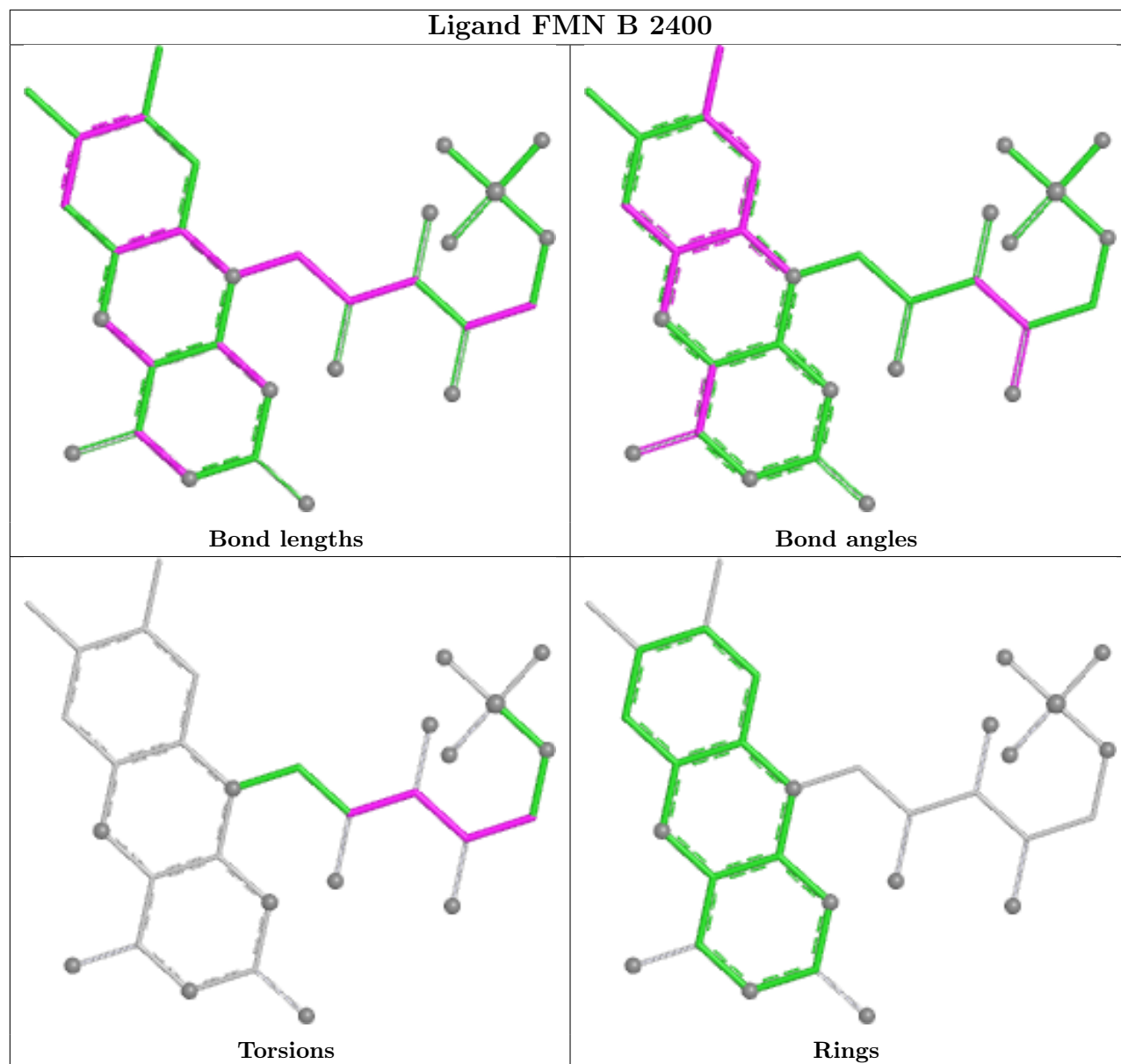
There are no ring outliers.

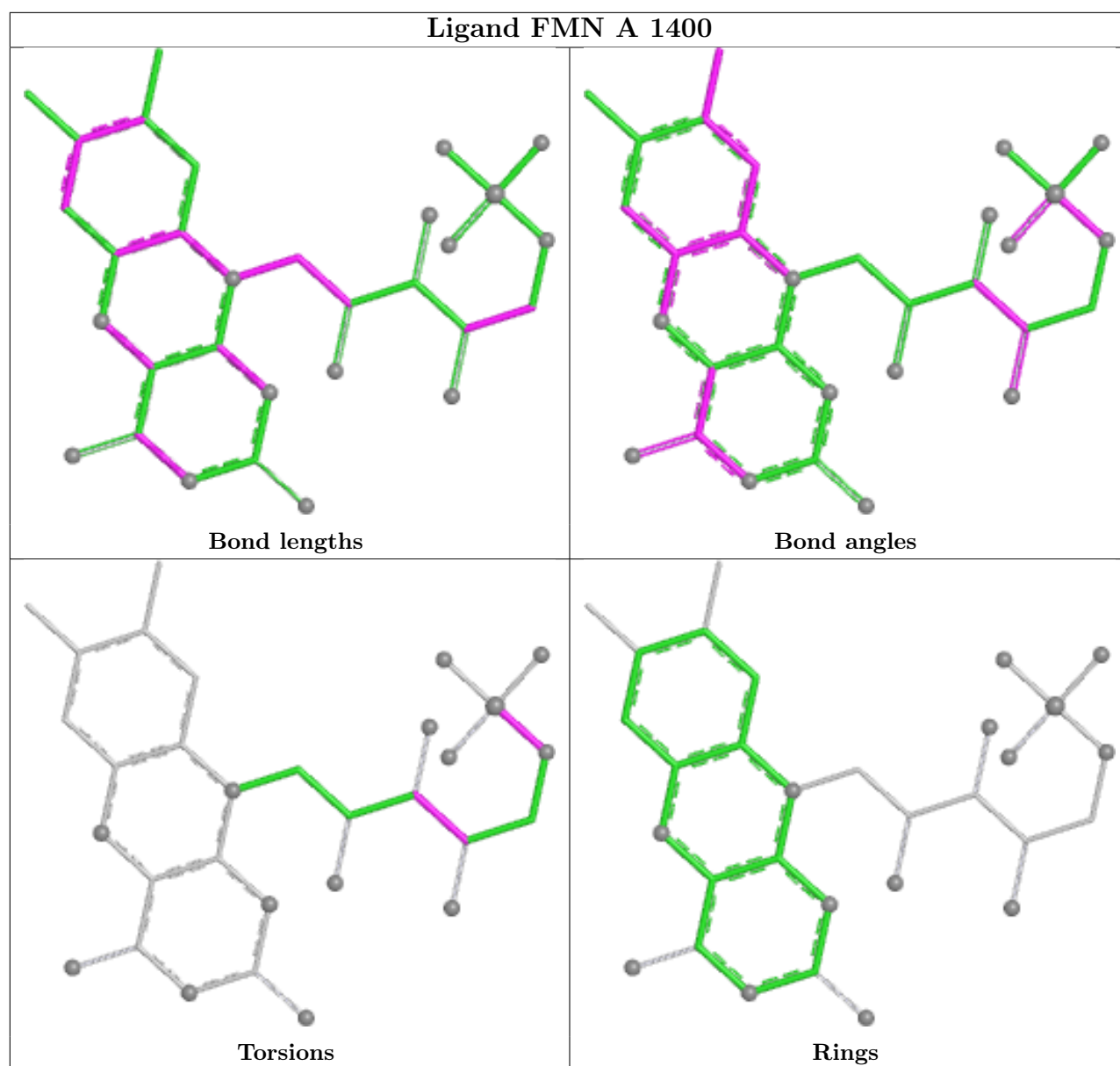
4 monomers are involved in 25 short contacts:

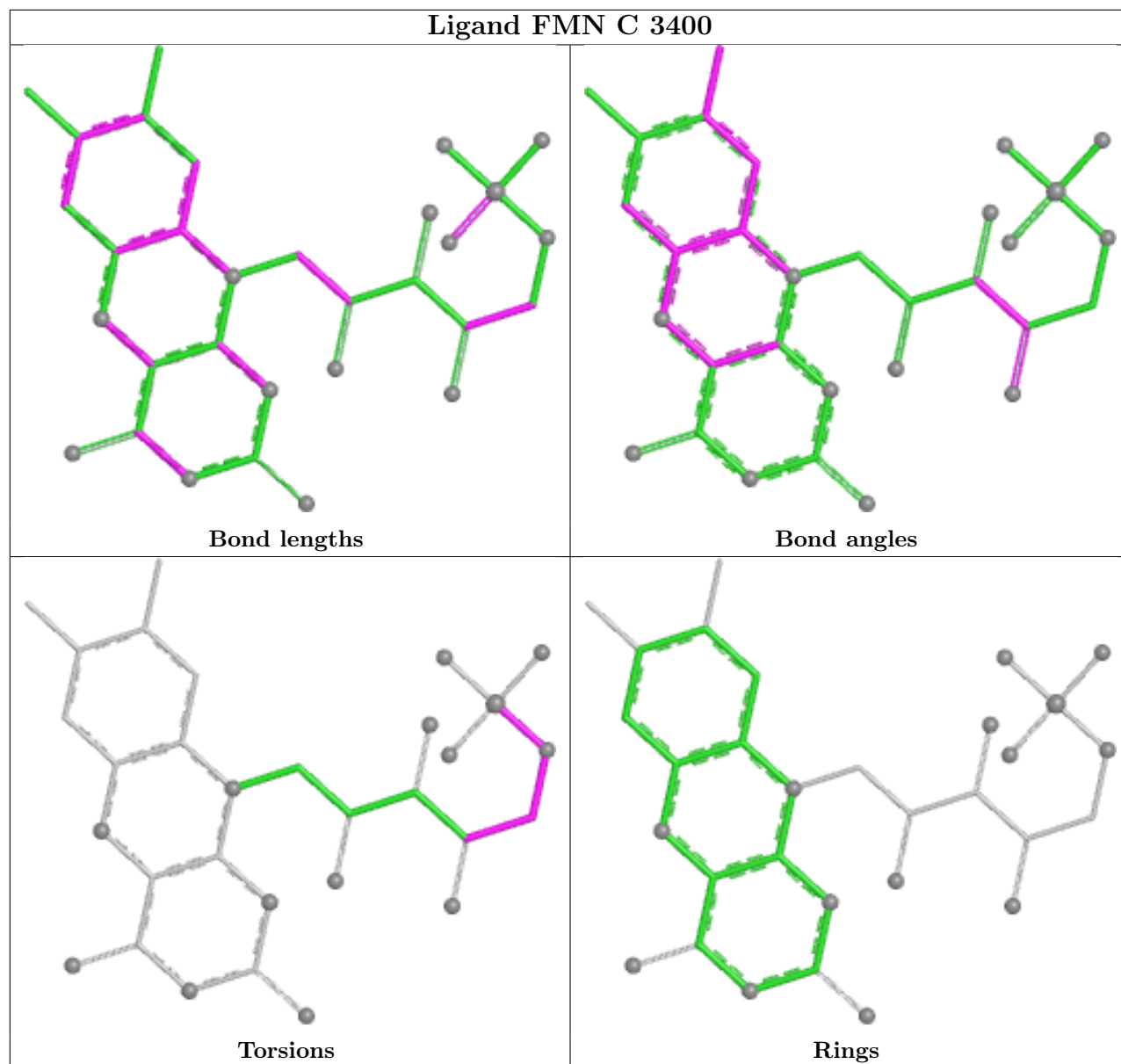
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4400	FMN	7	0
2	B	2400	FMN	9	0
2	A	1400	FMN	6	0
2	C	3400	FMN	3	0

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	365/365 (100%)	0.59	55 (15%) 5 6	16, 26, 104, 158	9 (2%)
1	B	365/365 (100%)	1.20	91 (24%) 2 1	20, 36, 124, 154	9 (2%)
1	C	365/365 (100%)	1.37	109 (29%) 1 1	19, 34, 147, 162	9 (2%)
1	D	365/365 (100%)	0.62	53 (14%) 6 6	17, 28, 85, 126	9 (2%)
All	All	1460/1460 (100%)	0.94	308 (21%) 2 2	16, 30, 122, 162	36 (2%)

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	ILE	10.5
1	C	103	SER	8.0
1	C	300	SER	7.8
1	B	271	PHE	7.6
1	D	115	ILE	7.3
1	A	118	PHE	7.1
1	C	58	LYS	6.9
1	A	96	ILE	6.7
1	A	53	PHE	6.7
1	C	118	PHE	6.7
1	B	52	VAL	6.6
1	C	302	PHE	6.6
1	A	54	ILE	6.5
1	A	56	PRO	6.5
1	C	100	PHE	6.4
1	C	319	LEU	6.4
1	B	118	PHE	6.4
1	B	263	ASN	6.3
1	C	56	PRO	6.3
1	C	53	PHE	6.1
1	C	310	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	317	CYS	6.1
1	A	52	VAL	6.1
1	A	94	ASP	6.1
1	B	270	GLY	6.0
1	C	48	GLY	6.0
1	C	122	GLY	6.0
1	C	315	CYS	5.9
1	C	99	LEU	5.9
1	C	304	PRO	5.8
1	A	115	ILE	5.8
1	B	53	PHE	5.8
1	B	56	PRO	5.7
1	C	52	VAL	5.7
1	D	118	PHE	5.7
1	A	93	TYR	5.7
1	B	93	TYR	5.5
1	A	88	ALA	5.4
1	B	214	ASN	5.3
1	B	122	GLY	5.2
1	B	54	ILE	5.2
1	D	96	ILE	5.1
1	B	264	ASP	5.1
1	C	55	THR	5.1
1	D	56	PRO	5.1
1	C	308	ILE	5.0
1	C	312	GLY	5.0
1	D	122	GLY	5.0
1	D	58	LYS	5.0
1	B	55	THR	5.0
1	D	121	GLY	5.0
1	C	318	LEU	4.9
1	C	104	HIS	4.9
1	A	117	ASP	4.9
1	A	49	GLY	4.9
1	B	120	GLY	4.9
1	C	96	ILE	4.9
1	C	121	GLY	4.8
1	C	305	GLN	4.8
1	C	49	GLY	4.8
1	B	88	ALA	4.8
1	C	54	ILE	4.7
1	B	265	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	211	ILE	4.7
1	C	307	THR	4.7
1	D	88	ALA	4.7
1	A	365	ASN	4.6
1	C	88	ALA	4.6
1	C	93	TYR	4.6
1	A	95	ASN	4.6
1	A	120	GLY	4.5
1	B	126	ALA	4.5
1	C	102	PRO	4.4
1	D	123	ARG	4.4
1	B	49	GLY	4.4
1	D	87	ARG	4.4
1	D	59	GLU	4.4
1	D	57	ARG	4.4
1	B	61	ASP	4.4
1	C	90	SER	4.3
1	B	58	LYS	4.3
1	D	55	THR	4.3
1	D	126	ALA	4.3
1	B	269	LYS	4.3
1	C	213	THR	4.3
1	C	214	ASN	4.3
1	C	321	GLY	4.3
1	C	92	ASP	4.3
1	C	313	ASN	4.2
1	B	213	THR	4.2
1	B	272	LEU	4.2
1	C	115	ILE	4.2
1	A	126	ALA	4.2
1	C	101	ARG	4.2
1	C	105	ALA	4.2
1	A	122	GLY	4.1
1	A	224	GLY	4.1
1	B	99	LEU	4.1
1	D	49	GLY	4.1
1	C	365	ASN	4.1
1	C	109	TYR	4.1
1	A	89	ARG	4.1
1	D	125	SER	4.1
1	B	123	ARG	4.0
1	B	115	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	95	ASN	4.0
1	C	124	SER	4.0
1	B	21	ILE	4.0
1	B	48	GLY	3.9
1	A	17	HIS	3.9
1	B	262	TYR	3.9
1	B	121	GLY	3.9
1	B	96	ILE	3.9
1	A	123	ARG	3.8
1	C	120	GLY	3.8
1	D	93	TYR	3.8
1	C	314	GLU	3.8
1	A	55	THR	3.8
1	C	316	GLU	3.8
1	D	85	ASN	3.8
1	A	121	GLY	3.7
1	C	85	ASN	3.7
1	C	57	ARG	3.7
1	C	20	VAL	3.7
1	A	58	LYS	3.7
1	B	302	PHE	3.7
1	B	211	ILE	3.6
1	D	21	ILE	3.6
1	B	273	SER	3.6
1	A	19	ASP	3.6
1	D	365	ASN	3.6
1	D	124	SER	3.6
1	D	116	ARG	3.6
1	C	61	ASP	3.6
1	D	117	ASP	3.6
1	C	59	GLU	3.5
1	C	270	GLY	3.5
1	A	214	ASN	3.5
1	D	224	GLY	3.5
1	B	266	MET	3.5
1	D	97	LYS	3.5
1	B	212	LYS	3.5
1	B	51	ASN	3.4
1	C	306	ARG	3.4
1	C	172	LYS	3.4
1	D	92	ASP	3.4
1	A	241	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	95	ASN	3.4
1	A	119	ARG	3.4
1	C	212	LYS	3.4
1	D	60	ASP	3.4
1	B	124	SER	3.4
1	B	85	ASN	3.4
1	C	320	LYS	3.3
1	C	86	GLN	3.3
1	B	301	ILE	3.3
1	C	15	GLU	3.3
1	B	89	ARG	3.3
1	A	124	SER	3.3
1	B	17	HIS	3.3
1	C	303	GLN	3.3
1	A	60	ASP	3.3
1	D	90	SER	3.3
1	C	161	LYS	3.2
1	B	87	ARG	3.2
1	C	98	ASN	3.2
1	D	120	GLY	3.2
1	B	117	ASP	3.2
1	D	94	ASP	3.2
1	A	61	ASP	3.2
1	A	85	ASN	3.1
1	D	54	ILE	3.1
1	A	50	ARG	3.1
1	D	89	ARG	3.1
1	B	100	PHE	3.1
1	C	62	LYS	3.1
1	C	323	HIS	3.1
1	D	364	GLU	3.1
1	C	114	GLY	3.1
1	B	309	ASP	3.0
1	A	57	ARG	3.0
1	C	107	PHE	3.0
1	B	300	SER	3.0
1	A	48	GLY	3.0
1	B	62	LYS	3.0
1	C	17	HIS	3.0
1	B	268	GLN	3.0
1	D	86	GLN	3.0
1	B	119	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	274	ASN	3.0
1	B	310	ILE	3.0
1	B	94	ASP	3.0
1	C	117	ASP	3.0
1	C	309	ASP	3.0
1	A	87	ARG	3.0
1	C	87	ARG	3.0
1	C	194	ILE	3.0
1	B	318	LEU	2.9
1	B	86	GLN	2.9
1	C	91	LYS	2.9
1	C	18	GLY	2.9
1	A	90	SER	2.9
1	B	321	GLY	2.9
1	C	269	LYS	2.9
1	D	172	LYS	2.9
1	C	123	ARG	2.9
1	C	322	ARG	2.9
1	D	119	ARG	2.9
1	C	125	SER	2.9
1	C	106	ASP	2.9
1	B	365	ASN	2.8
1	C	89	ARG	2.8
1	C	110	PHE	2.8
1	C	271	PHE	2.8
1	A	84	HIS	2.8
1	D	91	LYS	2.8
1	D	241	ASN	2.8
1	B	57	ARG	2.8
1	C	119	ARG	2.8
1	D	211	ILE	2.8
1	A	51	ASN	2.8
1	C	94	ASP	2.8
1	C	126	ALA	2.7
1	B	84	HIS	2.7
1	C	299	PRO	2.7
1	D	63	VAL	2.7
1	D	20	VAL	2.7
1	B	172	LYS	2.7
1	C	265	LEU	2.6
1	D	50	ARG	2.6
1	A	86	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	15	GLU	2.6
1	B	125	SER	2.6
1	C	51	ASN	2.6
1	B	102	PRO	2.6
1	A	20	VAL	2.6
1	B	90	SER	2.6
1	B	319	LEU	2.6
1	B	60	ASP	2.6
1	C	298	THR	2.6
1	B	317	CYS	2.5
1	B	104	HIS	2.5
1	D	17	HIS	2.5
1	A	47	GLN	2.5
1	B	95	ASN	2.5
1	C	215	GLN	2.5
1	C	224	GLY	2.5
1	D	48	GLY	2.5
1	D	321	GLY	2.5
1	A	116	ARG	2.5
1	A	322	ARG	2.5
1	C	21	ILE	2.5
1	A	215	GLN	2.5
1	C	364	GLU	2.5
1	B	19	ASP	2.5
1	D	84	HIS	2.4
1	C	60	ASP	2.4
1	C	13	PHE	2.4
1	B	267	ASP	2.4
1	C	200	ILE	2.4
1	B	47	GLN	2.4
1	B	308	ILE	2.4
1	A	114	GLY	2.4
1	B	315	CYS	2.4
1	D	61	ASP	2.3
1	B	170	ALA	2.3
1	C	83	ILE	2.3
1	C	97	LYS	2.3
1	A	16	SER	2.3
1	B	116	ARG	2.3
1	B	322	ARG	2.3
1	D	19	ASP	2.3
1	C	196	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	7	PHE	2.3
1	B	313	ASN	2.3
1	A	13	PHE	2.2
1	C	84	HIS	2.2
1	A	97	LYS	2.2
1	B	50	ARG	2.2
1	C	50	ARG	2.2
1	D	40	GLU	2.2
1	A	18	GLY	2.2
1	C	267	ASP	2.2
1	A	21	ILE	2.2
1	D	160	ILE	2.2
1	A	364	GLU	2.2
1	B	18	GLY	2.2
1	B	174	GLU	2.1
1	D	52	VAL	2.1
1	A	14	GLY	2.1
1	B	171	LEU	2.1
1	A	91	LYS	2.1
1	B	110	PHE	2.1
1	D	83	ILE	2.1
1	C	19	ASP	2.1
1	B	114	GLY	2.1
1	B	97	LYS	2.1
1	C	272	LEU	2.1
1	B	92	ASP	2.1
1	B	109	TYR	2.1
1	C	324	ASP	2.1
1	B	91	LYS	2.1
1	C	268	GLN	2.1
1	A	62	LYS	2.0
1	C	16	SER	2.0
1	B	98	ASN	2.0
1	B	46	ARG	2.0
1	B	14	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](#)

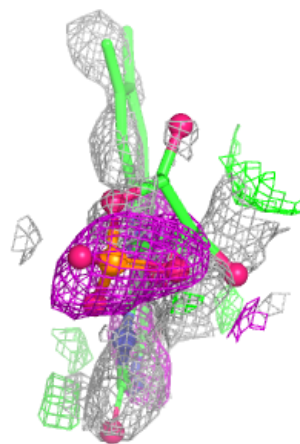
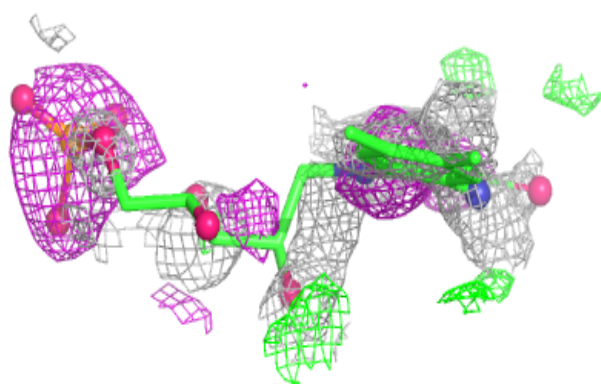
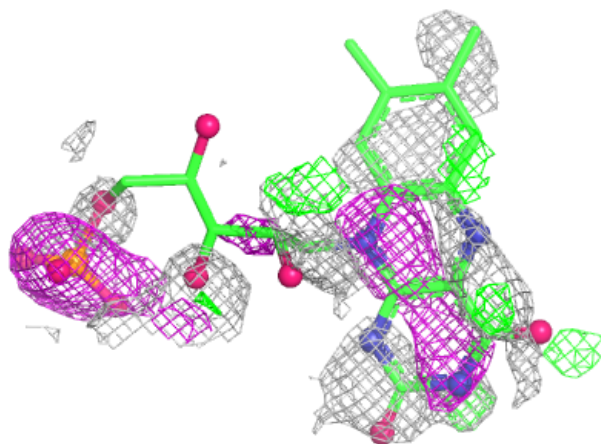
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FMN	C	3400	31/31	0.36	0.22	71,73,87,87	0
2	FMN	B	2400	31/31	0.47	0.22	62,69,82,82	0
2	FMN	A	1400	31/31	0.58	0.19	30,57,66,68	0
2	FMN	D	4400	31/31	0.58	0.20	45,61,70,71	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.

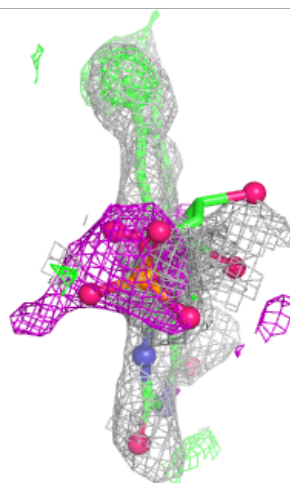
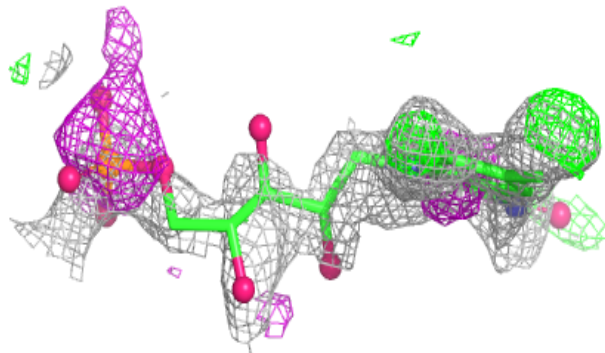
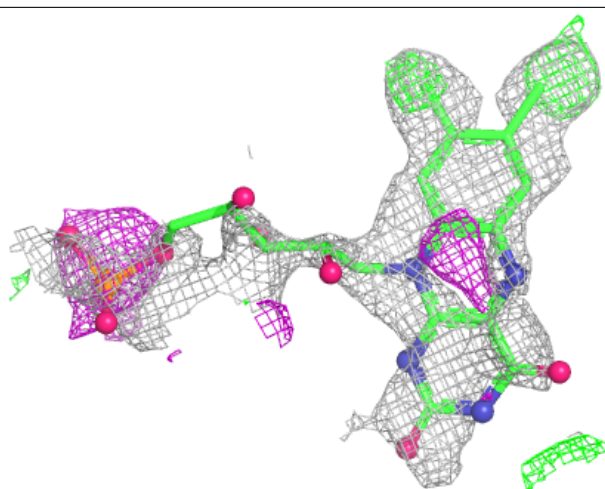
Electron density around FMN C 3400:

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



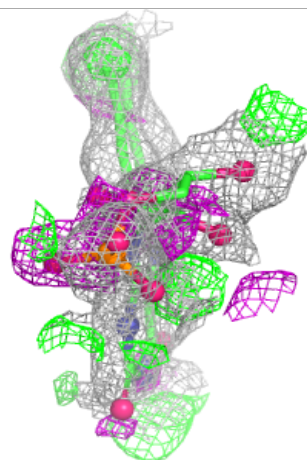
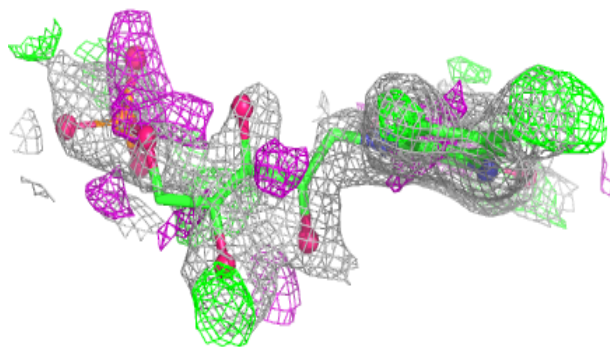
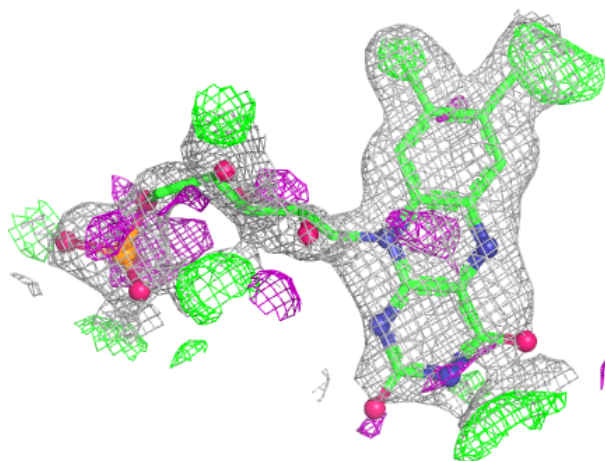
Electron density around FMN B 2400:

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



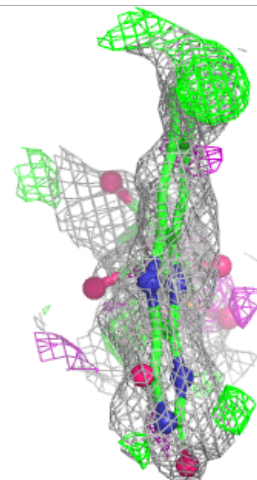
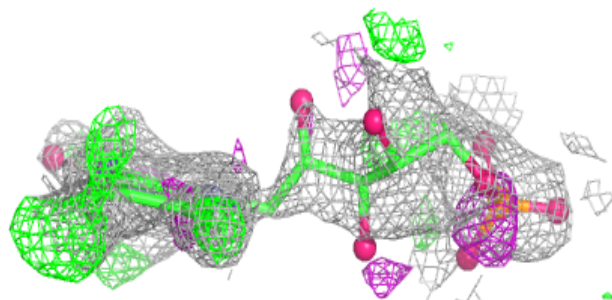
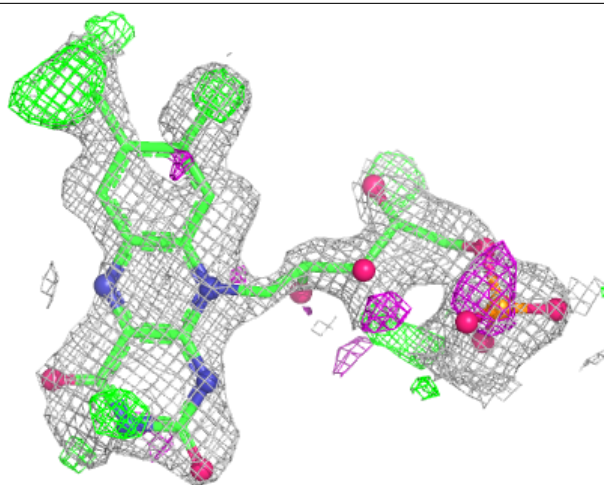
Electron density around FMN A 1400:

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



Electron density around FMN D 4400:

$2mF_o-DF_c$ (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.