



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID : 4YAO / pdb_00004yao
Title : Reduced CYPOR mutant - G143del
Authors : Xia, C.; Kim, J.J.P.
Deposited on : 2015-02-17
Resolution : 2.50 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

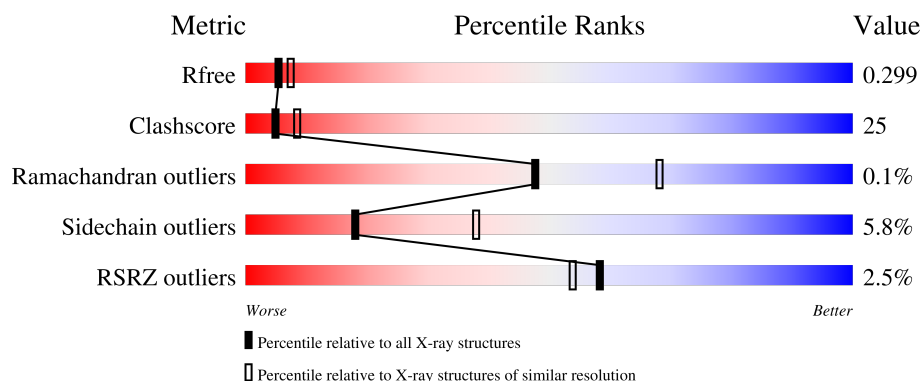
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	621	52% 41% • •
1	B	621	4% 47% 44% 5% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10066 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 NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4828	3061	834	910	23			
1	B	596	Total	C	N	O	S	0	0	0
			4729	2993	822	891	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P00388
B	?	-	GLY	deletion	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



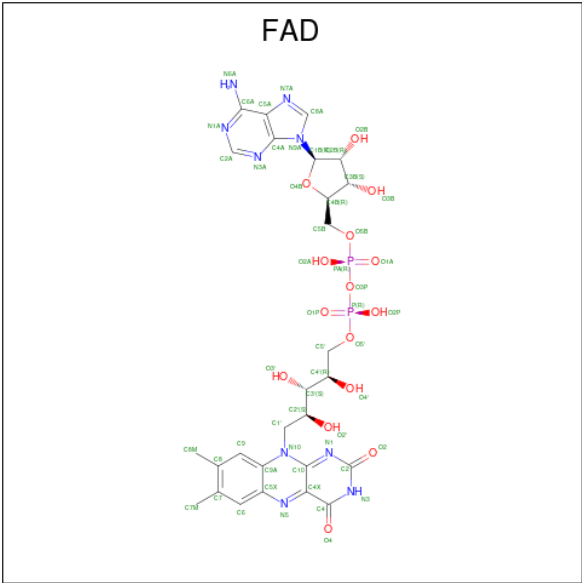
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

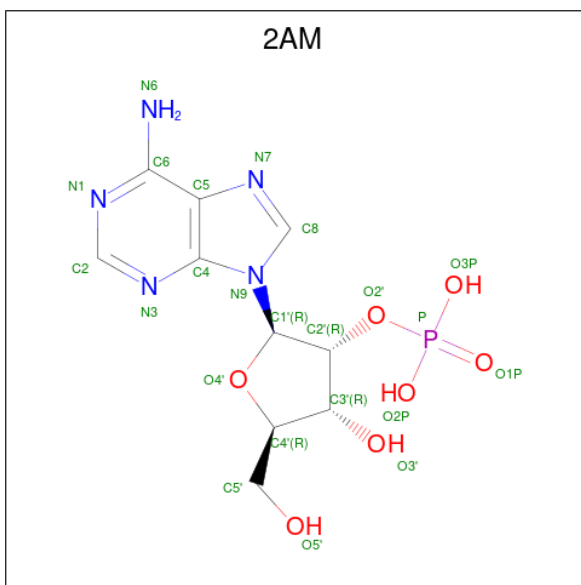
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

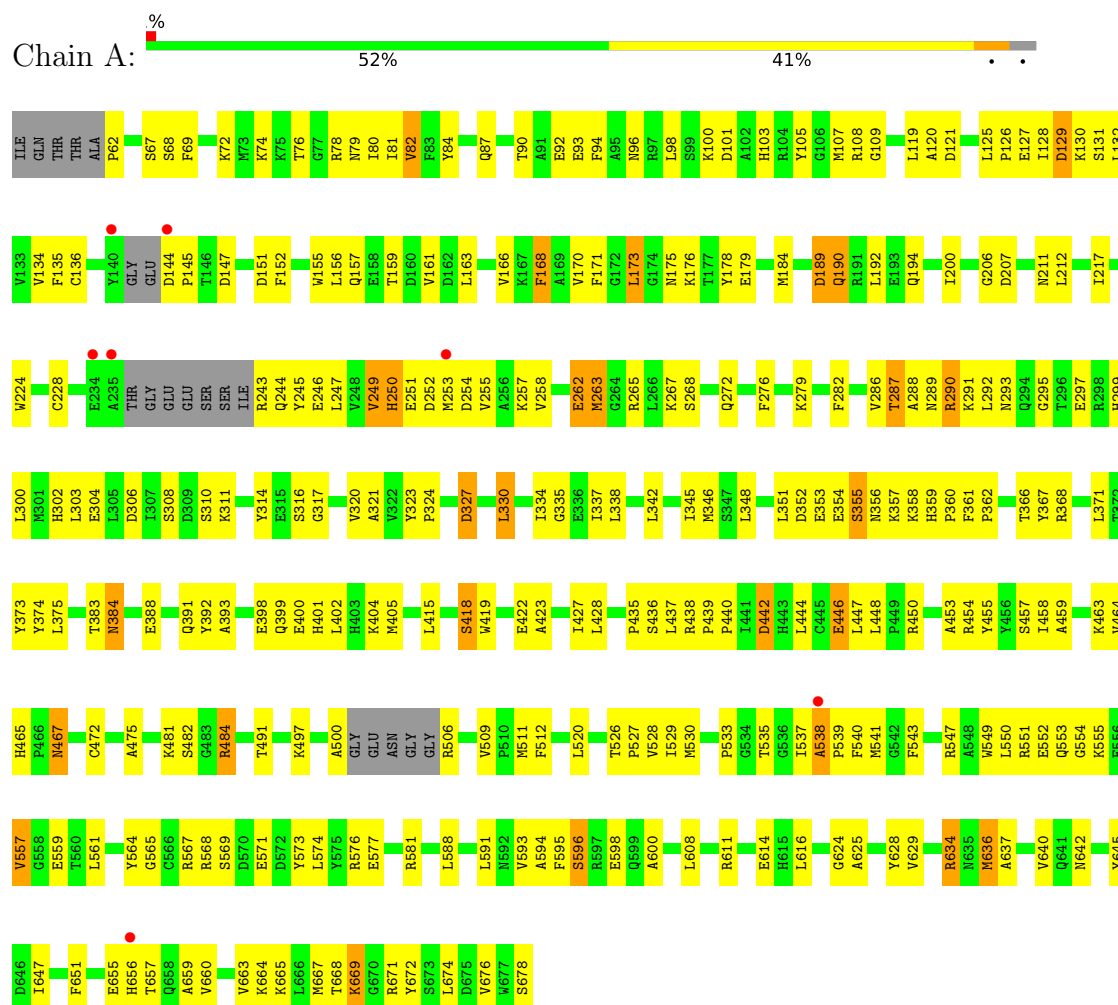
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	155	Total	O	0	0
			155	155		
6	B	120	Total	O	0	0
			120	120		

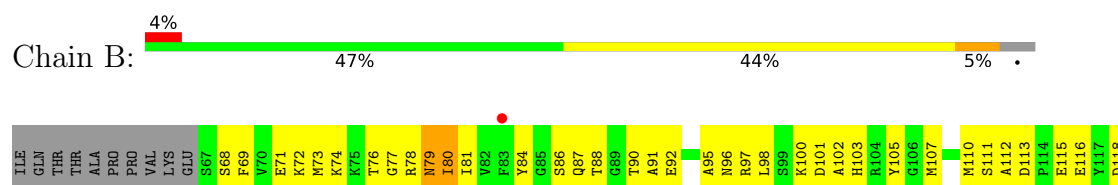
3 Residue-property plots

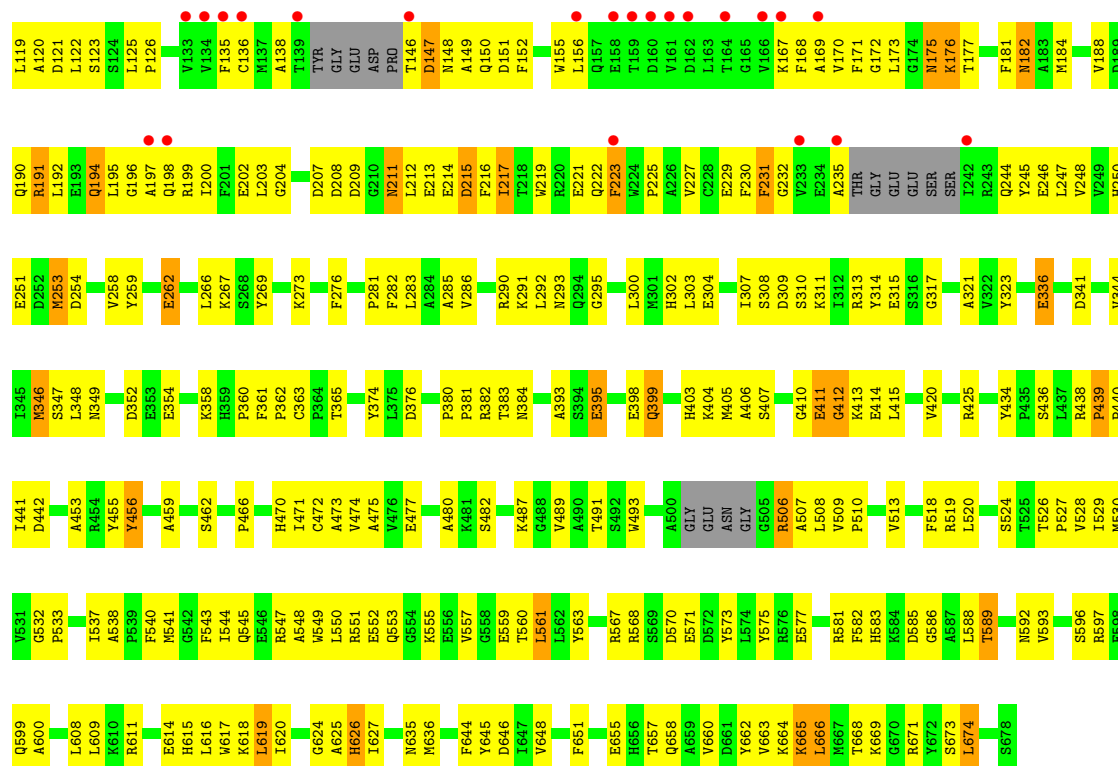
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NADPH-cytochrome P450 reductase



• Molecule 1: NADPH-cytochrome P450 reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.48Å 115.52Å 117.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.18 – 2.50 38.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.0 (38.18-2.50) 89.1 (38.18-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.51Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.234 , 0.298 0.236 , 0.299	Depositor DCC
R_{free} test set	2169 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10066	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0236e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, FAD, FMN, 2AM

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	0.52	3/4943 (0.1%)	1.00	22/6687 (0.3%)
1	B	0.49	0/4841	1.08	39/6550 (0.6%)
All	All	0.50	3/9784 (0.0%)	1.04	61/13237 (0.5%)

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
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	636	MET	SD-CE	-5.88	1.64	1.79
1	A	538	ALA	C-N	5.25	1.41	1.34
1	A	539	PRO	N-CD	5.23	1.55	1.47

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	GLY	N-CA-C	11.92	128.66	114.48
1	B	589	THR	N-CA-C	10.48	122.29	111.07
1	B	223	PHE	N-CA-C	9.65	121.56	111.14
1	B	230	PHE	CB-CA-C	9.40	125.64	110.88
1	B	230	PHE	N-CA-C	-9.23	101.19	111.07
1	B	125	LEU	N-CA-C	8.90	129.48	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	VAL	N-CA-C	8.75	118.82	110.42
1	B	231	PHE	N-CA-C	8.74	122.69	112.72
1	B	194	GLN	N-CA-C	8.72	120.56	111.14
1	A	249	VAL	CB-CA-C	-8.59	99.78	111.63
1	B	506	ARG	N-CA-CB	-8.45	96.21	110.49
1	B	251	GLU	N-CA-C	-7.85	103.84	113.50
1	B	596	SER	N-CA-C	7.03	119.97	111.82
1	B	506	ARG	N-CA-C	-6.96	95.97	110.80
1	B	232	GLY	N-CA-C	6.94	129.62	113.18
1	B	586	GLY	N-CA-C	-6.88	105.72	115.43
1	B	123	SER	CB-CA-C	-6.86	95.84	110.32
1	A	511	MET	N-CA-C	6.75	118.05	108.74
1	A	330	LEU	N-CA-C	-6.66	104.10	111.82
1	B	666	LEU	N-CA-C	-6.57	104.20	111.36
1	B	434	TYR	CA-C-N	6.36	126.85	119.47
1	B	434	TYR	C-N-CA	6.36	126.85	119.47
1	A	317	GLY	N-CA-C	-6.36	106.35	113.79
1	A	463	LYS	N-CA-C	-6.26	105.61	113.18
1	B	197	ALA	N-CA-C	6.17	118.67	110.53
1	B	123	SER	N-CA-C	6.12	119.85	112.38
1	A	168	PHE	N-CA-C	6.07	118.18	109.14
1	A	247	LEU	CB-CA-C	-6.05	99.32	109.48
1	A	557	VAL	N-CA-C	6.01	116.51	107.80
1	B	513	VAL	N-CA-C	5.94	116.42	107.80
1	A	346	MET	N-CA-C	5.90	116.07	108.34
1	B	395	GLU	CA-C-N	5.78	124.98	118.97
1	B	395	GLU	C-N-CA	5.78	124.98	118.97
1	A	596	SER	N-CA-C	5.75	118.01	111.11
1	A	263	MET	N-CA-C	5.72	118.38	111.40
1	B	412	GLY	N-CA-C	-5.65	108.45	114.67
1	B	489	VAL	N-CA-C	5.61	115.69	110.42
1	A	538	ALA	CA-C-N	-5.52	112.92	119.05
1	A	538	ALA	C-N-CA	-5.52	112.92	119.05
1	A	128	ILE	N-CA-C	-5.47	100.57	108.89
1	B	336	GLU	N-CA-C	5.43	117.00	111.14
1	A	373	TYR	N-CA-C	5.39	120.87	113.97
1	A	541	MET	N-CA-C	-5.39	105.81	112.38
1	B	290	ARG	N-CA-C	5.35	118.12	109.40
1	A	62	PRO	CA-C-N	-5.34	113.16	119.84
1	A	62	PRO	C-N-CA	-5.34	113.16	119.84
1	B	346	MET	N-CA-C	5.34	114.88	107.73
1	B	231	PHE	N-CA-CB	-5.30	102.80	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLU	CB-CA-C	-5.27	100.14	110.11
1	A	258	VAL	N-CA-C	5.22	115.38	107.80
1	B	665	LYS	N-CA-C	-5.21	107.05	113.41
1	B	438	ARG	CA-C-N	5.19	125.72	120.38
1	B	438	ARG	C-N-CA	5.19	125.72	120.38
1	A	90	THR	N-CA-C	5.13	116.87	111.28
1	B	112	ALA	N-CA-C	5.10	116.83	109.07
1	B	273	LYS	CA-C-N	5.05	123.34	119.66
1	B	273	LYS	C-N-CA	5.05	123.34	119.66
1	B	420	VAL	CB-CA-C	-5.04	106.65	111.44
1	A	355	SER	N-CA-CB	-5.01	102.96	110.17
1	B	217	ILE	N-CA-C	-5.00	105.29	112.35
1	B	253	MET	N-CA-C	5.00	117.91	109.95

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	581	ARG	Sidechain
1	B	456	TYR	Sidechain

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	4828	0	4679	228	0
1	B	4729	0	4510	259	0
2	A	31	0	19	0	0
2	B	31	0	19	1	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
5	A	10	0	0	1	0
5	B	10	0	0	1	0
6	A	155	0	0	16	0
6	B	120	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10066	0	9313	482	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (482) 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:A:144:ASP:CB	1:A:145:PRO:HD3	1.57	1.31
1:A:144:ASP:CB	1:A:145:PRO:CD	2.29	1.09
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.47	0.93
1:A:82:VAL:HG13	1:A:134:VAL:HB	1.51	0.93
1:A:78:ARG:HE	1:A:108:ARG:HE	1.16	0.92
1:A:352:ASP:OD2	1:A:355:SER:HB2	1.70	0.92
1:B:223:PHE:O	1:B:227:VAL:HG23	1.70	0.91
1:A:472:CYS:HB3	1:A:538:ALA:HB2	1.52	0.91
1:A:337:ILE:HB	1:B:600:ALA:HB1	1.52	0.91
1:A:245:TYR:OH	1:A:357:LYS:HD3	1.73	0.89
1:B:527:PRO:O	1:B:625:ALA:HB1	1.74	0.88
1:A:289:ASN:ND2	1:A:497:LYS:O	2.07	0.87
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.57	0.86
1:B:167:LYS:CB	1:B:200:ILE:HD11	2.06	0.85
1:B:227:VAL:HG13	1:B:231:PHE:CD2	2.12	0.84
1:B:227:VAL:HG13	1:B:231:PHE:CE2	2.13	0.84
1:A:634:ARG:HB3	1:A:634:ARG:HH11	1.43	0.82
1:B:152:PHE:CZ	1:B:156:LEU:HD11	2.15	0.82
1:B:262:GLU:HG2	1:B:269:TYR:HB2	1.61	0.81
1:B:541:MET:O	1:B:545:GLN:HG3	1.81	0.81
1:A:500:ALA:HB2	1:A:506:ARG:N	1.96	0.81
1:B:292:LEU:HD11	1:B:302:HIS:HB2	1.61	0.81
1:A:678:SER:HB2	6:A:925:HOH:O	1.82	0.79
1:B:529:ILE:HD13	1:B:616:LEU:HD22	1.66	0.78
1:A:384:ASN:O	1:A:388:GLU:HG2	1.83	0.78
1:B:581:ARG:HB2	6:B:898:HOH:O	1.84	0.78
1:B:404:LYS:HE2	1:B:407:SER:OG	1.85	0.77
1:B:188:VAL:O	1:B:192:LEU:HG	1.83	0.77
1:A:159:THR:OG1	1:A:161:VAL:HG13	1.83	0.77
1:A:217:ILE:HD11	1:A:383:THR:OG1	1.85	0.76
1:B:190:GLN:O	1:B:194:GLN:HG3	1.86	0.76
1:B:321:ALA:HB2	1:B:455:TYR:CE1	2.20	0.76
1:B:175:ASN:OD1	1:B:177:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HD12	1:A:132:LEU:O	1.85	0.74
1:A:78:ARG:NE	1:A:108:ARG:HE	1.84	0.74
1:B:175:ASN:O	1:B:181:PHE:CD1	2.41	0.74
1:A:79:ASN:OD1	1:A:107:MET:HE3	1.86	0.74
1:B:403:HIS:HB3	6:B:903:HOH:O	1.88	0.73
1:A:127:GLU:HB2	6:A:805:HOH:O	1.88	0.73
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.24	0.73
1:B:615:HIS:O	1:B:619:LEU:HD22	1.89	0.72
1:A:168:PHE:O	1:A:200:ILE:HG22	1.90	0.71
1:A:253:MET:HE3	1:A:254:ASP:H	1.55	0.71
1:B:286:VAL:HG23	1:B:507:ALA:O	1.91	0.70
1:B:80:ILE:HD11	1:B:107:MET:HB3	1.73	0.69
1:B:533:PRO:HG3	1:B:636:MET:HG3	1.74	0.69
1:A:354:GLU:O	6:A:801:HOH:O	2.09	0.68
1:B:247:LEU:HD22	1:B:442:ASP:CG	2.18	0.68
1:B:245:TYR:HB3	1:B:348:LEU:HB3	1.75	0.68
1:A:190:GLN:O	1:A:194:GLN:HG3	1.94	0.68
1:A:667:MET:HG2	1:A:672:TYR:HB3	1.74	0.68
1:B:616:LEU:HA	1:B:619:LEU:HD23	1.76	0.68
1:A:664:LYS:HA	1:A:667:MET:HE2	1.76	0.68
1:B:352:ASP:OD1	1:B:354:GLU:HB2	1.94	0.68
1:B:537:ILE:HG13	1:B:541:MET:HG2	1.75	0.68
1:B:175:ASN:O	1:B:181:PHE:HB2	1.94	0.67
1:B:213:GLU:O	1:B:217:ILE:HG13	1.95	0.67
1:A:388:GLU:HB2	1:A:447:LEU:HD11	1.76	0.67
1:B:300:LEU:HD12	1:B:300:LEU:N	2.11	0.66
1:A:76:THR:OG1	1:A:78:ARG:HD3	1.96	0.66
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.78	0.66
1:A:573:TYR:CD2	1:A:576:ARG:HG3	2.31	0.66
1:A:135:PHE:CE2	1:A:192:LEU:HD11	2.32	0.65
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.31	0.65
1:B:382:ARG:HG2	6:B:825:HOH:O	1.95	0.65
1:A:321:ALA:HB2	1:A:455:TYR:CE1	2.30	0.65
1:B:167:LYS:HA	1:B:198:GLN:O	1.95	0.65
1:B:477:GLU:HG3	1:B:487:LYS:HD2	1.79	0.65
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.79	0.65
1:A:543:PHE:O	1:A:547:ARG:HG2	1.97	0.64
1:B:459:ALA:HA	1:B:538:ALA:O	1.98	0.64
1:A:330:LEU:O	1:A:334:ILE:HG13	1.96	0.64
1:A:527:PRO:HB2	1:A:625:ALA:CB	2.27	0.64
1:B:617:TRP:HZ3	1:B:648:VAL:HG22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:PRO:HD2	1:B:625:ALA:HB2	1.81	0.63
1:A:400:GLU:HG3	1:A:404:LYS:HE3	1.81	0.63
1:A:459:ALA:HB2	1:A:538:ALA:HB1	1.80	0.63
1:A:561:LEU:N	1:A:561:LEU:HD12	2.13	0.63
1:A:655:GLU:O	1:A:657:THR:N	2.31	0.63
1:B:304:GLU:HG2	1:B:470:HIS:CD2	2.34	0.62
1:B:674:LEU:N	1:B:674:LEU:HD12	2.14	0.62
1:A:634:ARG:HH11	1:A:634:ARG:CB	2.10	0.62
1:B:663:VAL:HA	1:B:666:LEU:HD12	1.82	0.62
1:B:664:LYS:O	1:B:668:THR:HG23	1.99	0.62
1:A:262:GLU:HG2	6:A:930:HOH:O	1.98	0.61
1:B:74:LYS:O	1:B:74:LYS:HD3	2.00	0.61
1:B:87:GLN:HG3	1:B:146:THR:HB	1.82	0.61
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.82	0.61
1:A:642:ASN:HA	1:A:645:TYR:CD2	2.36	0.60
1:A:655:GLU:O	1:A:656:HIS:C	2.42	0.60
1:B:551:ARG:HG3	1:B:557:VAL:HG21	1.83	0.60
1:A:80:ILE:HD11	1:A:134:VAL:HG23	1.82	0.60
1:A:337:ILE:CB	1:B:600:ALA:HB1	2.29	0.60
1:B:227:VAL:CG1	1:B:231:PHE:CD2	2.85	0.60
1:B:227:VAL:CG1	1:B:231:PHE:HD2	2.15	0.60
1:B:527:PRO:HB2	1:B:625:ALA:CB	2.32	0.60
1:A:551:ARG:HG2	1:A:557:VAL:HG21	1.84	0.59
1:A:551:ARG:HG2	1:A:557:VAL:CG2	2.32	0.59
1:B:563:TYR:CE2	1:B:609:LEU:HD23	2.38	0.59
1:A:357:LYS:O	1:A:357:LYS:HG2	2.02	0.59
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.38	0.59
1:A:568:ARG:HD2	1:A:571:GLU:CD	2.27	0.58
1:B:472:CYS:HB3	1:B:538:ALA:HB2	1.85	0.58
1:B:666:LEU:HD23	1:B:671:ARG:NH1	2.17	0.58
1:A:600:ALA:HB2	1:B:336:GLU:CG	2.34	0.58
1:A:549:TRP:O	1:A:553:GLN:HG2	2.04	0.58
1:B:175:ASN:C	1:B:181:PHE:CD1	2.81	0.58
1:A:300:LEU:HD23	1:A:574:LEU:HD21	1.86	0.58
1:A:291:LYS:HD2	1:A:299:HIS:CE1	2.39	0.57
1:A:593:VAL:O	1:A:608:LEU:HD11	2.04	0.57
1:B:71:GLU:HG3	1:B:72:LYS:N	2.19	0.57
1:B:660:VAL:HG12	1:B:664:LYS:HE2	1.85	0.57
1:A:342:LEU:HA	1:A:367:TYR:HB2	1.86	0.57
1:B:540:PHE:HA	1:B:543:PHE:HB2	1.87	0.57
1:A:163:LEU:HD22	1:A:166:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ARG:HH11	1:A:576:ARG:HB3	1.70	0.57
1:B:79:ASN:H	1:B:79:ASN:ND2	2.02	0.57
1:A:660:VAL:HG12	1:A:664:LYS:HD2	1.85	0.57
1:A:491:THR:HG23	3:A:702:FAD:O1P	2.05	0.56
1:A:276:PHE:CG	1:A:282:PHE:HB2	2.41	0.56
1:A:279:LYS:HE3	6:A:947:HOH:O	2.05	0.56
1:A:105:TYR:CD1	1:A:228:CYS:SG	2.99	0.56
1:A:422:GLU:OE2	1:A:481:LYS:HE3	2.06	0.56
1:A:636:MET:CE	1:A:640:VAL:HG21	2.36	0.56
1:A:87:GLN:OE1	1:A:87:GLN:HA	2.06	0.56
1:B:152:PHE:CZ	1:B:156:LEU:CD1	2.88	0.56
1:A:176:LYS:HG3	1:A:207:ASP:CG	2.31	0.56
1:A:529:ILE:HD13	1:A:616:LEU:HD22	1.87	0.56
1:B:169:ALA:CB	1:B:223:PHE:HE1	2.19	0.56
1:A:472:CYS:HB3	1:A:538:ALA:CB	2.32	0.56
1:A:472:CYS:CB	1:A:538:ALA:HB2	2.31	0.55
1:B:352:ASP:C	1:B:354:GLU:H	2.13	0.55
1:B:559:GLU:OE1	1:B:619:LEU:HD11	2.06	0.55
1:B:570:ASP:HB3	6:B:880:HOH:O	2.05	0.55
1:A:81:ILE:HG23	1:A:81:ILE:O	2.05	0.55
1:A:321:ALA:HB3	1:A:512:PHE:CE1	2.41	0.55
1:A:400:GLU:OE2	1:A:404:LYS:HE3	2.06	0.55
1:A:564:TYR:CG	1:A:565:GLY:N	2.73	0.55
1:A:159:THR:HG1	1:A:161:VAL:HG13	1.71	0.55
1:B:404:LYS:HE2	1:B:407:SER:HG	1.69	0.55
1:A:100:LYS:HZ2	1:A:244:GLN:HG2	1.72	0.55
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.87	0.55
1:B:258:VAL:CG1	1:B:365:THR:HA	2.36	0.55
1:A:243:ARG:HH22	1:A:442:ASP:CB	2.20	0.55
1:B:281:PRO:HD2	6:B:870:HOH:O	2.07	0.55
1:B:347:SER:HB3	1:B:363:CYS:HB3	1.89	0.55
1:B:175:ASN:O	1:B:181:PHE:HD1	1.88	0.54
1:B:310:SER:O	1:B:311:LYS:HB2	2.06	0.54
1:B:227:VAL:HG13	1:B:231:PHE:HD2	1.66	0.54
1:A:80:ILE:HG23	1:A:109:GLY:CA	2.36	0.54
1:B:68:SER:O	1:B:71:GLU:HG2	2.07	0.54
1:B:493:TRP:CH2	1:B:509:VAL:HG13	2.42	0.54
1:A:267:LYS:HA	6:A:930:HOH:O	2.06	0.54
1:A:600:ALA:HB2	1:B:336:GLU:HG2	1.88	0.54
1:A:484:ARG:N	1:A:484:ARG:HD2	2.23	0.54
1:B:258:VAL:HG13	1:B:365:THR:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ALA:HA	1:B:508:LEU:HD23	1.90	0.54
1:A:475:ALA:HA	1:A:491:THR:HB	1.90	0.53
1:B:120:ALA:HA	1:B:155:TRP:CE2	2.42	0.53
1:B:346:MET:HE3	1:B:365:THR:O	2.08	0.53
1:B:559:GLU:HB3	1:B:561:LEU:HD21	1.89	0.53
1:A:249:VAL:HG12	1:A:250:HIS:N	2.24	0.53
1:B:441:ILE:HG22	6:B:820:HOH:O	2.08	0.53
1:B:456:TYR:HB3	1:B:471:ILE:HG23	1.90	0.53
1:B:592:ASN:HB3	1:B:608:LEU:HD13	1.91	0.53
1:B:614:GLU:O	1:B:614:GLU:HG3	2.06	0.53
1:A:300:LEU:N	1:A:300:LEU:HD12	2.24	0.53
1:A:577:GLU:OE1	1:A:577:GLU:N	2.42	0.53
1:B:188:VAL:O	1:B:188:VAL:HG12	2.08	0.53
1:B:358:LYS:H	1:B:358:LYS:HD2	1.73	0.53
1:B:175:ASN:H	1:B:181:PHE:HD1	1.56	0.53
1:A:300:LEU:CD2	1:A:574:LEU:HD21	2.39	0.53
1:A:179:GLU:CD	1:A:667:MET:HE1	2.33	0.53
1:A:243:ARG:HH22	1:A:442:ASP:HB3	1.74	0.53
1:B:69:PHE:HD1	1:B:69:PHE:H	1.56	0.53
1:A:152:PHE:CE2	1:A:156:LEU:HD11	2.44	0.53
1:A:345:ILE:HG12	1:A:366:THR:HG22	1.89	0.53
1:B:227:VAL:HG13	1:B:231:PHE:HE2	1.69	0.53
1:B:295:GLY:HA3	5:B:704:PO4:P	2.49	0.53
1:A:438:ARG:HB3	6:A:905:HOH:O	2.09	0.53
1:B:168:PHE:CE1	1:B:199:ARG:HB2	2.43	0.53
1:B:259:TYR:CD2	1:B:362:PRO:HB3	2.45	0.52
1:A:245:TYR:HB2	1:A:446:GLU:HG3	1.91	0.52
1:B:168:PHE:CD1	1:B:168:PHE:C	2.86	0.52
1:A:568:ARG:HD2	1:A:571:GLU:OE1	2.10	0.52
1:A:356:ASN:O	1:A:358:LYS:HG2	2.09	0.52
1:A:94:PHE:CD2	1:A:173:LEU:HD21	2.45	0.52
1:A:79:ASN:O	1:A:131:SER:HA	2.10	0.52
1:B:323:TYR:CE1	1:B:453:ALA:HB2	2.44	0.52
1:B:619:LEU:HD22	1:B:619:LEU:H	1.75	0.52
1:B:80:ILE:HD12	1:B:80:ILE:N	2.24	0.52
1:A:457:SER:O	1:A:458:ILE:C	2.53	0.52
1:A:464:VAL:HG12	1:A:465:HIS:CE1	2.45	0.51
1:B:493:TRP:CZ3	1:B:509:VAL:HG13	2.46	0.51
1:B:317:GLY:HA3	1:B:518:PHE:O	2.10	0.51
1:A:335:GLY:HA3	1:A:342:LEU:HD21	1.92	0.51
1:B:115:GLU:HB2	1:B:148:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG13	1:A:628:TYR:CE1	2.46	0.51
1:A:568:ARG:NH1	6:A:804:HOH:O	2.39	0.51
1:B:184:MET:HE3	1:B:188:VAL:HG21	1.91	0.51
1:B:191:ARG:HD2	1:B:195:LEU:HD11	1.91	0.51
1:B:302:HIS:HD1	1:B:575:TYR:HE1	1.57	0.51
1:A:393:ALA:HB1	1:A:436:SER:OG	2.11	0.51
1:B:91:ALA:HB2	1:B:173:LEU:HD22	1.93	0.51
1:A:173:LEU:HD12	1:A:173:LEU:N	2.26	0.51
1:A:637:ALA:HB2	1:A:676:VAL:HG11	1.94	0.50
1:B:74:LYS:HD3	1:B:74:LYS:C	2.35	0.50
1:B:528:VAL:HG23	1:B:528:VAL:O	2.10	0.50
1:A:246:GLU:O	1:A:348:LEU:HA	2.11	0.50
1:A:272:GLN:OE1	1:A:282:PHE:HA	2.11	0.50
1:A:135:PHE:HB2	1:A:170:VAL:HG22	1.93	0.50
1:A:559:GLU:HB3	1:A:561:LEU:HD11	1.93	0.50
1:A:175:ASN:HB3	1:A:178:TYR:HD2	1.77	0.50
1:B:393:ALA:HB3	1:B:399:GLN:HB2	1.93	0.50
1:B:395:GLU:H	1:B:436:SER:HB2	1.77	0.50
1:B:211:ASN:O	1:B:215:ASP:HB2	2.11	0.50
1:B:246:GLU:O	1:B:348:LEU:HA	2.11	0.50
1:B:608:LEU:O	1:B:611:ARG:HB3	2.12	0.50
1:B:167:LYS:CB	1:B:200:ILE:CD1	2.86	0.50
1:A:119:LEU:HG	1:A:152:PHE:CD1	2.47	0.50
1:B:583:HIS:HA	1:B:588:LEU:HB3	1.93	0.50
1:A:96:ASN:O	1:A:100:LYS:HG3	2.11	0.49
1:B:95:ALA:HB1	1:B:111:SER:OG	2.11	0.49
1:A:287:THR:HG21	1:A:306:ASP:HB2	1.94	0.49
1:B:69:PHE:HE1	1:B:121:ASP:HB2	1.76	0.49
1:B:620:ILE:HD11	1:B:627:ILE:HD11	1.94	0.49
1:B:673:SER:C	1:B:674:LEU:HD12	2.37	0.49
1:A:135:PHE:HE2	1:A:192:LEU:HD11	1.74	0.49
1:B:374:TYR:HA	6:B:845:HOH:O	2.13	0.49
1:B:527:PRO:CB	1:B:625:ALA:HB2	2.42	0.49
1:B:626:HIS:ND1	1:B:626:HIS:N	2.60	0.49
1:A:573:TYR:CE2	1:A:576:ARG:HG3	2.47	0.49
1:B:308:SER:O	1:B:309:ASP:HB2	2.13	0.49
1:A:550:LEU:O	1:A:555:LYS:HB2	2.13	0.49
1:A:636:MET:CE	1:A:640:VAL:CG2	2.90	0.49
1:B:302:HIS:ND1	1:B:575:TYR:HE1	2.11	0.49
1:B:618:LYS:HG2	6:B:872:HOH:O	2.12	0.49
1:B:136:CYS:HA	1:B:171:PHE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD22	1:B:191:ARG:HB3	1.94	0.49
1:B:214:GLU:OE1	1:B:413:LYS:HE3	2.13	0.49
1:A:668:THR:HG22	6:A:937:HOH:O	2.12	0.48
1:A:163:LEU:O	1:A:166:VAL:HG23	2.13	0.48
1:A:253:MET:CE	1:A:254:ASP:H	2.23	0.48
1:B:73:MET:O	1:B:77:GLY:N	2.46	0.48
1:B:168:PHE:CE2	1:B:192:LEU:HB2	2.48	0.48
1:B:291:LYS:HE3	1:B:293:ASN:O	2.13	0.48
1:B:221:GLU:O	1:B:225:PRO:HG2	2.13	0.48
1:B:222:GLN:C	1:B:225:PRO:HD2	2.37	0.48
1:B:425:ARG:HG3	1:B:425:ARG:HH11	1.77	0.48
1:A:74:LYS:NZ	6:A:805:HOH:O	2.46	0.48
1:A:415:LEU:HD12	1:A:419:TRP:HB2	1.95	0.48
1:A:569:SER:HB3	1:A:595:PHE:CZ	2.47	0.48
1:B:219:TRP:O	1:B:222:GLN:N	2.44	0.48
1:A:69:PHE:CE1	1:A:121:ASP:HB2	2.49	0.48
1:A:567:ARG:HA	1:A:596:SER:OG	2.13	0.48
1:B:76:THR:HG22	1:B:78:ARG:HE	1.79	0.48
1:B:105:TYR:HD1	1:B:235:ALA:HA	1.79	0.48
1:A:401:HIS:O	1:A:405:MET:HG2	2.13	0.48
1:B:172:GLY:C	1:B:182:ASN:HD21	2.21	0.48
1:B:568:ARG:HG3	1:B:571:GLU:HB2	1.96	0.48
1:B:665:LYS:O	1:B:669:LYS:HG3	2.13	0.48
1:B:341:ASP:O	1:B:344:VAL:HG23	2.13	0.48
1:A:588:LEU:HD13	1:A:591:LEU:HD13	1.96	0.48
1:A:147:ASP:HB2	6:A:884:HOH:O	2.13	0.48
1:B:118:ASP:OD2	1:B:120:ALA:HB3	2.14	0.48
1:B:151:ASP:O	1:B:152:PHE:C	2.55	0.48
1:A:100:LYS:HZ2	1:A:244:GLN:CG	2.26	0.47
1:A:101:ASP:HB3	1:A:224:TRP:CE2	2.49	0.47
1:A:291:LYS:HD2	1:A:299:HIS:ND1	2.28	0.47
1:A:338:LEU:CD2	1:A:439:PRO:HD2	2.44	0.47
1:B:98:LEU:C	1:B:100:LYS:H	2.22	0.47
1:A:151:ASP:HB2	6:A:822:HOH:O	2.13	0.47
1:B:135:PHE:HB2	1:B:170:VAL:HG22	1.96	0.47
1:A:262:GLU:CG	6:A:930:HOH:O	2.60	0.47
1:B:247:LEU:HD22	1:B:442:ASP:CB	2.44	0.47
1:B:383:THR:HB	1:B:406:ALA:HA	1.94	0.47
1:B:645:TYR:HD1	1:B:663:VAL:HG21	1.78	0.47
1:A:80:ILE:HD13	1:A:132:LEU:HB3	1.97	0.47
1:A:286:VAL:CG2	1:A:509:VAL:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASN:N	1:B:181:PHE:HD1	2.12	0.47
1:A:588:LEU:CD1	1:A:591:LEU:HD13	2.44	0.47
1:A:600:ALA:HB2	1:B:336:GLU:CD	2.40	0.47
1:B:175:ASN:O	1:B:181:PHE:CB	2.63	0.47
1:B:551:ARG:C	1:B:553:GLN:H	2.23	0.47
1:B:666:LEU:CD2	1:B:671:ARG:NH1	2.77	0.47
1:A:423:ALA:O	1:A:482:SER:HB3	2.15	0.47
1:A:310:SER:O	1:A:311:LYS:HB2	2.14	0.47
1:A:393:ALA:HA	1:A:436:SER:O	2.15	0.47
1:B:410:GLY:O	1:B:411:GLU:C	2.57	0.47
1:A:636:MET:HE2	1:A:640:VAL:CG2	2.45	0.46
1:B:146:THR:O	1:B:149:ALA:N	2.40	0.46
1:B:176:LYS:O	1:B:177:THR:C	2.58	0.46
1:B:462:SER:O	1:B:466:PRO:HD3	2.15	0.46
1:A:314:TYR:CD1	1:A:314:TYR:C	2.93	0.46
1:B:199:ARG:HB2	1:B:199:ARG:NH1	2.31	0.46
1:A:418:SER:HA	1:A:422:GLU:HB3	1.97	0.46
1:A:338:LEU:HD22	1:A:439:PRO:HD2	1.96	0.46
1:B:618:LYS:NZ	1:B:618:LYS:HB3	2.31	0.46
1:B:103:HIS:O	1:B:103:HIS:ND1	2.49	0.46
1:B:169:ALA:CB	1:B:223:PHE:CE1	2.98	0.46
1:B:190:GLN:HA	1:B:190:GLN:OE1	2.14	0.46
1:B:276:PHE:CG	1:B:282:PHE:HB2	2.51	0.46
1:B:567:ARG:HD3	1:B:597:ARG:CZ	2.46	0.46
1:B:615:HIS:CD2	1:B:619:LEU:HD21	2.51	0.46
1:B:79:ASN:H	1:B:79:ASN:HD22	1.64	0.46
1:B:98:LEU:HA	1:B:101:ASP:HB2	1.98	0.46
1:B:473:ALA:HA	3:B:702:FAD:O2	2.16	0.46
1:B:103:HIS:HA	1:B:107:MET:O	2.16	0.46
1:B:352:ASP:C	1:B:354:GLU:N	2.74	0.46
1:A:361:PHE:HB2	1:A:362:PRO:HD2	1.98	0.45
1:B:283:LEU:HD12	1:B:283:LEU:N	2.31	0.45
1:A:120:ALA:HA	1:A:155:TRP:CZ2	2.51	0.45
1:A:246:GLU:HB3	1:A:351:LEU:CD2	2.45	0.45
1:A:295:GLY:HA3	5:A:704:PO4:P	2.56	0.45
1:B:79:ASN:OD1	1:B:107:MET:HB3	2.16	0.45
1:A:189:ASP:OD1	1:A:189:ASP:C	2.58	0.45
1:A:342:LEU:HD12	1:A:368:ARG:CZ	2.46	0.45
1:B:624:GLY:HA2	1:B:671:ARG:NH2	2.31	0.45
1:A:361:PHE:HB2	1:A:362:PRO:CD	2.46	0.45
1:A:533:PRO:HG3	1:A:636:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:C	1:B:80:ILE:HG13	2.42	0.45
1:B:526:THR:HA	1:B:527:PRO:HD3	1.83	0.45
1:B:527:PRO:CD	1:B:625:ALA:HB2	2.46	0.45
1:A:98:LEU:O	1:A:101:ASP:HB2	2.16	0.45
1:A:105:TYR:HD1	1:A:228:CYS:SG	2.39	0.45
1:A:288:ALA:HB3	1:A:304:GLU:HB2	1.97	0.45
1:B:315:GLU:HB2	1:B:519:ARG:NE	2.31	0.45
1:A:287:THR:CG2	1:A:306:ASP:HB2	2.47	0.45
1:A:391:GLN:HA	1:A:399:GLN:HE21	1.82	0.45
1:B:168:PHE:CE1	1:B:199:ARG:HG3	2.52	0.45
1:A:402:LEU:HD11	1:A:437:LEU:HD22	1.99	0.45
1:A:263:MET:HE1	1:A:450:ARG:NH2	2.32	0.44
1:B:84:TYR:O	1:B:84:TYR:CD1	2.70	0.44
1:B:214:GLU:CD	1:B:413:LYS:HE3	2.43	0.44
1:B:348:LEU:HD12	1:B:360:PRO:HG3	1.99	0.44
1:A:84:TYR:CD1	1:A:84:TYR:O	2.70	0.44
1:A:101:ASP:HB3	1:A:224:TRP:CZ2	2.53	0.44
1:B:530:MET:HE1	1:B:544:ILE:CG1	2.46	0.44
1:B:207:ASP:C	1:B:209:ASP:H	2.25	0.44
1:B:552:GLU:HG3	6:B:882:HOH:O	2.16	0.44
1:A:206:GLY:HA3	1:A:212:LEU:CD1	2.48	0.44
1:A:245:TYR:CD2	1:A:360:PRO:HD3	2.52	0.44
1:B:102:ALA:C	1:B:107:MET:O	2.61	0.44
1:B:247:LEU:HD12	1:B:248:VAL:N	2.32	0.44
1:A:119:LEU:N	1:A:119:LEU:HD22	2.33	0.44
1:A:125:LEU:N	1:A:126:PRO:CD	2.80	0.44
1:A:265:ARG:O	1:A:268:SER:HB3	2.17	0.44
1:B:122:LEU:O	1:B:122:LEU:HD23	2.17	0.44
1:B:168:PHE:CE1	1:B:199:ARG:CB	3.01	0.44
1:B:216:PHE:CD1	1:B:216:PHE:C	2.95	0.44
1:B:532:GLY:HA3	1:B:540:PHE:HE2	1.82	0.44
1:A:103:HIS:HA	1:A:107:MET:O	2.18	0.44
1:A:637:ALA:CB	1:A:676:VAL:HG11	2.48	0.44
1:A:444:LEU:O	1:A:448:LEU:HG	2.18	0.44
1:A:600:ALA:CB	1:B:336:GLU:HG2	2.48	0.44
1:B:84:TYR:CZ	1:B:92:GLU:HG3	2.53	0.44
1:B:245:TYR:CB	1:B:348:LEU:HB3	2.46	0.44
1:A:659:ALA:O	1:A:663:VAL:HG23	2.17	0.43
1:B:283:LEU:HG	1:B:510:PRO:HG3	2.00	0.43
1:B:314:TYR:O	1:B:462:SER:HB3	2.18	0.43
1:A:243:ARG:HH12	1:A:442:ASP:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PHE:O	1:B:362:PRO:C	2.62	0.43
1:A:371:LEU:HD23	1:A:375:LEU:HD12	1.99	0.43
1:B:303:LEU:N	1:B:303:LEU:HD12	2.34	0.43
3:B:702:FAD:HM81	6:B:869:HOH:O	2.19	0.43
1:A:530:MET:HB3	1:A:540:PHE:CD1	2.54	0.43
1:B:96:ASN:O	1:B:100:LYS:HD3	2.18	0.43
1:B:245:TYR:HA	1:B:349:ASN:O	2.19	0.43
1:A:253:MET:HE2	1:A:257:LYS:HB2	2.00	0.43
1:A:292:LEU:HD21	1:A:302:HIS:HB2	2.01	0.43
1:A:348:LEU:HD12	1:A:360:PRO:HG3	2.01	0.43
1:A:665:LYS:HE2	1:A:669:LYS:HE3	2.01	0.43
1:B:520:LEU:HD21	1:B:543:PHE:CG	2.53	0.43
1:A:392:TYR:CD2	1:A:439:PRO:HB3	2.53	0.43
1:A:636:MET:HE2	1:A:636:MET:O	2.19	0.43
1:B:98:LEU:C	1:B:100:LYS:N	2.74	0.43
1:B:138:ALA:HB3	1:B:146:THR:HG21	2.00	0.43
1:B:307:ILE:O	1:B:308:SER:C	2.61	0.43
1:A:520:LEU:HD11	1:A:543:PHE:HA	2.00	0.43
1:B:97:ARG:NE	1:B:384:ASN:HB3	2.34	0.43
1:B:524:SER:HB2	1:B:550:LEU:HD13	2.00	0.43
1:B:549:TRP:HA	1:B:552:GLU:OE1	2.18	0.43
1:A:152:PHE:CE1	1:A:156:LEU:HD21	2.54	0.43
1:A:145:PRO:HG3	1:A:184:MET:SD	2.59	0.43
1:A:435:PRO:HA	1:A:438:ARG:HH12	1.83	0.43
1:B:69:PHE:O	1:B:73:MET:HG3	2.18	0.43
1:B:203:LEU:HD12	1:B:204:GLY:H	1.84	0.43
1:A:155:TRP:C	1:A:157:GLN:N	2.76	0.42
1:A:291:LYS:HZ1	1:A:293:ASN:ND2	2.16	0.42
1:A:374:TYR:O	1:A:450:ARG:HD2	2.18	0.42
1:A:608:LEU:O	1:A:611:ARG:HB3	2.18	0.42
1:A:593:VAL:HG12	1:A:594:ALA:N	2.34	0.42
1:B:266:LEU:O	1:B:267:LYS:HB2	2.17	0.42
1:B:635:ASN:O	1:B:636:MET:C	2.61	0.42
1:B:146:THR:O	1:B:147:ASP:C	2.62	0.42
1:B:248:VAL:HG12	1:B:250:HIS:CE1	2.54	0.42
1:B:259:TYR:CE2	1:B:362:PRO:HB3	2.54	0.42
1:B:480:ALA:C	1:B:482:SER:N	2.77	0.42
1:A:327:ASP:OD1	1:A:327:ASP:C	2.62	0.42
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.35	0.42
1:B:254:ASP:OD1	1:B:254:ASP:O	2.37	0.42
1:B:376:ASP:HA	6:B:830:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:LEU:N	1:B:674:LEU:CD1	2.82	0.42
1:B:71:GLU:HG3	1:B:72:LYS:H	1.85	0.42
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.85	0.42
1:B:212:LEU:HD21	2:B:701:FMN:O4'	2.20	0.42
1:B:346:MET:SD	1:B:346:MET:C	3.03	0.42
1:B:475:ALA:HA	1:B:491:THR:HB	2.01	0.42
1:B:550:LEU:O	1:B:555:LYS:HB2	2.19	0.42
1:A:92:GLU:O	1:A:93:GLU:C	2.62	0.42
1:A:253:MET:HE3	1:A:253:MET:HA	2.01	0.42
1:A:308:SER:HA	1:A:467:ASN:OD1	2.19	0.42
1:A:440:PRO:C	1:A:442:ASP:N	2.77	0.42
1:A:526:THR:HA	1:A:527:PRO:HD3	1.91	0.42
1:A:647:ILE:O	1:A:651:PHE:HD1	2.03	0.42
1:B:208:ASP:HB2	1:B:212:LEU:HD22	2.02	0.42
1:B:582:PHE:HB3	1:B:588:LEU:HB2	2.01	0.42
1:A:530:MET:HB3	1:A:540:PHE:CE1	2.54	0.42
1:A:636:MET:HE2	1:A:640:VAL:HG23	2.02	0.42
1:B:76:THR:HG21	1:B:78:ARG:NH2	2.35	0.42
1:A:129:ASP:O	1:A:130:LYS:C	2.63	0.42
1:A:564:TYR:OH	1:A:574:LEU:HG	2.19	0.42
1:B:669:LYS:HB3	1:B:669:LYS:HE2	1.83	0.42
1:A:535:THR:C	1:A:537:ILE:H	2.28	0.41
1:A:175:ASN:HB3	1:A:178:TYR:CD2	2.55	0.41
1:A:176:LYS:HB3	6:A:847:HOH:O	2.18	0.41
1:B:173:LEU:N	1:B:173:LEU:HD12	2.35	0.41
1:B:548:ALA:O	1:B:552:GLU:HG2	2.20	0.41
1:A:291:LYS:NZ	1:A:293:ASN:ND2	2.69	0.41
1:A:358:LYS:C	1:A:359:HIS:ND1	2.78	0.41
1:B:103:HIS:ND1	1:B:103:HIS:C	2.77	0.41
1:B:651:PHE:CD1	1:B:651:PHE:N	2.88	0.41
1:A:84:TYR:CE2	1:A:92:GLU:HG3	2.56	0.41
1:A:291:LYS:HD2	1:A:299:HIS:HD1	1.85	0.41
1:B:81:ILE:HG13	1:B:110:MET:HG3	2.02	0.41
1:B:321:ALA:HB2	1:B:455:TYR:HE1	1.77	0.41
1:B:405:MET:HE2	1:B:415:LEU:HD23	2.02	0.41
1:A:288:ALA:O	1:A:303:LEU:HA	2.20	0.41
1:A:440:PRO:C	1:A:442:ASP:H	2.28	0.41
1:B:84:TYR:CE2	1:B:92:GLU:HG3	2.55	0.41
1:B:169:ALA:HB2	1:B:223:PHE:HE1	1.85	0.41
1:A:136:CYS:HA	1:A:171:PHE:O	2.21	0.41
1:A:464:VAL:HG12	1:A:465:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PRO:HA	1:B:381:PRO:HD3	1.84	0.41
1:B:474:VAL:O	1:B:474:VAL:HG13	2.21	0.41
1:B:71:GLU:CG	1:B:72:LYS:N	2.82	0.41
1:B:168:PHE:CZ	1:B:199:ARG:HB2	2.55	0.41
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.86	0.41
1:A:400:GLU:CG	1:A:404:LYS:HE3	2.49	0.41
1:A:569:SER:HB3	1:A:595:PHE:CE1	2.55	0.41
1:B:199:ARG:CB	1:B:199:ARG:HH11	2.33	0.41
1:B:244:GLN:O	1:B:244:GLN:HG3	2.21	0.41
1:A:356:ASN:O	1:A:358:LYS:N	2.53	0.41
1:A:552:GLU:C	1:A:554:GLY:H	2.29	0.41
1:B:113:ASP:HB3	1:B:116:GLU:HG2	2.03	0.41
1:B:116:GLU:HA	6:B:907:HOH:O	2.20	0.41
1:B:300:LEU:N	1:B:300:LEU:CD1	2.82	0.41
1:B:410:GLY:O	1:B:412:GLY:N	2.54	0.41
1:B:644:PHE:C	1:B:646:ASP:N	2.78	0.41
1:B:665:LYS:HB3	1:B:665:LYS:HE2	1.85	0.41
1:A:290:ARG:HG2	1:A:302:HIS:HB3	2.03	0.41
1:B:253:MET:HE3	1:B:253:MET:HB2	1.89	0.41
1:A:316:SER:HB3	6:A:857:HOH:O	2.20	0.40
1:A:323:TYR:CE1	1:A:453:ALA:HB2	2.56	0.40
1:B:573:TYR:OH	1:B:593:VAL:HG21	2.21	0.40
1:B:635:ASN:HB2	6:B:822:HOH:O	2.20	0.40
1:A:528:VAL:HG13	1:A:628:TYR:HE1	1.85	0.40
1:B:302:HIS:CD2	1:B:302:HIS:C	2.99	0.40
1:B:439:PRO:HA	1:B:440:PRO:HD3	1.91	0.40
1:B:527:PRO:C	1:B:625:ALA:HB1	2.41	0.40
1:A:67:SER:O	1:A:68:SER:C	2.64	0.40
1:A:398:GLU:O	1:A:399:GLN:C	2.64	0.40
1:A:454:ARG:HA	6:A:886:HOH:O	2.19	0.40
1:A:576:ARG:HB3	1:A:576:ARG:NH1	2.35	0.40
1:B:398:GLU:OE2	1:B:436:SER:OG	2.32	0.40
1:B:411:GLU:H	1:B:411:GLU:HG2	1.53	0.40
1:A:67:SER:O	1:A:72:LYS:HE3	2.21	0.40
1:A:250:HIS:HB2	1:A:345:ILE:O	2.21	0.40
1:B:528:VAL:CG2	1:B:560:THR:HA	2.52	0.40
1:B:544:ILE:HG21	1:B:582:PHE:CD2	2.56	0.40
1:B:662:TYR:CD1	1:B:662:TYR:C	3.00	0.40
1:A:427:ILE:HG23	1:A:428:LEU:N	2.37	0.40

There are no symmetry-related clashes.

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	594/621 (96%)	546 (92%)	47 (8%)	1 (0%)	43	63
1	B	588/621 (95%)	532 (90%)	56 (10%)	0	100	100
All	All	1182/1242 (95%)	1078 (91%)	103 (9%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	GLU

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	514/531 (97%)	488 (95%)	26 (5%)	21	43
1	B	490/531 (92%)	458 (94%)	32 (6%)	15	32
All	All	1004/1062 (94%)	946 (94%)	58 (6%)	18	38

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	129	ASP
1	A	173	LEU
1	A	189	ASP
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	211	ASN
1	A	250	HIS
1	A	251	GLU
1	A	252	ASP
1	A	262	GLU
1	A	287	THR
1	A	290	ARG
1	A	297	GLU
1	A	320	VAL
1	A	324	PRO
1	A	327	ASP
1	A	384	ASN
1	A	418	SER
1	A	442	ASP
1	A	446	GLU
1	A	467	ASN
1	A	484	ARG
1	A	598	GLU
1	A	614	GLU
1	A	634	ARG
1	A	669	LYS
1	B	79	ASN
1	B	80	ILE
1	B	88	THR
1	B	90	THR
1	B	126	PRO
1	B	147	ASP
1	B	150	GLN
1	B	175	ASN
1	B	176	LYS
1	B	182	ASN
1	B	191	ARG
1	B	202	GLU
1	B	211	ASN
1	B	215	ASP
1	B	262	GLU
1	B	399	GLN
1	B	411	GLU
1	B	414	GLU
1	B	439	PRO
1	B	506	ARG
1	B	547	ARG

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Mol	Chain	Res	Type
1	B	561	LEU
1	B	577	GLU
1	B	585	ASP
1	B	589	THR
1	B	599	GLN
1	B	619	LEU
1	B	626	HIS
1	B	655	GLU
1	B	657	THR
1	B	658	GLN
1	B	674	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	399	GLN
1	A	553	GLN
1	A	601	HIS
1	B	150	GLN
1	B	157	GLN
1	B	211	ASN
1	B	250	HIS
1	B	333	GLN
1	B	356	ASN
1	B	401	HIS
1	B	545	GLN
1	B	642	ASN
1	B	656	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	701	-	33,33,33	2.68	13 (39%)	48,50,50	1.66	12 (25%)
3	FAD	B	702	-	58,58,58	2.31	13 (22%)	85,89,89	1.96	19 (22%)
2	FMN	A	701	-	33,33,33	2.56	13 (39%)	48,50,50	1.64	13 (27%)
5	PO4	B	705	-	4,4,4	1.71	1 (25%)	6,6,6	0.47	0
4	2AM	B	703	-	25,25,25	1.71	7 (28%)	38,38,38	2.13	11 (28%)
5	PO4	A	705	-	4,4,4	1.66	0	6,6,6	0.46	0
5	PO4	B	704	-	4,4,4	1.75	2 (50%)	6,6,6	0.42	0
3	FAD	A	702	-	58,58,58	2.32	14 (24%)	85,89,89	1.93	16 (18%)
5	PO4	A	704	-	4,4,4	1.76	1 (25%)	6,6,6	0.50	0
4	2AM	A	703	-	25,25,25	1.71	7 (28%)	38,38,38	2.16	13 (34%)

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	701	-	-	0/18/18/18	0/3/3/3
3	FAD	B	702	-	-	3/34/50/50	0/6/6/6
2	FMN	A	701	-	-	0/18/18/18	0/3/3/3
4	2AM	B	703	-	-	3/11/27/27	0/3/3/3
3	FAD	A	702	-	-	0/34/50/50	0/6/6/6
4	2AM	A	703	-	-	4/11/27/27	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C8A-N7A	8.62	1.48	1.31
3	B	702	FAD	C8A-N7A	8.53	1.48	1.31
2	A	701	FMN	C8M-C8	-6.89	1.38	1.51
2	B	701	FMN	C8M-C8	-6.74	1.38	1.51
3	A	702	FAD	C8A-N9A	6.26	1.48	1.37
3	B	702	FAD	C8A-N9A	6.18	1.48	1.37
3	B	702	FAD	C7M-C7	-6.16	1.39	1.51
3	A	702	FAD	C7M-C7	-6.13	1.39	1.51
3	B	702	FAD	C8M-C8	-6.12	1.39	1.51
3	A	702	FAD	C8M-C8	-6.10	1.39	1.51
2	B	701	FMN	C4A-N5	5.34	1.42	1.30
2	B	701	FMN	C10-N10	5.19	1.48	1.37
2	B	701	FMN	C9-C9A	5.15	1.48	1.39
2	A	701	FMN	C10-N10	5.01	1.48	1.37
2	A	701	FMN	C4A-N5	4.92	1.41	1.30
2	A	701	FMN	C9-C9A	4.39	1.46	1.39
2	A	701	FMN	C9A-C5A	4.32	1.48	1.41
2	B	701	FMN	C9A-N10	4.28	1.48	1.41
2	B	701	FMN	C9A-C5A	4.15	1.47	1.41
2	A	701	FMN	C9A-N10	4.09	1.48	1.41
2	A	701	FMN	C8-C7	3.92	1.50	1.40
3	A	702	FAD	C9A-N10	-3.84	1.34	1.41
2	B	701	FMN	C8-C7	3.79	1.50	1.40
3	B	702	FAD	C9A-N10	-3.79	1.34	1.41
4	B	703	2AM	C2-N3	3.63	1.40	1.33
3	A	702	FAD	C2A-N1A	3.63	1.40	1.33
4	B	703	2AM	C2-N1	3.62	1.40	1.33
3	A	702	FAD	C2A-N3A	3.62	1.40	1.33
3	A	702	FAD	C10-N1	3.61	1.40	1.33
3	B	702	FAD	C10-N1	3.61	1.40	1.33
3	B	702	FAD	C2A-N3A	3.60	1.40	1.33
4	A	703	2AM	C2-N1	3.60	1.40	1.33
4	A	703	2AM	C2-N3	3.59	1.40	1.33
3	B	702	FAD	C2A-N1A	3.55	1.40	1.33
2	B	701	FMN	C10-N1	3.50	1.40	1.33
4	A	703	2AM	C5-C4	-3.12	1.33	1.39
4	A	703	2AM	C5-N7	-3.09	1.33	1.39
4	B	703	2AM	C5-C4	-3.08	1.33	1.39
4	B	703	2AM	C5-N7	-3.03	1.33	1.39
3	B	702	FAD	C5A-N7A	-3.03	1.33	1.39
3	A	702	FAD	C5A-N7A	-2.98	1.33	1.39
2	B	701	FMN	C6-C5A	2.94	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C5A-C4A	-2.93	1.33	1.39
2	A	701	FMN	C10-N1	2.89	1.39	1.33
3	A	702	FAD	C5A-C4A	-2.87	1.34	1.39
2	A	701	FMN	C4'-C3'	2.83	1.58	1.53
2	A	701	FMN	C1'-C2'	2.76	1.56	1.52
3	B	702	FAD	C5X-N5	-2.74	1.34	1.39
3	A	702	FAD	C5A-C6A	-2.67	1.33	1.41
2	B	701	FMN	C4'-C3'	2.67	1.58	1.53
3	A	702	FAD	C5X-N5	-2.66	1.34	1.39
4	A	703	2AM	C5-C6	-2.66	1.33	1.41
4	B	703	2AM	C5-C6	-2.65	1.33	1.41
3	B	702	FAD	C5A-C6A	-2.65	1.33	1.41
2	B	701	FMN	O2'-C2'	2.60	1.48	1.43
2	A	701	FMN	C6-C5A	2.42	1.43	1.40
4	B	703	2AM	C8-N9	-2.38	1.33	1.37
4	A	703	2AM	C8-N9	-2.38	1.33	1.37
5	A	704	PO4	P-O2	-2.21	1.48	1.54
2	A	701	FMN	C7M-C7	2.20	1.55	1.51
2	B	701	FMN	C6-C7	2.18	1.42	1.39
4	A	703	2AM	C4-N9	-2.08	1.33	1.37
2	A	701	FMN	O2'-C2'	2.08	1.47	1.43
4	B	703	2AM	C4-N9	-2.07	1.33	1.37
3	A	702	FAD	P-O3P	2.07	1.61	1.59
5	B	704	PO4	P-O2	-2.06	1.48	1.54
5	B	704	PO4	P-O4	-2.04	1.48	1.54
5	B	705	PO4	P-O2	-2.03	1.48	1.54
2	B	701	FMN	C7M-C7	2.01	1.54	1.51
3	B	702	FAD	PA-O3P	2.01	1.61	1.59
3	A	702	FAD	PA-O3P	2.00	1.61	1.59

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N9A-C8A-N7A	-9.91	99.88	113.94
3	B	702	FAD	N9A-C8A-N7A	-9.31	100.72	113.94
3	B	702	FAD	N3A-C2A-N1A	-7.41	117.37	128.58
3	A	702	FAD	N3A-C2A-N1A	-7.40	117.38	128.58
4	B	703	2AM	N3-C2-N1	-7.08	117.86	128.58
4	A	703	2AM	N3-C2-N1	-6.99	118.00	128.58
3	B	702	FAD	C5A-C4A-N3A	-4.71	120.23	126.72
4	B	703	2AM	N9-C8-N7	-4.65	107.34	113.94
3	A	702	FAD	C5A-C4A-N3A	-4.54	120.47	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	2AM	N9-C8-N7	-4.51	107.54	113.94
3	B	702	FAD	C5A-C4A-N9A	4.37	110.57	105.81
4	B	703	2AM	C5-C4-N3	-4.24	120.88	126.72
2	A	701	FMN	C9A-C5A-N5	4.10	126.81	122.45
4	A	703	2AM	C5-C4-N3	-3.94	121.28	126.72
2	B	701	FMN	C9A-C5A-N5	3.93	126.62	122.45
3	B	702	FAD	C2A-N3A-C4A	3.69	120.85	111.83
3	A	702	FAD	C2A-N3A-C4A	3.59	120.59	111.83
2	B	701	FMN	O4'-C4'-C3'	-3.51	101.04	109.25
2	B	701	FMN	C4'-C3'-C2'	-3.49	107.77	113.57
2	A	701	FMN	C4'-C3'-C2'	-3.33	108.03	113.57
3	B	702	FAD	C5A-N7A-C8A	3.30	108.64	103.45
4	A	703	2AM	O4'-C1'-C2'	-3.29	100.92	106.59
4	B	703	2AM	C2-N3-C4	3.28	119.84	111.83
2	A	701	FMN	O4'-C4'-C3'	-3.27	101.59	109.25
3	B	702	FAD	C4-N3-C2	-3.24	119.89	125.64
4	B	703	2AM	C5-N7-C8	3.23	108.53	103.45
4	A	703	2AM	C2-N3-C4	3.11	119.42	111.83
3	A	702	FAD	C5A-N7A-C8A	3.08	108.28	103.45
4	A	703	2AM	C5-N7-C8	3.02	108.19	103.45
3	A	702	FAD	C4-N3-C2	-3.01	120.30	125.64
3	B	702	FAD	C5A-C6A-N6A	-3.00	115.85	123.29
3	A	702	FAD	C2B-C3B-C4B	-2.95	96.90	102.61
3	A	702	FAD	C5A-C6A-N6A	-2.93	116.02	123.29
2	B	701	FMN	C5A-C9A-N10	-2.93	115.32	117.97
2	B	701	FMN	O3P-P-O5'	-2.88	99.15	106.67
3	B	702	FAD	C4A-N9A-C8A	2.84	108.72	105.74
3	A	702	FAD	C10-C4X-N5	-2.82	119.04	124.81
4	A	703	2AM	C5-C6-N6	-2.80	116.35	123.29
3	B	702	FAD	C10-C4X-N5	-2.78	119.13	124.81
4	B	703	2AM	C5-C6-N6	-2.78	116.40	123.29
2	A	701	FMN	O4-C4-N3	-2.78	114.90	120.11
2	B	701	FMN	O4-C4-N3	-2.78	114.90	120.11
4	B	703	2AM	C4-N9-C8	2.74	108.62	105.74
2	A	701	FMN	C5A-C9A-N10	-2.72	115.51	117.97
3	B	702	FAD	C4X-C4-N3	2.61	119.89	113.25
4	A	703	2AM	C4-N9-C8	2.60	108.47	105.74
3	A	702	FAD	C4X-C4-N3	2.53	119.69	113.25
3	A	702	FAD	C5A-C4A-N9A	2.53	108.56	105.81
2	A	701	FMN	O2P-P-O1P	2.52	120.67	110.83
2	B	701	FMN	C8M-C8-C7	2.50	125.86	120.76
4	B	703	2AM	C6-C5-C4	2.46	120.54	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	O4-C4-C4X	-2.45	120.06	126.53
4	B	703	2AM	C4-C5-N7	-2.44	107.79	110.58
2	A	701	FMN	C8M-C8-C7	2.43	125.72	120.76
4	A	703	2AM	C6-C5-C4	2.42	120.48	117.18
2	A	701	FMN	C5A-N5-C4A	-2.40	114.21	118.09
2	B	701	FMN	C5A-N5-C4A	-2.37	114.26	118.09
3	B	702	FAD	O4-C4-C4X	-2.36	120.31	126.53
2	B	701	FMN	O2P-P-O1P	2.35	119.99	110.83
3	B	702	FAD	C9A-C5X-N5	-2.30	120.01	122.45
2	A	701	FMN	C8M-C8-C9	-2.28	115.56	119.57
3	A	702	FAD	C6A-C5A-C4A	2.28	120.29	117.18
3	B	702	FAD	C6A-C5A-C4A	2.28	120.29	117.18
3	B	702	FAD	C4'-C3'-C2'	-2.28	109.78	113.57
3	B	702	FAD	C2B-C3B-C4B	-2.26	98.24	102.61
4	A	703	2AM	C4'-O4'-C1'	-2.25	104.50	109.47
2	A	701	FMN	C6-C5A-N5	-2.24	114.72	118.44
4	A	703	2AM	C3'-C2'-C1'	-2.24	98.53	102.81
2	B	701	FMN	C9-C9A-N10	2.23	124.86	121.85
4	A	703	2AM	C4-C5-N7	-2.22	108.04	110.58
4	A	703	2AM	N3-C4-N9	2.22	130.94	127.17
2	A	701	FMN	C9-C9A-N10	2.21	124.83	121.85
2	A	701	FMN	O3P-P-O5'	-2.20	100.92	106.67
3	A	702	FAD	C4'-C3'-C2'	-2.20	109.92	113.57
4	B	703	2AM	C3'-C2'-C1'	-2.18	98.63	102.81
3	B	702	FAD	C4-C4X-C10	2.18	120.67	116.93
4	B	703	2AM	N3-C4-N9	2.15	130.82	127.17
2	B	701	FMN	C7M-C7-C6	-2.12	115.84	119.57
2	B	701	FMN	C8M-C8-C9	-2.12	115.84	119.57
3	A	702	FAD	C9A-C5X-N5	-2.11	120.21	122.45
2	A	701	FMN	C7M-C7-C6	-2.10	115.87	119.57
3	B	702	FAD	C5A-C6A-N1A	2.08	122.79	117.51
3	B	702	FAD	C5X-C9A-N10	2.05	119.82	117.97
3	A	702	FAD	C4-C4X-C10	2.01	120.38	116.93

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	2AM	C2'-C1'-N9-C8
4	A	703	2AM	C2'-C1'-N9-C4
4	B	703	2AM	C2'-C1'-N9-C4
4	A	703	2AM	C2'-C1'-N9-C8

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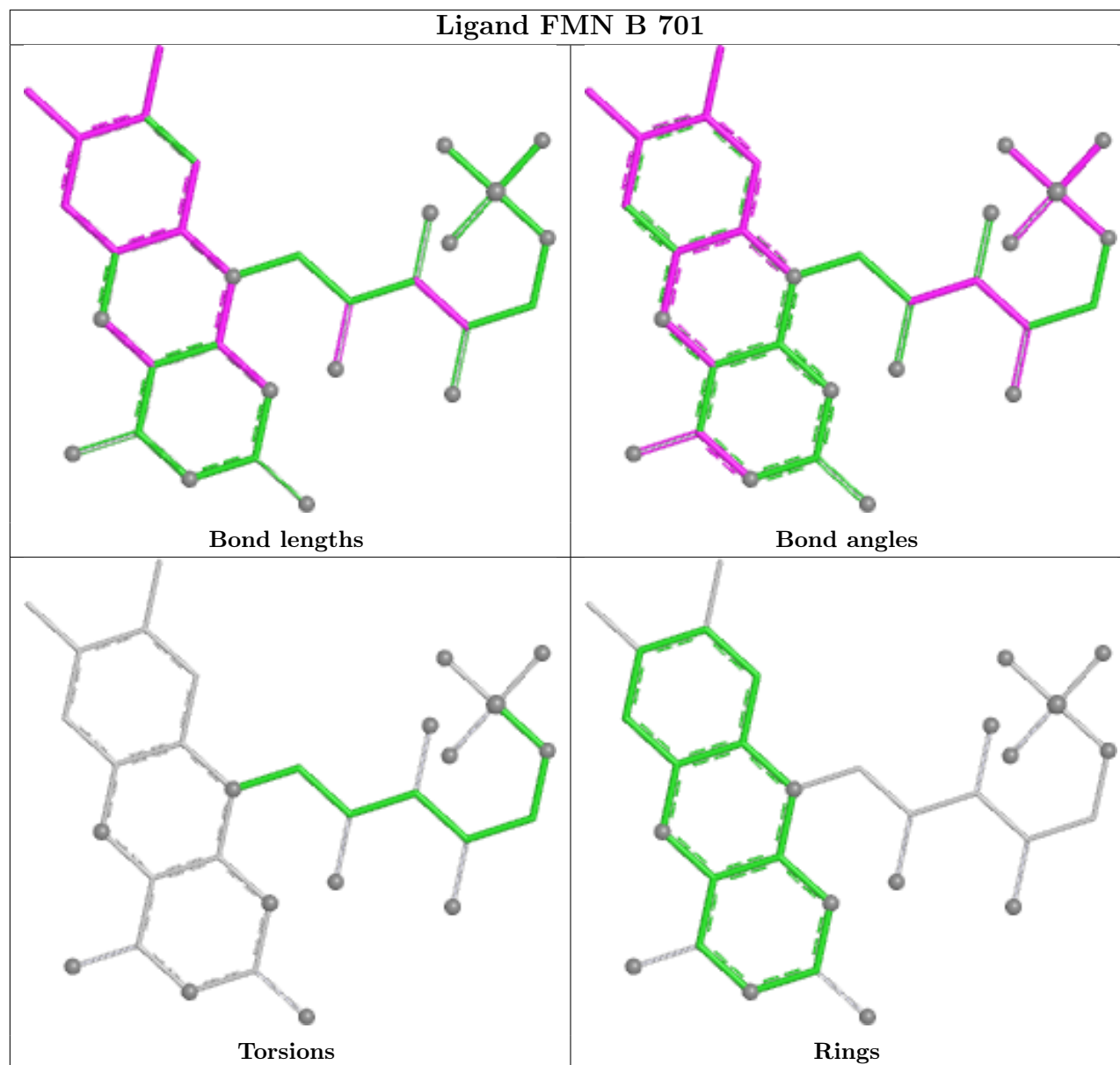
Mol	Chain	Res	Type	Atoms
3	B	702	FAD	PA-O3P-P-O1P
4	B	703	2AM	C2'-O2'-P-O1P
3	B	702	FAD	C5'-O5'-P-O1P
3	B	702	FAD	PA-O3P-P-O2P
4	A	703	2AM	O4'-C1'-N9-C8
4	A	703	2AM	C2'-O2'-P-O1P

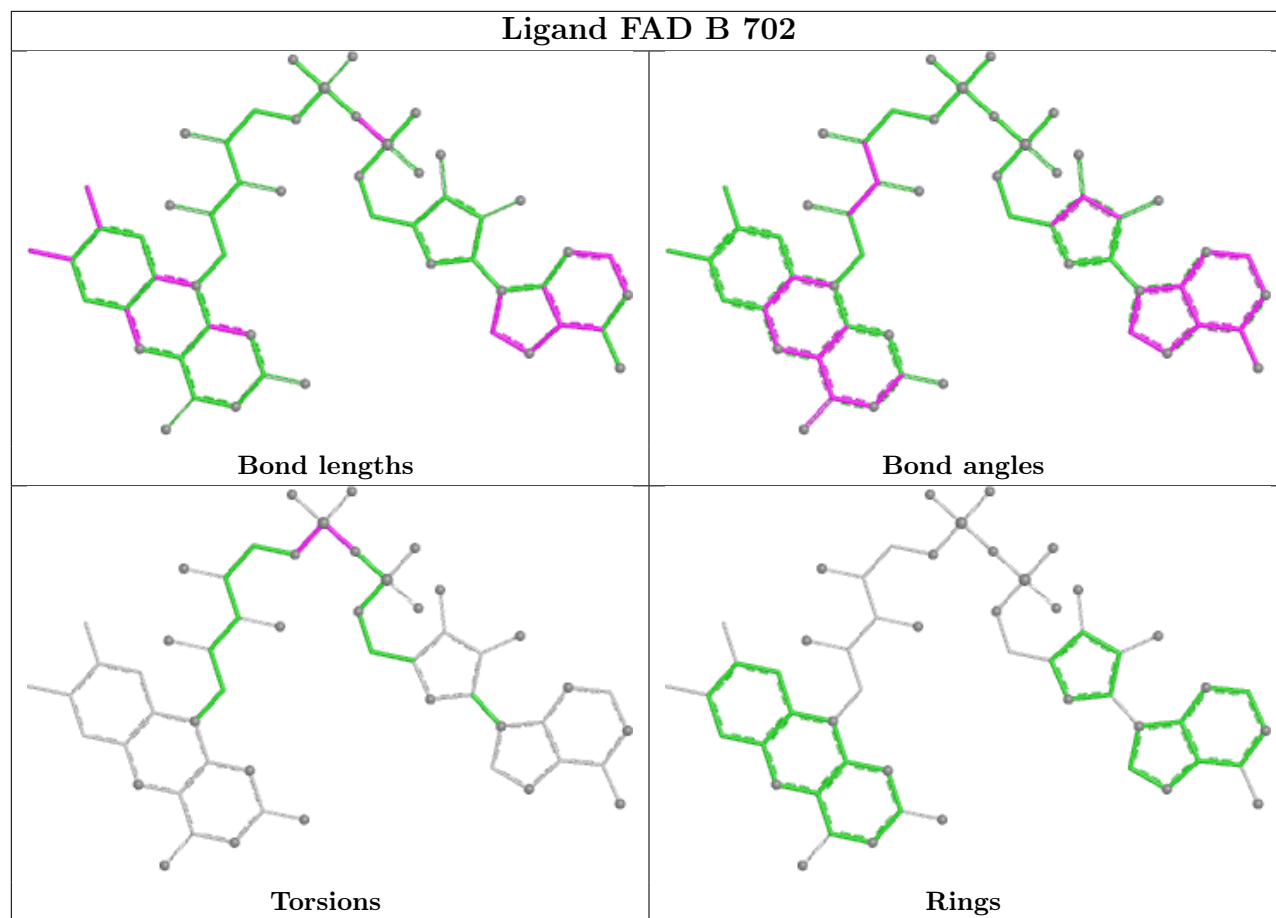
There are no ring outliers.

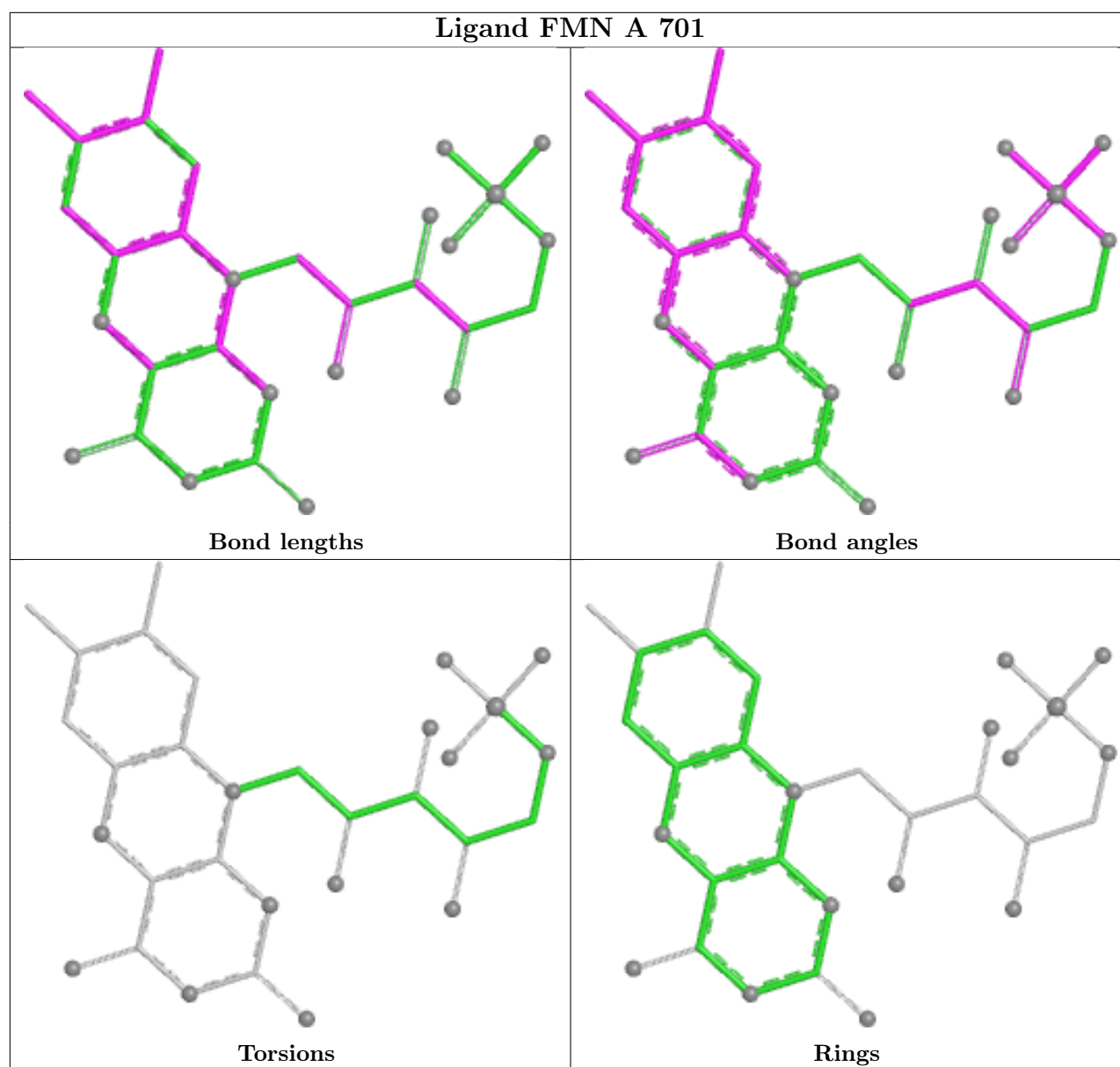
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FMN	1	0
3	B	702	FAD	2	0
5	B	704	PO4	1	0
3	A	702	FAD	1	0
5	A	704	PO4	1	0

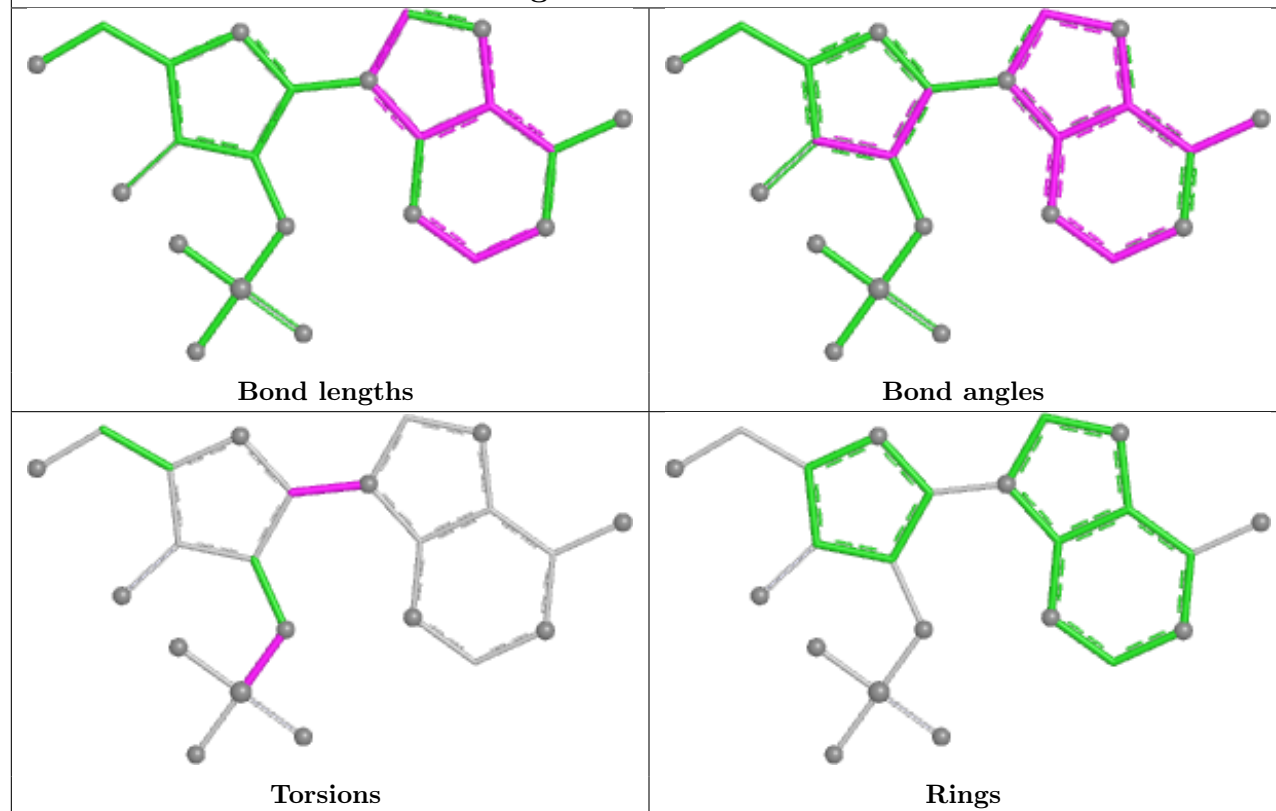
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



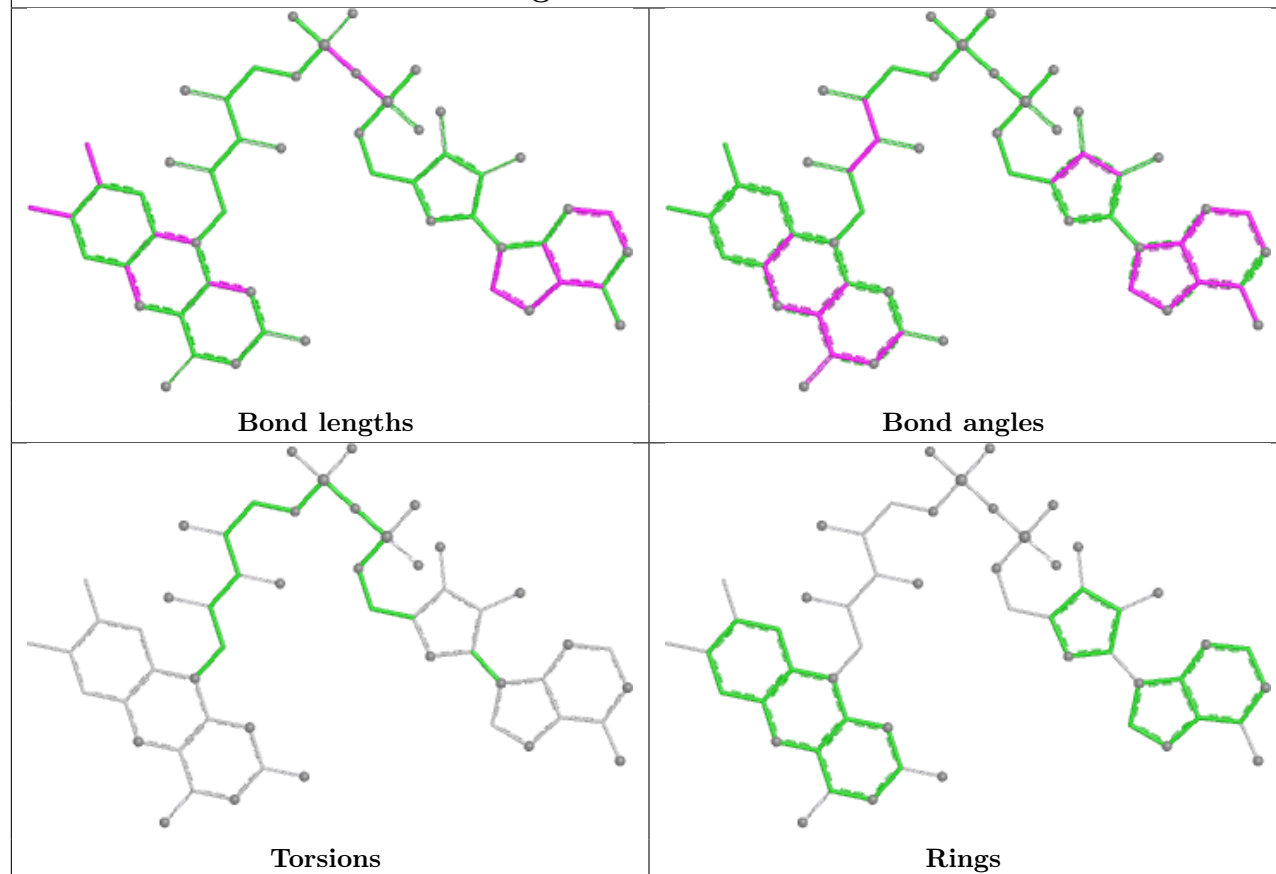


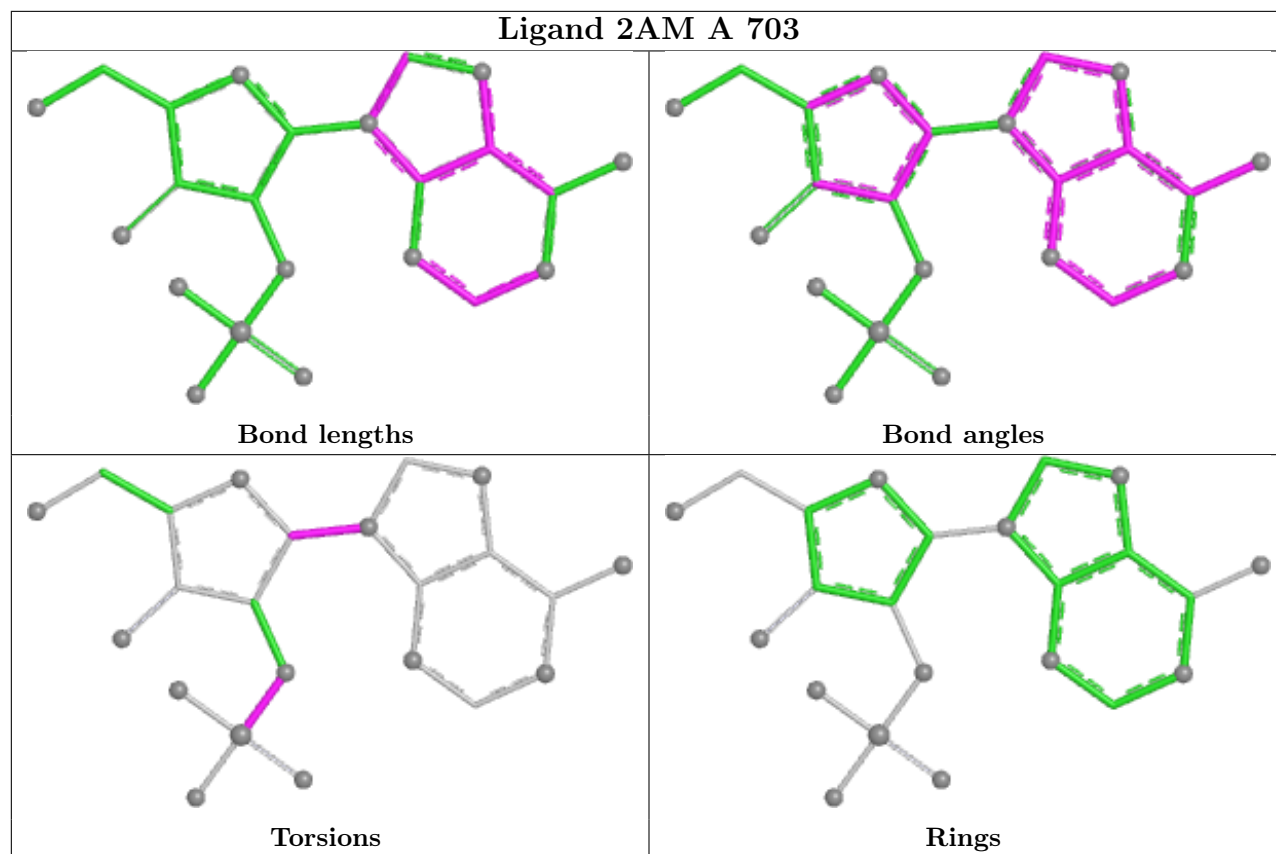


Ligand 2AM B 703



Ligand FAD A 702





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	602/621 (96%)	0.08	7 (1%) 76 73	26, 54, 78, 102	0
1	B	596/621 (95%)	0.33	23 (3%) 43 38	26, 61, 108, 133	0
All	All	1198/1242 (96%)	0.21	30 (2%) 58 54	26, 57, 103, 133	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	TYR	6.6
1	B	161	VAL	4.1
1	A	144	ASP	3.9
1	A	235	ALA	3.4
1	B	164	THR	3.4
1	B	160	ASP	3.2
1	B	139	THR	3.0
1	B	169	ALA	3.0
1	B	166	VAL	2.9
1	B	156	LEU	2.9
1	B	133	VAL	2.7
1	B	146	THR	2.7
1	B	233	VAL	2.6
1	A	538	ALA	2.6
1	B	162	ASP	2.6
1	B	158	GLU	2.5
1	B	136	CYS	2.5
1	B	223	PHE	2.5
1	A	656	HIS	2.4
1	B	235	ALA	2.4
1	B	159	THR	2.4
1	A	234	GLU	2.4
1	B	83	PHE	2.3
1	B	135	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	167	LYS	2.2
1	B	134	VAL	2.2
1	B	197	ALA	2.1
1	B	242	ILE	2.1
1	B	198	GLN	2.1
1	A	253	MET	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](#)

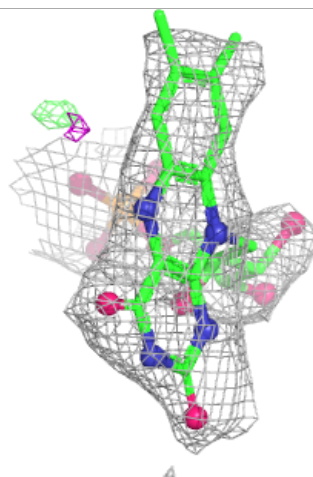
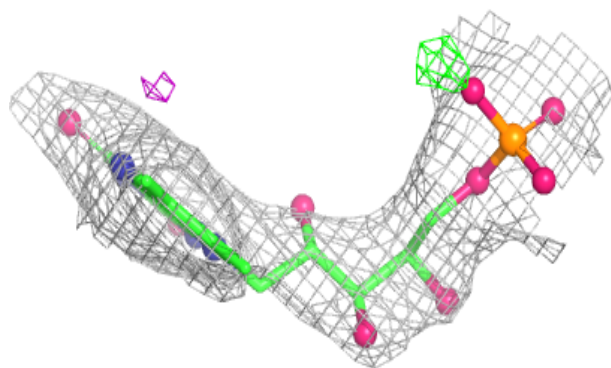
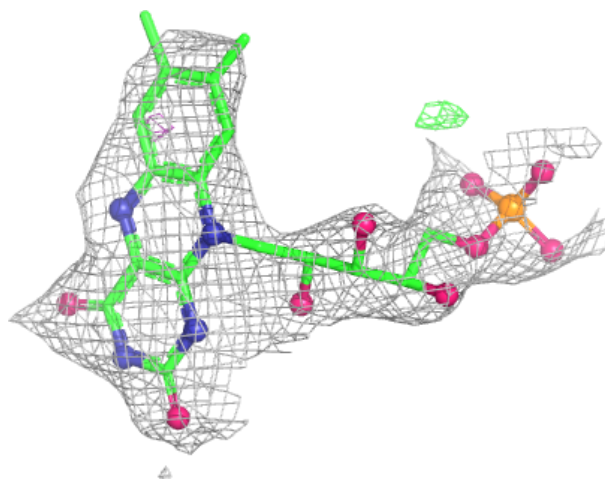
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	705	5/5	0.81	0.10	103,103,104,104	0
5	PO4	B	705	5/5	0.87	0.10	97,97,98,99	0
2	FMN	B	701	31/31	0.90	0.10	77,79,80,81	0
5	PO4	A	704	5/5	0.90	0.10	49,50,54,57	0
4	2AM	B	703	23/23	0.94	0.08	43,46,49,51	0
2	FMN	A	701	31/31	0.94	0.09	44,52,58,60	0
5	PO4	B	704	5/5	0.95	0.06	43,44,48,51	0
3	FAD	B	702	53/53	0.96	0.07	29,43,52,53	0
3	FAD	A	702	53/53	0.96	0.06	32,38,47,47	0
4	2AM	A	703	23/23	0.97	0.05	29,40,45,46	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.

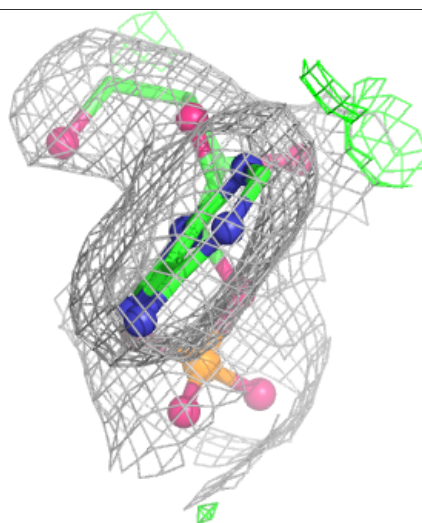
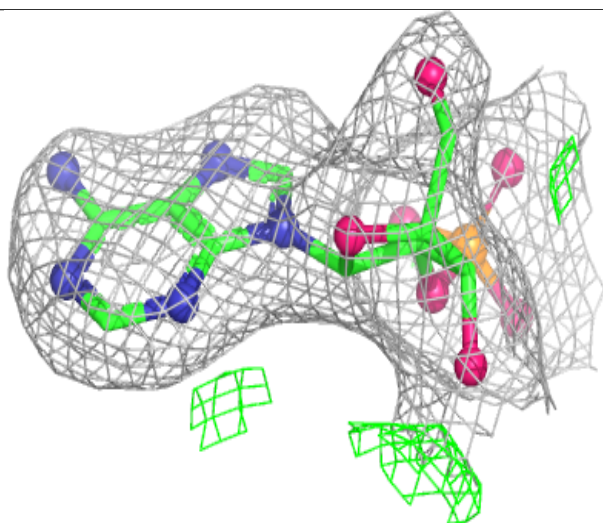
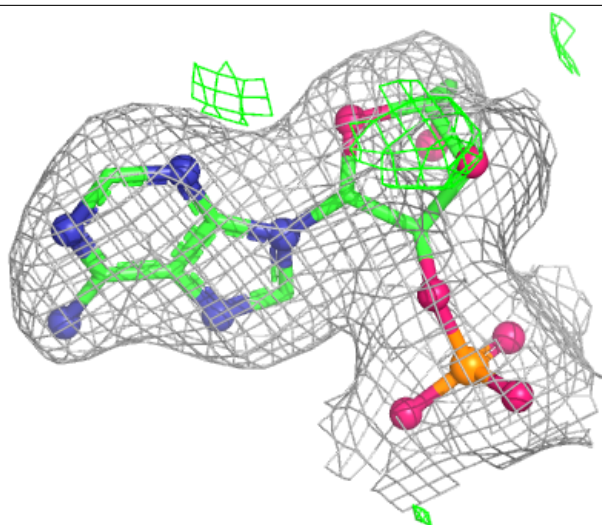
Electron density around FMN B 701:

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



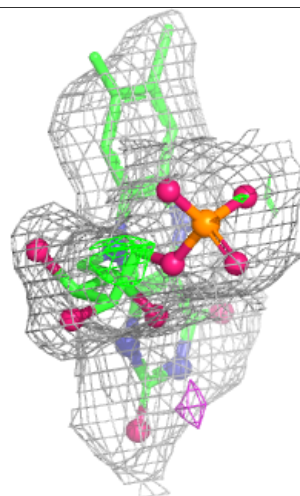
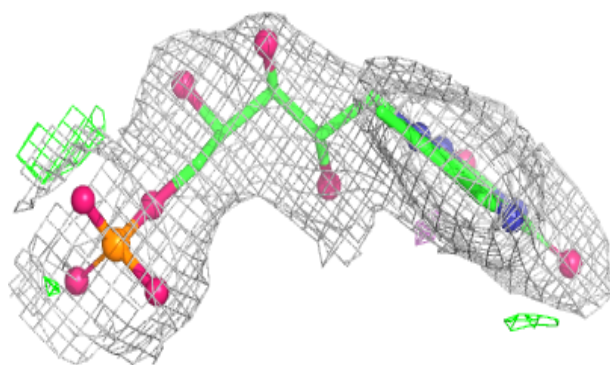
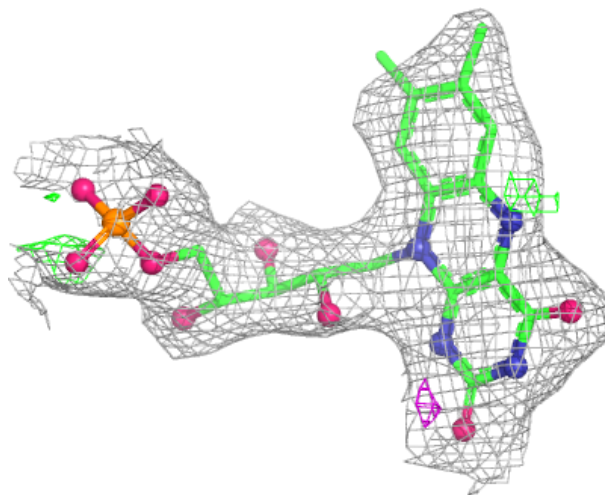
Electron density around 2AM B 703:

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



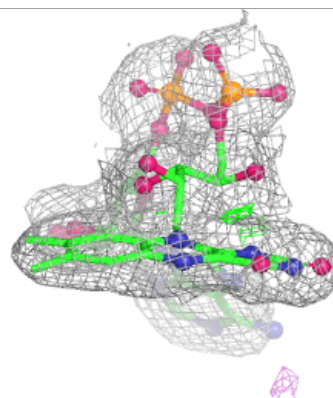
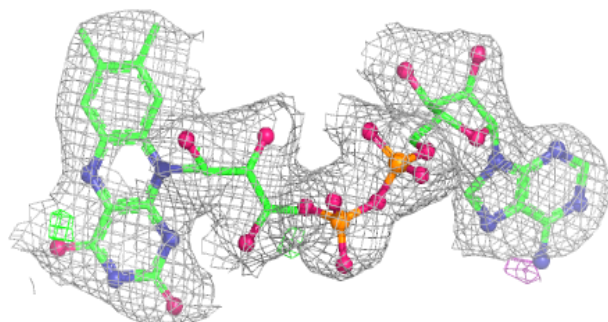
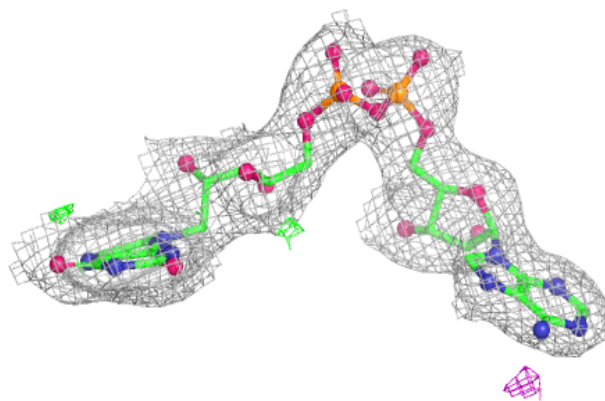
Electron density around FMN A 701:

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

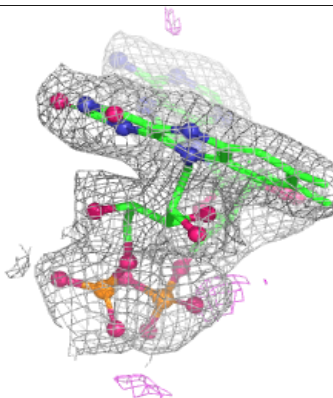
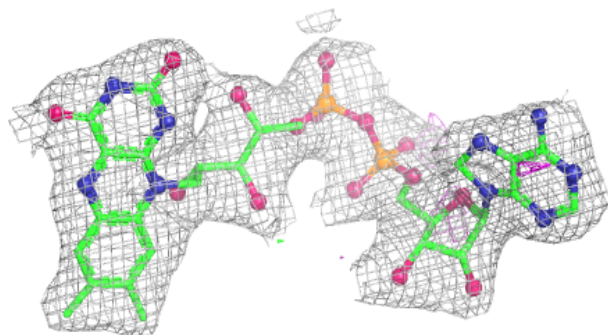
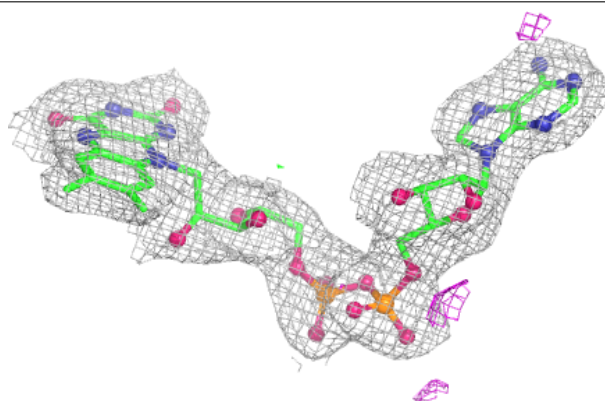


Electron density around FAD B 702:

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

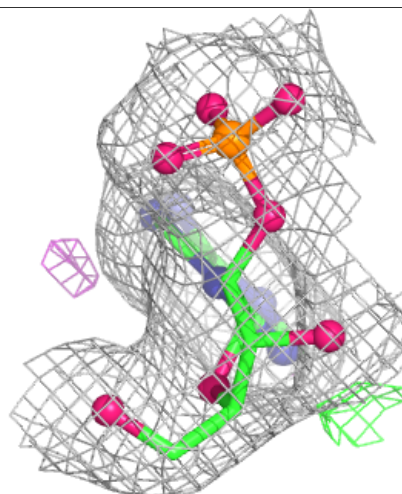
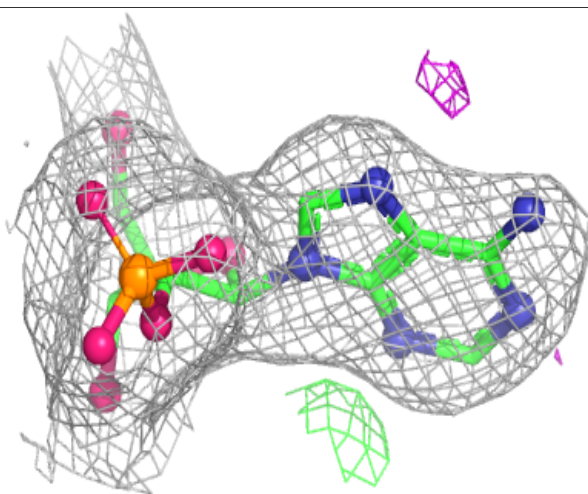
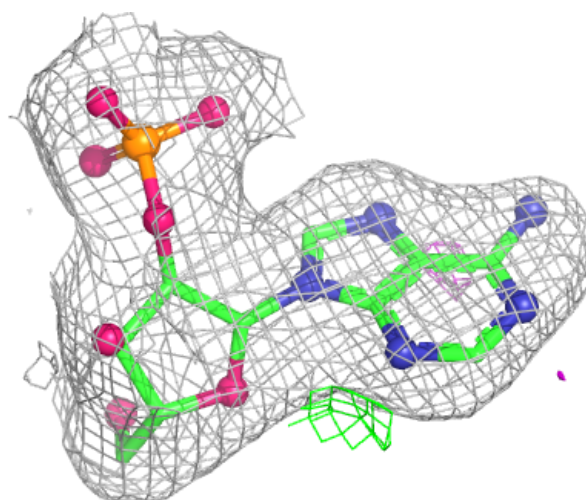
**Electron density around FAD A 702:**

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



Electron density around 2AM A 703:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.