



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:59 PM UTC

PDB ID : 1T6Y / pdb_00001t6y
Title : Crystal structure of ADP, AMP, and FMN bound TM379
Authors : Shin, D.H.; Wang, W.; Kim, R.; Yokota, H.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2004-05-07
Resolution : 2.80 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

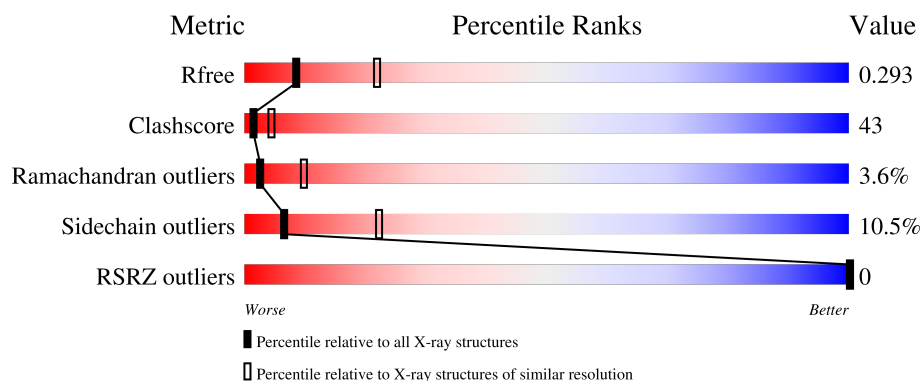
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	293	
1	B	293	

2 Entry composition [i](#)

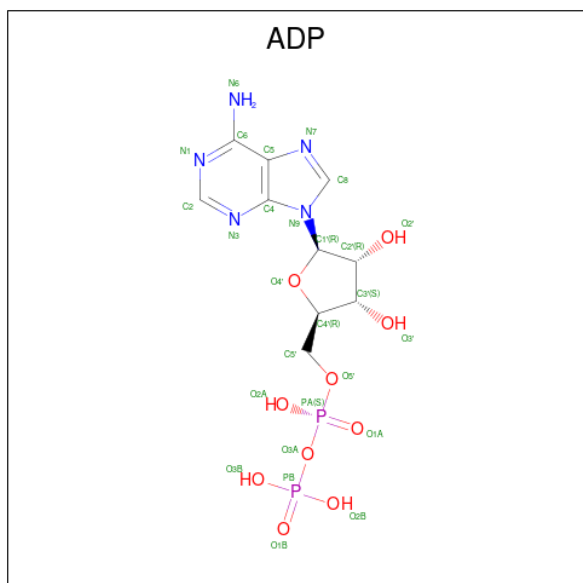
There are 5 unique types of molecules in this entry. The entry contains 4560 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 riboflavin kinase/FMN adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2176	1400	378	392	6			
1	B	270	Total	C	N	O	S	0	0	0
			2189	1413	373	397	6			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



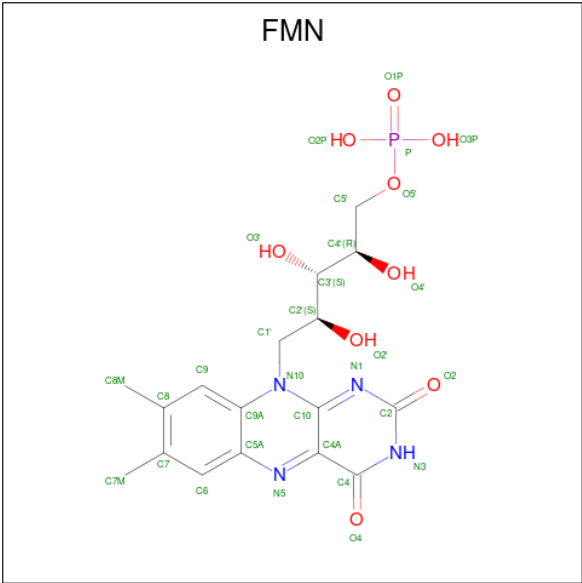
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

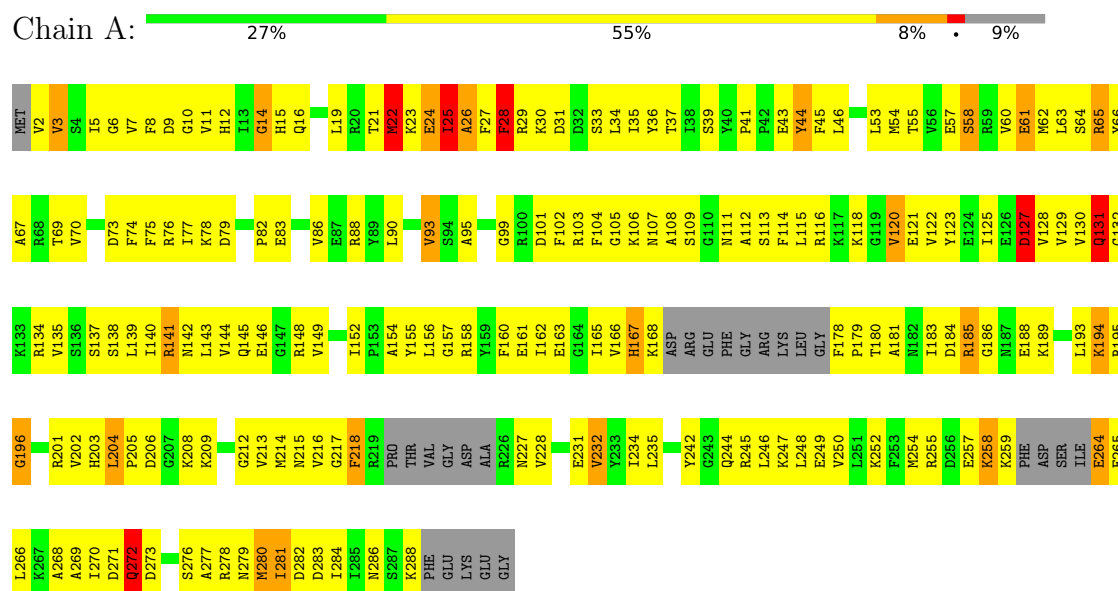
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total 18	O 18	0	0
5	B	15	Total 15	O 15	0	0

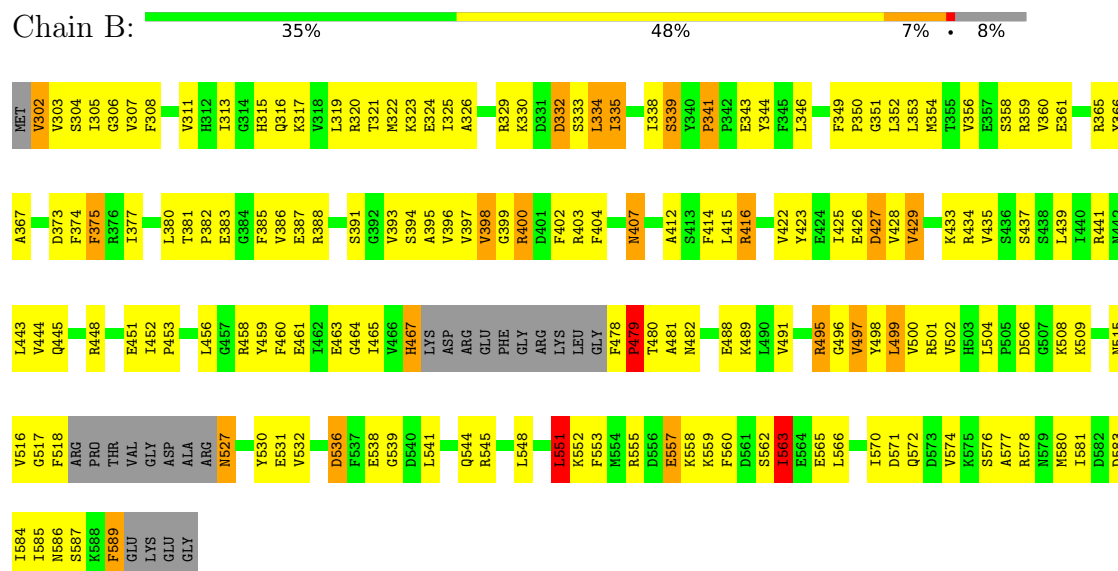
3 Residue-property plots

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: riboflavin kinase/FMN adenylyltransferase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.80Å 82.66Å 66.72Å 90.00° 116.42° 90.00°	Depositor
Resolution (Å)	19.92 – 2.80 19.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.92-2.80) 98.9 (19.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.298 0.229 , 0.293	Depositor DCC
R_{free} test set	1639 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4560	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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, AMP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/2213	1.15	16/2968 (0.5%)
1	B	0.61	0/2229	1.08	9/2994 (0.3%)
All	All	0.65	0/4442	1.12	25/5962 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	GLN	N-CA-C	-8.59	101.88	111.07
1	A	127	ASP	N-CA-C	8.03	122.04	110.24
1	A	3	VAL	N-CA-C	7.51	119.56	108.45
1	A	218	PHE	N-CA-C	7.39	119.50	110.41
1	A	196	GLY	N-CA-C	6.97	120.28	110.38
1	B	499	LEU	N-CA-C	-6.83	98.48	109.96
1	B	504	LEU	CA-C-N	6.66	126.16	119.24
1	B	504	LEU	C-N-CA	6.66	126.16	119.24
1	A	61	GLU	N-CA-C	-6.47	105.52	113.41
1	B	551	LEU	N-CA-C	6.45	121.41	112.45
1	A	33	SER	N-CA-C	6.12	119.22	109.24
1	A	14	GLY	N-CA-C	-6.00	107.22	114.66
1	A	194	LYS	N-CA-C	-5.86	101.98	110.24
1	A	280	MET	N-CA-C	-5.79	104.97	111.28
1	B	381	THR	N-CA-C	-5.47	103.03	110.36
1	A	258	LYS	N-CA-C	5.44	118.58	110.14
1	A	157	GLY	N-CA-C	-5.41	108.16	115.36
1	A	22	MET	N-CA-C	-5.39	105.49	111.36
1	B	374	PHE	N-CA-C	-5.26	105.19	111.03
1	A	252	LYS	N-CA-C	5.24	117.78	109.50
1	A	118	LYS	N-CA-C	-5.23	105.61	112.41
1	B	330	LYS	N-CA-C	-5.15	106.58	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	SER	N-CA-C	5.13	117.27	111.11
1	B	367	ALA	N-CA-C	5.10	115.08	107.88
1	B	572	GLN	N-CA-C	-5.07	105.94	111.82

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	2176	0	2221	216	0
1	B	2189	0	2221	179	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
3	A	23	0	12	4	0
3	B	23	0	12	2	0
4	A	31	0	19	1	0
4	B	31	0	19	4	0
5	A	18	0	0	2	1
5	B	15	0	0	2	1
All	All	4560	0	4528	392	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (392) 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:214:MET:HB2	1:A:232:VAL:HG23	1.37	1.06
1:A:103:ARG:HD3	1:A:108:ALA:HB1	1.34	1.04
1:A:3:VAL:HG12	1:A:34:LEU:HB3	1.38	1.03
1:A:212:GLY:HA2	1:A:235:LEU:HD13	1.49	0.93
1:B:354:MET:HE2	1:B:359:ARG:HA	1.51	0.90
1:B:495:ARG:HH11	1:B:495:ARG:H	1.12	0.90
1:A:21:THR:HG21	1:A:125:ILE:HD11	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HD12	1:A:271:ASP:N	1.88	0.88
1:A:280:MET:O	1:A:283:ASP:HB2	1.74	0.87
1:A:3:VAL:CG1	1:A:34:LEU:HB3	2.04	0.87
1:B:322:MET:HE3	1:B:333:SER:HB3	1.60	0.82
1:A:161:GLU:OE1	1:A:247:LYS:HE3	1.80	0.81
1:A:269:ALA:HA	1:A:272:GLN:NE2	1.95	0.81
1:A:166:VAL:HG12	1:A:167:HIS:H	1.45	0.81
1:A:140:ILE:O	1:A:144:VAL:HG23	1.80	0.81
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.46	0.80
1:B:388:ARG:HD3	5:B:629:HOH:O	1.81	0.80
1:A:166:VAL:HG23	1:A:244:GLN:O	1.81	0.80
1:B:321:THR:HG21	1:B:425:ILE:HD11	1.64	0.80
1:B:354:MET:HE2	1:B:359:ARG:CA	2.11	0.79
1:A:75:PHE:HA	1:A:78:LYS:HE3	1.65	0.79
1:B:465:ILE:HD11	1:B:545:ARG:HG2	1.64	0.79
1:A:88:ARG:HH11	1:A:88:ARG:HB2	1.47	0.79
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.47	0.78
1:A:41:PRO:HB2	1:A:43:GLU:OE2	1.84	0.77
1:B:517:GLY:O	1:B:518:PHE:HB2	1.84	0.77
1:B:463:GLU:HG2	1:B:464:GLY:N	2.00	0.77
1:A:203:HIS:ND1	1:A:209:LYS:HG2	2.00	0.76
1:A:9:ASP:OD1	1:A:141:ARG:NH1	2.18	0.76
1:B:382:PRO:O	1:B:386:VAL:HG23	1.85	0.75
1:A:178:PHE:N	1:A:179:PRO:HA	2.02	0.75
1:A:29:ARG:C	1:A:30:LYS:HD2	2.12	0.74
1:A:139:LEU:HD12	1:B:506:ASP:OD1	1.86	0.74
1:B:465:ILE:CD1	1:B:545:ARG:HG2	2.16	0.74
1:B:501:ARG:HB2	1:B:551:LEU:HD11	1.70	0.73
1:A:166:VAL:HB	1:A:242:TYR:O	1.89	0.73
1:A:129:VAL:HG12	1:A:134:ARG:HA	1.71	0.72
1:A:202:VAL:HG22	1:A:248:LEU:HD22	1.72	0.71
1:B:495:ARG:H	1:B:495:ARG:NH1	1.88	0.71
1:A:178:PHE:N	5:A:625:HOH:O	2.24	0.71
1:B:501:ARG:HG2	1:B:501:ARG:HH11	1.55	0.71
1:A:83:GLU:CD	1:A:83:GLU:H	1.99	0.70
1:A:127:ASP:HA	3:A:295:AMP:C2	2.27	0.70
1:A:103:ARG:CD	1:A:108:ALA:HB1	2.16	0.70
1:A:202:VAL:HG22	1:A:248:LEU:CD2	2.23	0.69
1:B:570:ILE:O	1:B:574:VAL:HG13	1.93	0.69
1:B:577:ALA:O	1:B:581:ILE:HG13	1.92	0.69
1:B:315:HIS:O	1:B:319:LEU:HG	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:VAL:O	1:B:308:PHE:HB2	1.93	0.68
1:B:437:SER:O	1:B:441:ARG:HG3	1.93	0.68
1:B:495:ARG:HH11	1:B:495:ARG:N	1.87	0.68
1:B:407:ASN:N	1:B:407:ASN:HD22	1.92	0.68
1:A:12:HIS:O	1:A:15:HIS:HB2	1.92	0.68
1:B:356:VAL:O	1:B:360:VAL:HG23	1.94	0.68
1:B:383:GLU:H	1:B:383:GLU:CD	2.02	0.67
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.08	0.67
1:A:8:PHE:HA	1:A:15:HIS:CE1	2.30	0.67
1:A:166:VAL:HG12	1:A:167:HIS:N	2.08	0.67
1:A:88:ARG:HB2	1:A:88:ARG:NH1	2.09	0.66
1:A:245:ARG:C	1:A:246:LEU:HD12	2.20	0.66
1:B:358:SER:O	1:B:361:GLU:HB3	1.95	0.66
1:B:343:GLU:H	1:B:343:GLU:CD	2.04	0.66
1:B:325:ILE:HD13	1:B:423:TYR:CD2	2.31	0.65
1:A:167:HIS:O	1:A:168:LYS:HB3	1.96	0.65
1:B:302:VAL:CG1	1:B:326:ALA:HB2	2.27	0.65
1:A:60:VAL:HG12	1:A:60:VAL:O	1.96	0.64
1:A:158:ARG:HG2	1:A:158:ARG:NH1	2.10	0.64
1:A:34:LEU:HD11	1:A:70:VAL:HG23	1.80	0.64
1:A:130:VAL:HG21	1:A:154:ALA:O	1.97	0.64
1:A:11:VAL:HA	1:A:15:HIS:ND1	2.12	0.64
1:A:43:GLU:CD	1:A:43:GLU:H	2.06	0.64
1:A:178:PHE:CZ	1:A:270:ILE:HD13	2.33	0.64
1:B:316:GLN:HG2	1:B:366:TYR:OH	1.96	0.64
1:A:195:ARG:HD2	1:A:257:GLU:HG2	1.81	0.63
1:A:178:PHE:HD2	1:A:178:PHE:O	1.81	0.63
1:B:329:ARG:HH12	1:B:394:SER:HB2	1.63	0.63
1:A:149:VAL:HG11	1:A:250:VAL:CG1	2.29	0.63
1:A:19:LEU:O	1:A:22:MET:HB3	1.99	0.62
1:B:481:ALA:O	1:B:531:GLU:HA	1.99	0.62
1:B:562:SER:HB3	1:B:565:GLU:CD	2.25	0.62
1:B:377:ILE:HA	1:B:380:LEU:HG	1.81	0.62
1:A:12:HIS:O	1:A:16:GLN:HG3	1.98	0.62
1:A:112:ALA:HB1	1:A:122:VAL:HG11	1.80	0.62
1:A:258:LYS:HG2	1:A:259:LYS:N	2.13	0.62
1:A:254:MET:HG2	1:A:280:MET:HE1	1.80	0.62
1:A:127:ASP:N	1:A:127:ASP:OD2	2.32	0.61
1:B:316:GLN:HB3	1:B:320:ARG:HH12	1.65	0.61
1:A:28:PHE:HD1	1:A:28:PHE:O	1.83	0.61
1:A:45:PHE:HE2	1:A:74:PHE:CD2	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PHE:O	1:A:46:LEU:HD23	2.00	0.61
1:A:21:THR:CG2	1:A:125:ILE:HD11	2.28	0.61
1:A:3:VAL:HG12	1:A:34:LEU:CB	2.23	0.60
1:B:352:LEU:O	1:B:491:VAL:HG12	2.00	0.60
1:B:322:MET:HE3	1:B:333:SER:CB	2.29	0.60
1:A:178:PHE:HZ	1:A:270:ILE:HD13	1.67	0.60
1:A:37:THR:HB	1:A:63:LEU:HD13	1.84	0.60
1:B:354:MET:HE2	1:B:359:ARG:N	2.15	0.60
1:B:373:ASP:OD1	1:B:375:PHE:N	2.35	0.60
1:A:130:VAL:HB	1:A:155:TYR:CE1	2.36	0.60
1:B:580:MET:O	1:B:583:ASP:HB2	2.01	0.60
1:B:555:ARG:NH2	4:B:596:FMN:N5	2.50	0.59
1:A:269:ALA:HA	1:A:272:GLN:HE22	1.65	0.59
1:A:58:SER:O	1:A:61:GLU:HB3	2.02	0.59
1:A:83:GLU:HG3	1:A:114:PHE:HZ	1.67	0.59
1:A:130:VAL:HG12	1:A:131:GLN:HG3	1.85	0.59
1:B:354:MET:CE	1:B:359:ARG:HA	2.31	0.59
1:B:488:GLU:HG3	1:B:489:LYS:N	2.18	0.59
1:B:495:ARG:N	1:B:495:ARG:HD3	2.16	0.59
1:B:365:ARG:HG3	1:B:365:ARG:HH11	1.67	0.59
1:A:99:GLY:HA3	3:A:295:AMP:O2'	2.03	0.59
1:B:325:ILE:HD12	1:B:397:VAL:HG22	1.84	0.59
1:B:498:TYR:CE1	1:B:553:PHE:HD1	2.21	0.58
1:A:23:LYS:O	1:A:26:ALA:HB3	2.03	0.58
1:A:134:ARG:NH2	1:B:539:GLY:HA3	2.18	0.58
1:B:311:VAL:HA	1:B:315:HIS:ND1	2.18	0.58
1:B:501:ARG:HG2	1:B:501:ARG:NH1	2.16	0.58
1:A:53:LEU:HD12	1:A:53:LEU:H	1.68	0.58
1:B:576:SER:O	1:B:580:MET:HG3	2.03	0.58
1:A:37:THR:HG23	1:A:37:THR:O	2.02	0.58
1:B:536:ASP:OD2	1:B:578:ARG:NH2	2.35	0.58
1:A:62:MET:O	1:A:63:LEU:C	2.47	0.57
1:A:53:LEU:HD11	1:A:141:ARG:HD3	1.86	0.57
1:B:563:ILE:O	1:B:563:ILE:HD12	2.04	0.57
1:A:103:ARG:HH11	1:A:108:ALA:HB3	1.69	0.57
1:B:365:ARG:HG3	1:B:365:ARG:NH1	2.19	0.57
1:A:24:GLU:O	1:A:26:ALA:N	2.38	0.56
1:B:383:GLU:HG3	1:B:414:PHE:HZ	1.70	0.56
1:B:517:GLY:O	1:B:518:PHE:CB	2.52	0.56
1:B:527:ASN:HA	5:B:616:HOH:O	2.04	0.56
1:A:19:LEU:HD12	1:A:66:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ARG:HB3	1:B:451:GLU:OE1	2.06	0.56
1:A:73:ASP:OD2	1:A:75:PHE:HB2	2.06	0.55
1:B:429:VAL:HA	1:B:433:LYS:O	2.07	0.55
1:A:129:VAL:HG23	1:A:129:VAL:O	2.05	0.55
1:B:488:GLU:HG3	1:B:489:LYS:H	1.71	0.55
1:B:555:ARG:NH1	4:B:596:FMN:O4	2.38	0.55
1:B:398:VAL:HG11	1:B:402:PHE:CD2	2.41	0.55
1:A:64:SER:O	1:A:66:TYR:N	2.40	0.55
1:B:502:VAL:HG22	1:B:548:LEU:HD22	1.88	0.55
1:A:166:VAL:CG1	1:A:167:HIS:H	2.19	0.54
1:A:27:PHE:C	1:A:29:ARG:H	2.16	0.54
1:B:302:VAL:N	1:B:332:ASP:O	2.40	0.54
1:A:178:PHE:N	1:A:179:PRO:CA	2.70	0.54
1:A:64:SER:C	1:A:66:TYR:H	2.15	0.54
1:B:325:ILE:HD13	1:B:423:TYR:HD2	1.72	0.54
1:B:427:ASP:HB2	1:B:434:ARG:HH21	1.71	0.54
1:A:35:ILE:CD1	1:A:67:ALA:HB3	2.38	0.54
1:A:203:HIS:CE1	1:A:209:LYS:HG2	2.42	0.54
1:A:212:GLY:HA2	1:A:235:LEU:CD1	2.31	0.54
1:A:205:PRO:O	1:A:206:ASP:HB2	2.08	0.54
1:A:88:ARG:HH11	1:A:88:ARG:CB	2.18	0.54
1:A:142:ASN:O	1:A:145:GLN:N	2.42	0.53
1:B:441:ARG:O	1:B:445:GLN:HG3	2.08	0.53
1:B:399:GLY:HA2	1:B:425:ILE:H	1.72	0.53
1:A:43:GLU:O	1:A:45:PHE:N	2.41	0.53
1:A:138:SER:HB2	1:B:508:LYS:HD2	1.89	0.53
1:A:216:VAL:HG12	1:A:228:VAL:CG1	2.39	0.53
1:B:558:LYS:HG2	1:B:559:LYS:N	2.23	0.53
1:A:116:ARG:HA	1:A:120:VAL:O	2.09	0.53
1:A:29:ARG:NH1	1:A:29:ARG:HG2	2.24	0.53
1:A:272:GLN:O	1:A:276:SER:HB2	2.09	0.53
1:A:149:VAL:HG11	1:A:250:VAL:HG12	1.91	0.53
1:B:463:GLU:HG2	1:B:464:GLY:H	1.74	0.53
1:A:53:LEU:HD12	1:A:53:LEU:N	2.24	0.52
1:A:24:GLU:C	1:A:26:ALA:H	2.16	0.52
1:B:329:ARG:NH1	1:B:394:SER:HB2	2.24	0.52
1:A:43:GLU:O	1:A:44:TYR:C	2.53	0.52
1:A:265:GLU:HG2	1:A:268:ALA:HB3	1.91	0.52
1:A:106:LYS:O	1:A:107:ASN:HB2	2.10	0.52
1:B:496:GLY:HA2	1:B:557:GLU:HB2	1.90	0.52
1:A:254:MET:HG2	1:A:280:MET:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ARG:H	1:B:495:ARG:CD	2.22	0.51
1:A:103:ARG:HH11	1:A:108:ALA:CB	2.23	0.51
1:B:344:TYR:HA	1:B:349:PHE:CD2	2.45	0.51
1:B:353:LEU:HD23	1:B:491:VAL:HG11	1.92	0.51
1:B:495:ARG:H	1:B:495:ARG:HD3	1.76	0.51
1:A:22:MET:HE1	1:A:67:ALA:HB2	1.91	0.51
1:A:24:GLU:C	1:A:26:ALA:N	2.65	0.51
1:A:138:SER:CB	1:B:508:LYS:HD2	2.41	0.51
1:B:344:TYR:OH	1:B:489:LYS:HG2	2.10	0.51
1:A:216:VAL:HG12	1:A:228:VAL:HG13	1.93	0.51
1:B:467:HIS:O	1:B:467:HIS:CG	2.63	0.51
1:B:495:ARG:NH1	1:B:495:ARG:HG2	2.25	0.51
1:B:303:VAL:HG22	1:B:334:LEU:HB3	1.93	0.51
1:A:270:ILE:HD12	1:A:270:ILE:C	2.36	0.50
1:A:286:ASN:O	1:A:288:LYS:N	2.43	0.50
1:A:90:LEU:O	1:A:93:VAL:HG12	2.11	0.50
1:A:257:GLU:HA	1:A:257:GLU:OE2	2.10	0.50
1:B:325:ILE:O	1:B:325:ILE:HG22	2.11	0.50
1:B:563:ILE:O	1:B:566:LEU:HB3	2.12	0.50
1:A:202:VAL:O	1:A:209:LYS:HA	2.11	0.50
1:B:571:ASP:O	1:B:574:VAL:HG22	2.11	0.50
1:A:19:LEU:O	1:A:22:MET:CB	2.58	0.50
1:B:343:GLU:HA	1:B:346:LEU:HD12	1.94	0.50
1:A:134:ARG:NH2	1:B:538:GLU:O	2.44	0.50
1:A:95:ALA:HA	1:A:121:GLU:O	2.11	0.50
1:A:105:GLY:O	1:A:106:LYS:C	2.54	0.50
1:A:29:ARG:HH21	1:A:121:GLU:CD	2.20	0.50
1:B:398:VAL:HG21	1:B:402:PHE:HD2	1.77	0.50
1:B:552:LYS:HD3	1:B:580:MET:CE	2.41	0.50
1:B:324:GLU:C	1:B:326:ALA:N	2.68	0.50
1:A:14:GLY:HA2	1:A:128:VAL:HG21	1.93	0.49
1:A:204:LEU:HB2	1:A:208:LYS:HB2	1.94	0.49
1:B:532:VAL:HG11	1:B:548:LEU:HD11	1.94	0.49
1:A:149:VAL:HG11	1:A:250:VAL:HG11	1.94	0.49
1:B:338:ILE:O	1:B:339:SER:C	2.55	0.49
1:B:460:PHE:CD1	1:B:461:GLU:N	2.81	0.49
1:A:37:THR:HB	1:A:63:LEU:CD1	2.41	0.49
1:B:396:VAL:HG12	1:B:396:VAL:O	2.11	0.49
1:A:28:PHE:O	1:A:28:PHE:CD1	2.64	0.49
1:A:103:ARG:HD3	1:A:108:ALA:CB	2.23	0.49
1:A:111:ASN:OD1	1:A:113:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:C	1:A:186:GLY:H	2.21	0.49
1:A:288:LYS:HB2	5:A:630:HOH:O	2.12	0.49
1:A:7:VAL:O	1:A:8:PHE:HB2	2.13	0.49
1:B:404:PHE:CZ	1:B:415:LEU:HD21	2.48	0.49
1:A:193:LEU:O	1:A:194:LYS:C	2.55	0.48
1:A:204:LEU:N	1:A:204:LEU:HD22	2.28	0.48
1:B:349:PHE:CZ	1:B:352:LEU:HD23	2.48	0.48
1:A:73:ASP:HB3	1:A:76:ARG:HD3	1.95	0.48
1:A:167:HIS:HB3	1:A:168:LYS:H	1.47	0.48
1:B:516:VAL:HG22	1:B:530:TYR:CD1	2.48	0.48
1:A:268:ALA:O	1:A:272:GLN:OE1	2.31	0.48
1:A:195:ARG:CD	1:A:217:GLY:HA2	2.44	0.48
1:B:320:ARG:HG3	1:B:320:ARG:HH11	1.79	0.48
1:A:264:GLU:OE2	1:A:264:GLU:O	2.31	0.48
1:B:407:ASN:N	1:B:407:ASN:ND2	2.61	0.48
1:A:232:VAL:CG1	1:A:234:ILE:HG13	2.44	0.48
1:B:349:PHE:HZ	1:B:352:LEU:HD23	1.79	0.48
1:B:560:PHE:CD1	1:B:566:LEU:HA	2.49	0.48
1:A:34:LEU:HD11	1:A:70:VAL:CG2	2.44	0.47
1:A:113:SER:O	1:A:116:ARG:HB2	2.13	0.47
1:B:341:PRO:HB2	1:B:343:GLU:OE2	2.14	0.47
1:B:584:ILE:HG22	1:B:584:ILE:O	2.13	0.47
1:B:302:VAL:HG13	1:B:326:ALA:HB2	1.95	0.47
1:B:502:VAL:HG13	1:B:548:LEU:CD2	2.45	0.47
1:A:158:ARG:NH1	1:A:158:ARG:CG	2.75	0.47
1:B:415:LEU:HB2	1:B:422:VAL:CG2	2.44	0.47
1:A:112:ALA:CB	1:A:122:VAL:HG11	2.44	0.47
1:B:316:GLN:HB3	1:B:320:ARG:NH1	2.28	0.47
1:B:416:ARG:HG3	1:B:416:ARG:HH11	1.79	0.47
1:B:571:ASP:HA	1:B:574:VAL:HG22	1.96	0.47
1:A:116:ARG:NH2	1:A:122:VAL:O	2.48	0.47
3:A:295:AMP:H5'1	3:A:295:AMP:H8	1.79	0.47
1:A:26:ALA:O	1:A:27:PHE:C	2.58	0.47
1:B:322:MET:HA	1:B:397:VAL:HG21	1.96	0.47
1:B:552:LYS:CD	1:B:580:MET:HE2	2.45	0.46
1:A:265:GLU:O	1:A:268:ALA:HB3	2.14	0.46
1:B:465:ILE:HD13	1:B:545:ARG:HG2	1.95	0.46
1:A:3:VAL:HG11	1:A:34:LEU:HD23	1.98	0.46
1:A:254:MET:HE3	1:A:280:MET:CE	2.45	0.46
1:A:284:ILE:H	1:A:284:ILE:HG13	1.58	0.46
1:A:201:ARG:HD2	1:A:201:ARG:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:CG1	1:A:228:VAL:CG1	2.94	0.46
1:B:415:LEU:HB2	1:B:422:VAL:HG21	1.97	0.46
1:B:497:VAL:HG22	1:B:515:ASN:HD22	1.80	0.46
1:A:142:ASN:O	1:A:143:LEU:C	2.59	0.46
1:A:25:ILE:HG22	1:A:29:ARG:HD2	1.98	0.46
1:B:452:ILE:O	1:B:453:PRO:C	2.59	0.45
1:A:64:SER:C	1:A:66:TYR:N	2.73	0.45
1:A:269:ALA:O	1:A:272:GLN:HB2	2.16	0.45
1:B:322:MET:CE	1:B:333:SER:HB3	2.40	0.45
1:B:427:ASP:CB	1:B:434:ARG:HE	2.28	0.45
1:B:585:ILE:C	1:B:587:SER:H	2.23	0.45
1:A:258:LYS:CG	1:A:259:LYS:N	2.80	0.45
1:A:277:ALA:O	1:A:278:ARG:C	2.60	0.45
1:B:527:ASN:C	1:B:527:ASN:HD22	2.24	0.45
1:B:562:SER:O	1:B:563:ILE:C	2.60	0.45
1:B:429:VAL:HG12	1:B:433:LYS:H	1.82	0.45
1:B:495:ARG:HA	1:B:516:VAL:HG12	1.97	0.45
1:A:27:PHE:O	1:A:29:ARG:N	2.49	0.45
1:A:60:VAL:O	1:A:60:VAL:CG1	2.65	0.45
1:A:103:ARG:O	1:A:104:PHE:HB3	2.15	0.45
1:A:137:SER:O	1:A:141:ARG:HB2	2.17	0.45
1:A:195:ARG:HD3	1:A:218:PHE:HD1	1.82	0.45
1:B:495:ARG:HH11	1:B:495:ARG:HG2	1.81	0.45
1:B:391:SER:O	1:B:393:VAL:HG23	2.17	0.45
1:B:427:ASP:HA	3:B:595:AMP:N1	2.32	0.45
1:B:302:VAL:HB	1:B:395:ALA:HB3	1.99	0.44
1:B:412:ALA:HB1	1:B:422:VAL:HG11	1.98	0.44
1:B:313:ILE:HD11	1:B:435:VAL:HG21	2.00	0.44
1:B:558:LYS:CG	1:B:559:LYS:N	2.80	0.44
1:B:303:VAL:O	1:B:396:VAL:HA	2.17	0.44
1:B:502:VAL:HG13	1:B:548:LEU:HD21	1.99	0.44
1:B:563:ILE:HD12	1:B:563:ILE:C	2.43	0.44
1:A:2:VAL:HA	1:A:95:ALA:O	2.18	0.44
1:B:459:TYR:O	1:B:460:PHE:C	2.58	0.44
1:A:43:GLU:C	1:A:45:PHE:N	2.75	0.44
1:B:437:SER:O	1:B:441:ARG:CG	2.62	0.44
1:B:463:GLU:CG	1:B:464:GLY:N	2.77	0.44
1:B:566:LEU:O	1:B:570:ILE:HG13	2.17	0.44
1:B:400:ARG:HH11	1:B:400:ARG:HB3	1.83	0.44
1:A:28:PHE:CD1	1:A:28:PHE:C	2.96	0.44
1:A:9:ASP:OD1	1:A:53:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:O	1:A:276:SER:HB3	2.17	0.43
1:B:317:LYS:HE3	1:B:425:ILE:HG23	1.99	0.43
1:B:324:GLU:C	1:B:326:ALA:H	2.26	0.43
1:B:456:LEU:HD12	1:B:456:LEU:O	2.17	0.43
1:B:586:ASN:HA	1:B:589:PHE:HE1	1.83	0.43
1:A:10:GLY:HA2	1:A:54:MET:SD	2.58	0.43
1:A:167:HIS:O	1:A:168:LYS:CB	2.66	0.43
1:A:281:ILE:O	1:A:283:ASP:N	2.51	0.43
1:B:319:LEU:HD22	1:B:335:ILE:HD13	2.01	0.43
1:A:165:ILE:HG22	1:A:166:VAL:N	2.33	0.43
1:A:144:VAL:O	1:A:193:LEU:HD23	2.19	0.43
1:B:416:ARG:HG3	1:B:416:ARG:NH1	2.33	0.43
1:A:115:LEU:O	1:A:120:VAL:HG23	2.19	0.43
1:A:286:ASN:O	1:A:288:LYS:HG3	2.18	0.43
1:B:305:ILE:HG22	1:B:306:GLY:N	2.33	0.43
1:B:325:ILE:O	1:B:329:ARG:HG3	2.18	0.43
1:B:496:GLY:HA2	1:B:557:GLU:H	1.83	0.43
1:A:146:GLU:O	1:A:148:ARG:HG3	2.19	0.43
1:A:281:ILE:C	1:A:283:ASP:N	2.76	0.43
1:A:45:PHE:CE2	1:A:74:PHE:CD2	3.05	0.43
4:A:296:FMN:H1'1	4:A:296:FMN:H9	1.79	0.42
1:B:541:LEU:HA	1:B:544:GLN:OE1	2.19	0.42
1:A:195:ARG:CD	1:A:218:PHE:HD1	2.32	0.42
1:A:217:GLY:O	1:A:228:VAL:HA	2.19	0.42
1:A:245:ARG:O	1:A:246:LEU:HD12	2.18	0.42
1:A:254:MET:HE3	1:A:280:MET:HE3	2.01	0.42
1:B:428:VAL:HG23	3:B:595:AMP:N1	2.35	0.42
1:A:8:PHE:CE1	1:A:19:LEU:HD21	2.53	0.42
1:B:478:PHE:HB3	1:B:479:PRO:HD2	2.01	0.42
1:A:55:THR:OG1	1:A:58:SER:HB2	2.20	0.42
1:A:127:ASP:HA	3:A:295:AMP:N1	2.34	0.42
1:B:480:THR:HB	1:B:531:GLU:HB3	2.02	0.42
1:A:152:ILE:HD13	1:A:160:PHE:HB2	2.01	0.42
1:B:576:SER:O	1:B:577:ALA:C	2.63	0.42
1:A:139:LEU:C	1:A:139:LEU:HD23	2.45	0.42
1:A:180:THR:O	2:A:294:ADP:O1B	2.38	0.42
1:A:181:ALA:O	1:A:231:GLU:HA	2.19	0.42
1:A:201:ARG:HB3	1:A:249:GLU:HB2	2.01	0.42
1:B:320:ARG:HG3	1:B:320:ARG:NH1	2.34	0.42
1:B:531:GLU:OE1	4:B:596:FMN:H4'	2.19	0.42
1:B:552:LYS:HD3	1:B:580:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:VAL:O	1:B:577:ALA:HB3	2.19	0.42
1:A:78:LYS:NZ	1:B:589:PHE:CZ	2.88	0.42
1:A:82:PRO:O	1:A:86:VAL:HG23	2.20	0.42
1:A:25:ILE:HG22	1:A:25:ILE:O	2.19	0.42
1:A:178:PHE:C	1:A:178:PHE:CD2	2.96	0.42
1:B:308:PHE:HA	1:B:315:HIS:CE1	2.55	0.42
1:A:205:PRO:O	1:A:206:ASP:CB	2.66	0.41
1:A:25:ILE:O	1:A:29:ARG:HB2	2.20	0.41
1:A:79:ASP:HA	1:A:106:LYS:HE3	2.01	0.41
1:A:105:GLY:O	1:A:108:ALA:N	2.53	0.41
1:A:137:SER:HB3	1:A:141:ARG:NH1	2.34	0.41
1:B:350:PRO:O	1:B:491:VAL:HA	2.20	0.41
1:B:385:PHE:C	1:B:385:PHE:CD2	2.98	0.41
1:A:5:ILE:HG22	1:A:6:GLY:N	2.36	0.41
1:A:27:PHE:C	1:A:29:ARG:N	2.78	0.41
1:A:195:ARG:HD3	1:A:217:GLY:HA2	2.02	0.41
1:A:232:VAL:HG13	1:A:234:ILE:HG13	2.02	0.41
1:B:304:SER:C	1:B:305:ILE:HG13	2.45	0.41
1:B:479:PRO:HA	2:B:594:ADP:O2A	2.21	0.41
1:B:502:VAL:O	1:B:509:LYS:HG2	2.20	0.41
1:B:349:PHE:CE2	1:B:351:GLY:HA2	2.56	0.41
1:B:412:ALA:CB	1:B:422:VAL:HG11	2.50	0.41
1:B:499:LEU:HD12	1:B:500:VAL:N	2.36	0.41
1:A:11:VAL:CA	1:A:15:HIS:ND1	2.83	0.41
1:A:258:LYS:O	1:A:259:LYS:C	2.63	0.41
1:B:552:LYS:HD3	1:B:580:MET:HE2	2.03	0.41
1:A:107:ASN:C	1:A:109:SER:N	2.74	0.41
1:A:6:GLY:O	1:A:37:THR:HA	2.21	0.41
1:A:45:PHE:O	1:A:46:LEU:CD2	2.68	0.41
1:A:196:GLY:O	1:A:215:ASN:HA	2.21	0.41
1:A:266:LEU:C	1:A:268:ALA:N	2.76	0.41
1:A:277:ALA:C	1:A:279:ASN:N	2.78	0.41
1:B:516:VAL:HG22	1:B:530:TYR:CE1	2.56	0.41
1:B:560:PHE:HD1	1:B:566:LEU:HD13	1.86	0.41
4:B:596:FMN:H9	4:B:596:FMN:H1'1	1.96	0.41
1:A:218:PHE:HA	1:A:227:ASN:O	2.21	0.41
1:A:8:PHE:HB3	1:A:63:LEU:HD21	2.03	0.40
1:A:25:ILE:HD12	1:A:123:TYR:CD1	2.55	0.40
1:A:144:VAL:O	1:A:193:LEU:HA	2.21	0.40
1:B:495:ARG:N	1:B:495:ARG:CD	2.80	0.40
1:A:29:ARG:NH2	1:A:121:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HG	1:A:158:ARG:NH1	2.36	0.40
1:A:276:SER:O	1:A:279:ASN:HB2	2.21	0.40
1:B:443:LEU:O	1:B:444:VAL:C	2.64	0.40
1:B:453:PRO:HA	1:B:458:ARG:O	2.21	0.40
1:B:585:ILE:C	1:B:587:SER:N	2.79	0.40
1:B:343:GLU:CD	1:B:343:GLU:N	2.75	0.40
1:B:308:PHE:CE1	1:B:319:LEU:HD21	2.56	0.40
1:B:311:VAL:O	1:B:311:VAL:HG12	2.21	0.40
1:B:358:SER:O	1:B:361:GLU:CB	2.67	0.40
1:B:383:GLU:CD	1:B:383:GLU:N	2.76	0.40
1:B:400:ARG:HB3	1:B:400:ARG:NH1	2.36	0.40
1:A:143:LEU:H	1:A:143:LEU:HG	1.74	0.40
1:A:162:ILE:HD12	1:A:185:ARG:NE	2.36	0.40
1:A:167:HIS:CD2	1:A:242:TYR:HD1	2.39	0.40
1:B:402:PHE:CD1	1:B:403:ARG:N	2.89	0.40
1:B:500:VAL:HG21	1:B:548:LEU:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:602:HOH:O	5:B:629:HOH:O[2_656]	2.10	0.10

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	260/293 (89%)	210 (81%)	39 (15%)	11 (4%)	2	7
1	B	264/293 (90%)	222 (84%)	34 (13%)	8 (3%)	3	12
All	All	524/586 (89%)	432 (82%)	73 (14%)	19 (4%)	2	10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	44	TYR
1	A	65	ARG
1	B	398	VAL
1	A	25	ILE
1	A	26	ALA
1	A	102	PHE
1	A	131	GLN
1	A	185	ARG
1	A	282	ASP
1	B	375	PHE
1	B	479	PRO
1	B	341	PRO
1	B	557	GLU
1	A	281	ILE
1	B	323	LYS
1	B	339	SER
1	B	563	ILE
1	A	132	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/257 (92%)	209 (88%)	28 (12%)	5	17
1	B	239/257 (93%)	217 (91%)	22 (9%)	8	27
All	All	476/514 (93%)	426 (90%)	50 (10%)	6	22

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	24	GLU
1	A	25	ILE
1	A	28	PHE

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Mol	Chain	Res	Type
1	A	31	ASP
1	A	36	TYR
1	A	57	GLU
1	A	58	SER
1	A	65	ARG
1	A	69	THR
1	A	77	ILE
1	A	93	VAL
1	A	101	ASP
1	A	120	VAL
1	A	127	ASP
1	A	131	GLN
1	A	135	VAL
1	A	141	ARG
1	A	163	GLU
1	A	167	HIS
1	A	183	ILE
1	A	188	GLU
1	A	189	LYS
1	A	204	LEU
1	A	213	VAL
1	A	232	VAL
1	A	264	GLU
1	A	272	GLN
1	B	302	VAL
1	B	332	ASP
1	B	334	LEU
1	B	335	ILE
1	B	387	GLU
1	B	400	ARG
1	B	407	ASN
1	B	416	ARG
1	B	426	GLU
1	B	427	ASP
1	B	429	VAL
1	B	439	LEU
1	B	467	HIS
1	B	479	PRO
1	B	482	ASN
1	B	495	ARG
1	B	497	VAL
1	B	527	ASN

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Mol	Chain	Res	Type
1	B	536	ASP
1	B	551	LEU
1	B	563	ILE
1	B	589	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	131	GLN
1	A	167	HIS
1	A	244	GLN
1	A	272	GLN
1	A	279	ASN
1	B	407	ASN
1	B	515	ASN
1	B	527	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	AMP	A	295	-	25,25,25	1.65	5 (20%)	37,38,38	1.74	10 (27%)
2	ADP	B	594	-	28,29,29	1.57	5 (17%)	43,45,45	2.01	8 (18%)
2	ADP	A	294	-	28,29,29	1.69	9 (32%)	43,45,45	2.11	10 (23%)
4	FMN	A	296	-	33,33,33	2.32	11 (33%)	48,50,50	2.63	21 (43%)
4	FMN	B	596	-	33,33,33	2.38	10 (30%)	48,50,50	2.57	20 (41%)
3	AMP	B	595	-	25,25,25	2.04	6 (24%)	37,38,38	1.60	10 (27%)

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
3	AMP	A	295	-	-	0/10/26/26	0/3/3/3
2	ADP	B	594	-	-	9/16/32/32	0/3/3/3
2	ADP	A	294	-	-	8/16/32/32	0/3/3/3
4	FMN	A	296	-	-	7/18/18/18	0/3/3/3
4	FMN	B	596	-	-	8/18/18/18	0/3/3/3
3	AMP	B	595	-	-	0/10/26/26	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	596	FMN	C9-C9A	5.72	1.48	1.39
3	B	595	AMP	C3'-C4'	5.70	1.67	1.53
4	B	596	FMN	C9A-C5A	5.70	1.50	1.41
4	A	296	FMN	C9-C9A	5.62	1.48	1.39
4	A	296	FMN	C9A-C5A	4.83	1.48	1.41
2	A	294	ADP	C5-N7	-4.66	1.30	1.39
4	A	296	FMN	C6-C7	4.57	1.45	1.39
4	B	596	FMN	C6-C7	4.54	1.45	1.39
4	A	296	FMN	C2-N3	4.50	1.48	1.39
4	B	596	FMN	C5'-C4'	4.41	1.57	1.51
3	A	295	AMP	C3'-C4'	4.24	1.63	1.53
2	B	594	ADP	C5-N7	-4.19	1.31	1.39
4	B	596	FMN	C2-N3	4.15	1.48	1.39
4	A	296	FMN	C5'-C4'	4.05	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	595	AMP	O3'-C3'	3.67	1.52	1.43
4	B	596	FMN	C4A-C10	3.62	1.54	1.44
4	A	296	FMN	C4A-C10	3.54	1.54	1.44
3	A	295	AMP	O3'-C3'	3.46	1.51	1.43
3	B	595	AMP	C2'-C1'	3.29	1.63	1.53
4	B	596	FMN	C4-N3	3.05	1.44	1.38
3	B	595	AMP	C8-N9	2.91	1.42	1.37
2	A	294	ADP	C5-C4	2.82	1.44	1.39
4	A	296	FMN	C8-C7	2.76	1.47	1.40
4	B	596	FMN	C4'-C3'	2.69	1.58	1.53
4	A	296	FMN	C9A-N10	-2.54	1.36	1.41
3	B	595	AMP	C5-C4	2.52	1.43	1.39
2	A	294	ADP	C4-N3	2.52	1.39	1.34
4	B	596	FMN	C8-C7	2.51	1.47	1.40
3	A	295	AMP	C8-N9	2.48	1.41	1.37
2	A	294	ADP	C1'-N9	2.43	1.53	1.46
2	B	594	ADP	C4-N9	-2.41	1.32	1.37
2	B	594	ADP	PA-O3A	2.39	1.62	1.59
2	A	294	ADP	C4-N9	-2.36	1.32	1.37
4	A	296	FMN	C4-N3	2.32	1.43	1.38
2	B	594	ADP	C4-N3	2.29	1.38	1.34
2	A	294	ADP	C5'-C4'	2.23	1.58	1.51
3	A	295	AMP	C2'-C1'	2.22	1.60	1.53
2	B	594	ADP	C5-C4	2.19	1.43	1.39
4	B	596	FMN	P-O1P	2.18	1.57	1.50
2	A	294	ADP	C2-N1	2.17	1.37	1.33
3	A	295	AMP	C5-C4	2.16	1.42	1.39
2	A	294	ADP	C2-N3	2.15	1.37	1.33
4	A	296	FMN	P-O1P	2.09	1.57	1.50
4	A	296	FMN	C1'-C2'	-2.09	1.49	1.52
2	A	294	ADP	PA-O2A	-2.02	1.46	1.55
3	B	595	AMP	C8-N7	2.02	1.35	1.31

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	296	FMN	C5A-C9A-N10	7.60	124.84	117.97
4	B	596	FMN	C5A-C9A-N10	7.33	124.59	117.97
2	B	594	ADP	N3-C2-N1	-6.86	118.20	128.58
2	A	294	ADP	N3-C2-N1	-6.76	118.36	128.58
4	A	296	FMN	C7M-C7-C6	-6.18	108.69	119.57
4	B	596	FMN	C7M-C7-C6	-5.83	109.30	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	294	ADP	C5-C4-N3	-5.39	119.30	126.72
4	B	596	FMN	C9A-C5A-N5	-5.24	116.89	122.45
2	B	594	ADP	C5-C4-N3	-5.16	119.61	126.72
4	A	296	FMN	C7M-C7-C8	4.99	130.95	120.76
4	A	296	FMN	C9A-C5A-N5	-4.83	117.33	122.45
4	B	596	FMN	C7M-C7-C8	4.79	130.55	120.76
2	A	294	ADP	N3-C4-N9	4.53	134.86	127.17
2	B	594	ADP	C2-N3-C4	4.48	122.78	111.83
2	A	294	ADP	C2-N3-C4	4.38	122.53	111.83
2	B	594	ADP	N3-C4-N9	4.11	134.15	127.17
4	B	596	FMN	C1'-N10-C9A	4.03	128.46	120.63
4	A	296	FMN	C4'-C3'-C2'	4.02	120.25	113.57
4	B	596	FMN	O2-C2-N1	4.01	128.46	121.80
4	B	596	FMN	C4'-C3'-C2'	3.96	120.16	113.57
4	A	296	FMN	O2-C2-N1	3.81	128.12	121.80
4	A	296	FMN	C9A-N10-C10	-3.80	114.95	120.75
3	A	295	AMP	O4'-C4'-C5'	-3.65	97.64	109.33
4	B	596	FMN	C9A-N10-C10	-3.56	115.33	120.75
4	B	596	FMN	C4A-C10-N10	3.49	121.47	116.48
4	A	296	FMN	C10-N1-C2	3.48	124.38	116.85
4	B	596	FMN	C10-N1-C2	3.45	124.33	116.85
4	A	296	FMN	C4A-C10-N10	3.34	121.27	116.48
2	B	594	ADP	C5-N7-C8	3.32	108.66	103.45
4	A	296	FMN	C1'-C2'-C3'	-3.29	100.75	109.66
3	A	295	AMP	N6-C6-N1	3.28	125.69	118.38
2	A	294	ADP	C5-N7-C8	3.27	108.58	103.45
4	A	296	FMN	C9-C9A-N10	-3.25	117.48	121.85
3	A	295	AMP	C4-C5-N7	3.23	114.28	110.58
4	B	596	FMN	C5'-C4'-C3'	3.21	118.28	112.22
3	A	295	AMP	O3'-C3'-C4'	-3.19	101.91	111.08
3	A	295	AMP	C5-N7-C8	-3.16	98.49	103.45
3	B	595	AMP	O4'-C4'-C5'	-3.11	99.37	109.33
3	B	595	AMP	C2-N1-C6	3.05	123.75	118.73
4	A	296	FMN	C5'-C4'-C3'	3.04	117.96	112.22
3	B	595	AMP	N6-C6-N1	2.97	124.98	118.38
4	A	296	FMN	C2'-C1'-N10	2.96	124.17	110.20
3	B	595	AMP	C5-N7-C8	-2.92	98.85	103.45
4	A	296	FMN	O4-C4-N3	-2.92	114.63	120.11
3	A	295	AMP	C2-N1-C6	2.88	123.46	118.73
3	B	595	AMP	C4-C5-N7	2.87	113.86	110.58
4	B	596	FMN	O4-C4-N3	-2.85	114.75	120.11
2	B	594	ADP	C4-C5-N7	-2.83	107.35	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	296	FMN	C4A-C10-N1	-2.81	117.70	124.59
2	B	594	ADP	N9-C8-N7	-2.75	110.04	113.94
4	B	596	FMN	O2-C2-N3	-2.72	113.38	118.58
4	A	296	FMN	C4-C4A-C10	2.69	121.54	116.93
4	B	596	FMN	C1'-C2'-C3'	-2.68	102.39	109.66
4	A	296	FMN	C1'-N10-C9A	2.65	125.78	120.63
2	A	294	ADP	C1'-N9-C8	-2.63	121.26	127.09
3	A	295	AMP	N3-C2-N1	-2.60	124.65	128.58
4	A	296	FMN	O2-C2-N3	-2.60	113.60	118.58
2	A	294	ADP	C4-C5-N7	-2.59	107.62	110.58
3	A	295	AMP	N9-C8-N7	2.58	117.60	113.94
4	B	596	FMN	C9-C9A-N10	-2.58	118.38	121.85
4	A	296	FMN	O3'-C3'-C4'	-2.58	103.06	108.93
4	B	596	FMN	C4A-C10-N1	-2.56	118.32	124.59
3	B	595	AMP	N3-C2-N1	-2.47	124.85	128.58
2	A	294	ADP	N9-C8-N7	-2.46	110.45	113.94
4	B	596	FMN	C6-C5A-N5	2.46	122.52	118.44
3	B	595	AMP	O3'-C3'-C4'	-2.44	104.08	111.08
2	A	294	ADP	C2'-C3'-C4'	2.36	107.16	102.61
3	B	595	AMP	N9-C8-N7	2.33	117.25	113.94
3	A	295	AMP	C2'-C1'-N9	-2.31	107.56	113.30
4	A	296	FMN	C6-C5A-N5	2.28	122.23	118.44
2	A	294	ADP	O4'-C1'-N9	2.27	112.45	108.09
4	B	596	FMN	O2'-C2'-C3'	2.25	114.52	109.25
3	B	595	AMP	C3'-C2'-C1'	2.22	105.66	101.46
4	A	296	FMN	O2'-C2'-C3'	2.18	114.36	109.25
4	B	596	FMN	C4-C4A-C10	2.18	120.67	116.93
3	B	595	AMP	O4'-C4'-C3'	2.17	109.45	105.15
4	B	596	FMN	O3'-C3'-C4'	-2.06	104.25	108.93
3	A	295	AMP	C3'-C2'-C1'	2.03	105.30	101.46
2	B	594	ADP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	294	ADP	PA-O3A-PB-O2B
2	A	294	ADP	C5'-O5'-PA-O1A
2	A	294	ADP	C5'-O5'-PA-O2A
2	A	294	ADP	C5'-O5'-PA-O3A
2	B	594	ADP	C5'-O5'-PA-O1A
2	B	594	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	594	ADP	C5'-O5'-PA-O3A
4	A	296	FMN	C2'-C1'-N10-C10
4	A	296	FMN	C1'-C2'-C3'-O3'
4	A	296	FMN	C1'-C2'-C3'-C4'
4	A	296	FMN	O2'-C2'-C3'-O3'
4	A	296	FMN	C3'-C4'-C5'-O5'
4	A	296	FMN	O4'-C4'-C5'-O5'
4	B	596	FMN	C1'-C2'-C3'-O3'
4	B	596	FMN	C1'-C2'-C3'-C4'
4	B	596	FMN	O2'-C2'-C3'-O3'
4	B	596	FMN	O2'-C2'-C3'-C4'
4	A	296	FMN	O2'-C2'-C3'-C4'
4	B	596	FMN	O4'-C4'-C5'-O5'
2	B	594	ADP	PA-O3A-PB-O1B
2	B	594	ADP	PA-O3A-PB-O2B
4	B	596	FMN	C3'-C4'-C5'-O5'
2	B	594	ADP	PB-O3A-PA-O1A
4	B	596	FMN	C4'-C5'-O5'-P
2	A	294	ADP	C3'-C4'-C5'-O5'
2	A	294	ADP	PA-O3A-PB-O1B
2	A	294	ADP	PA-O3A-PB-O3B
2	A	294	ADP	O4'-C1'-N9-C8
4	B	596	FMN	C2'-C3'-C4'-C5'
2	B	594	ADP	C3'-C4'-C5'-O5'
2	B	594	ADP	O4'-C1'-N9-C8
2	B	594	ADP	PB-O3A-PA-O2A

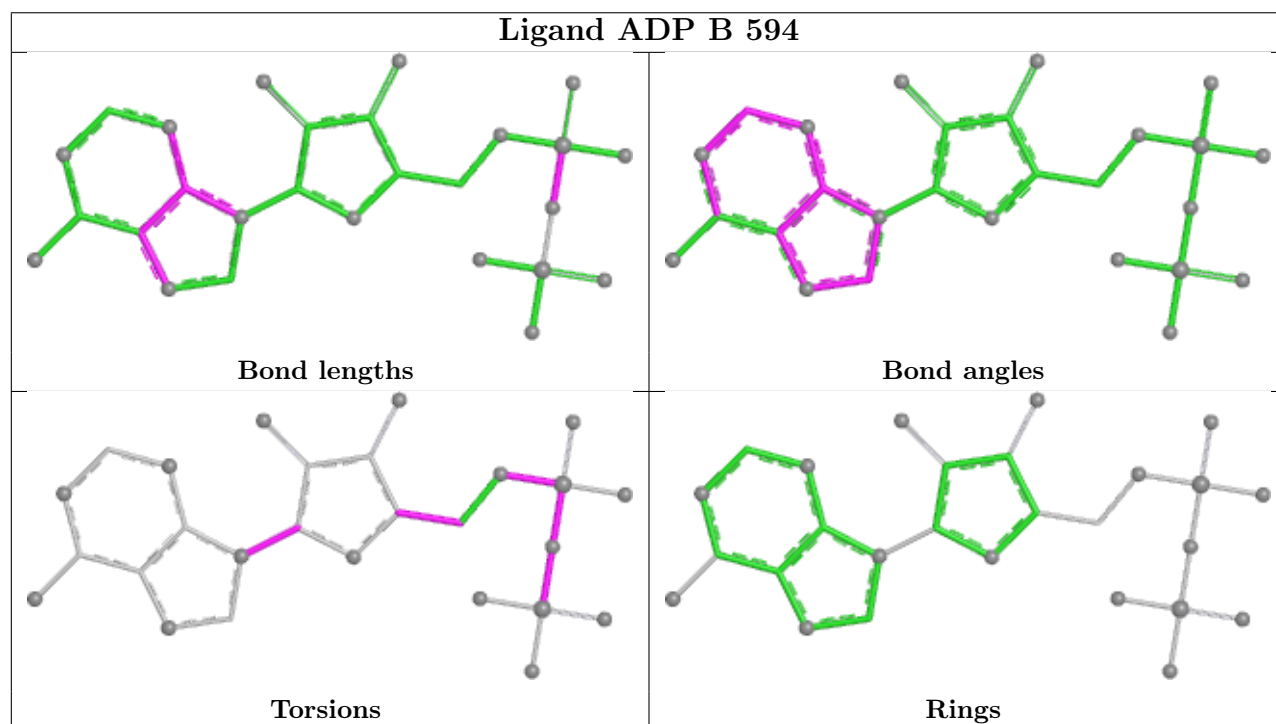
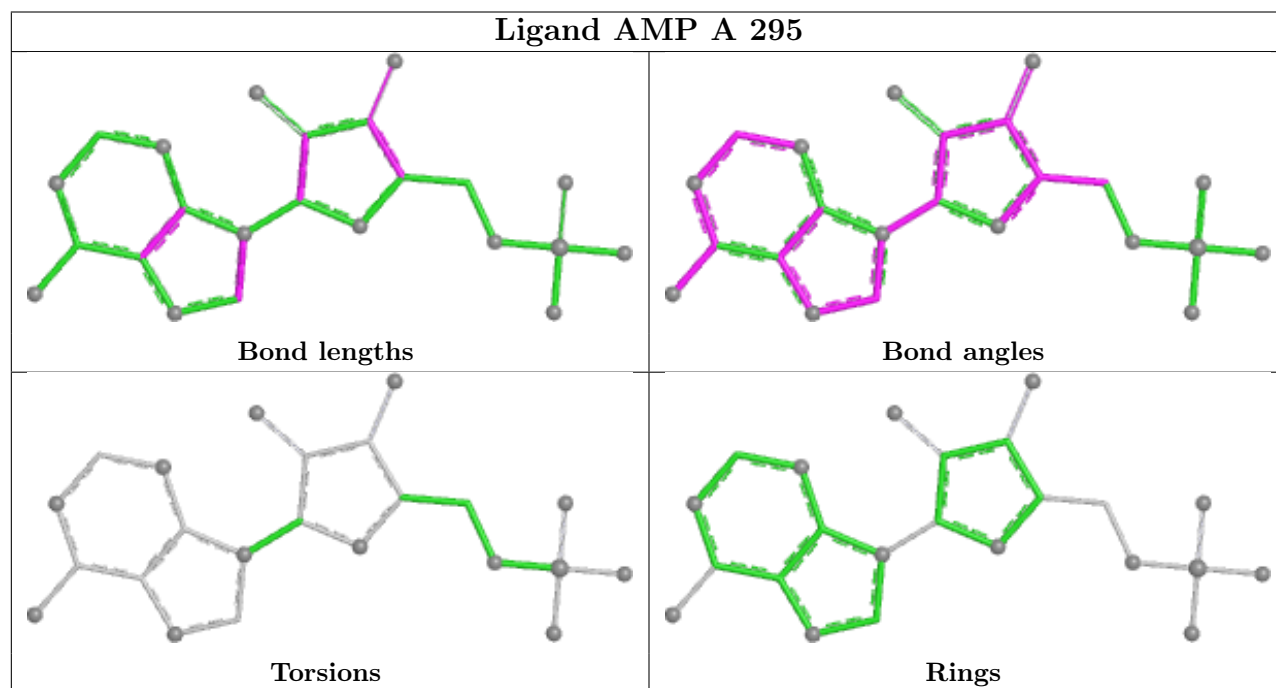
There are no ring outliers.

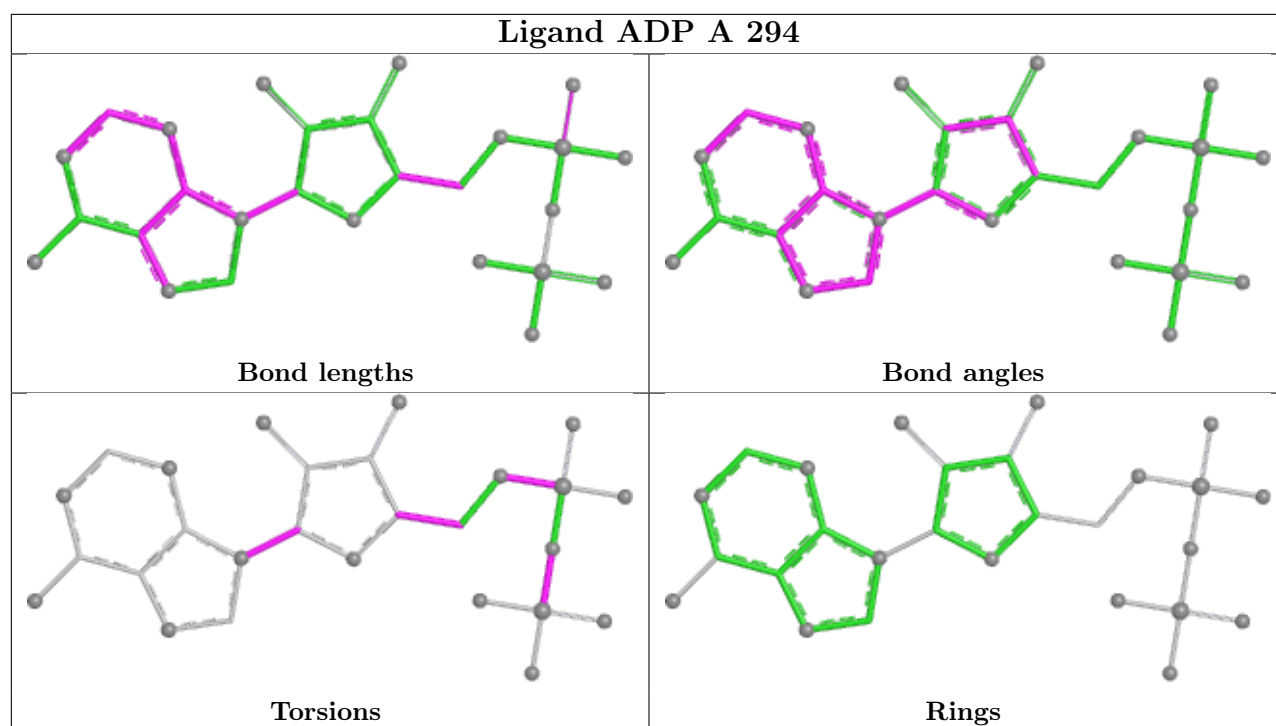
6 monomers are involved in 13 short contacts:

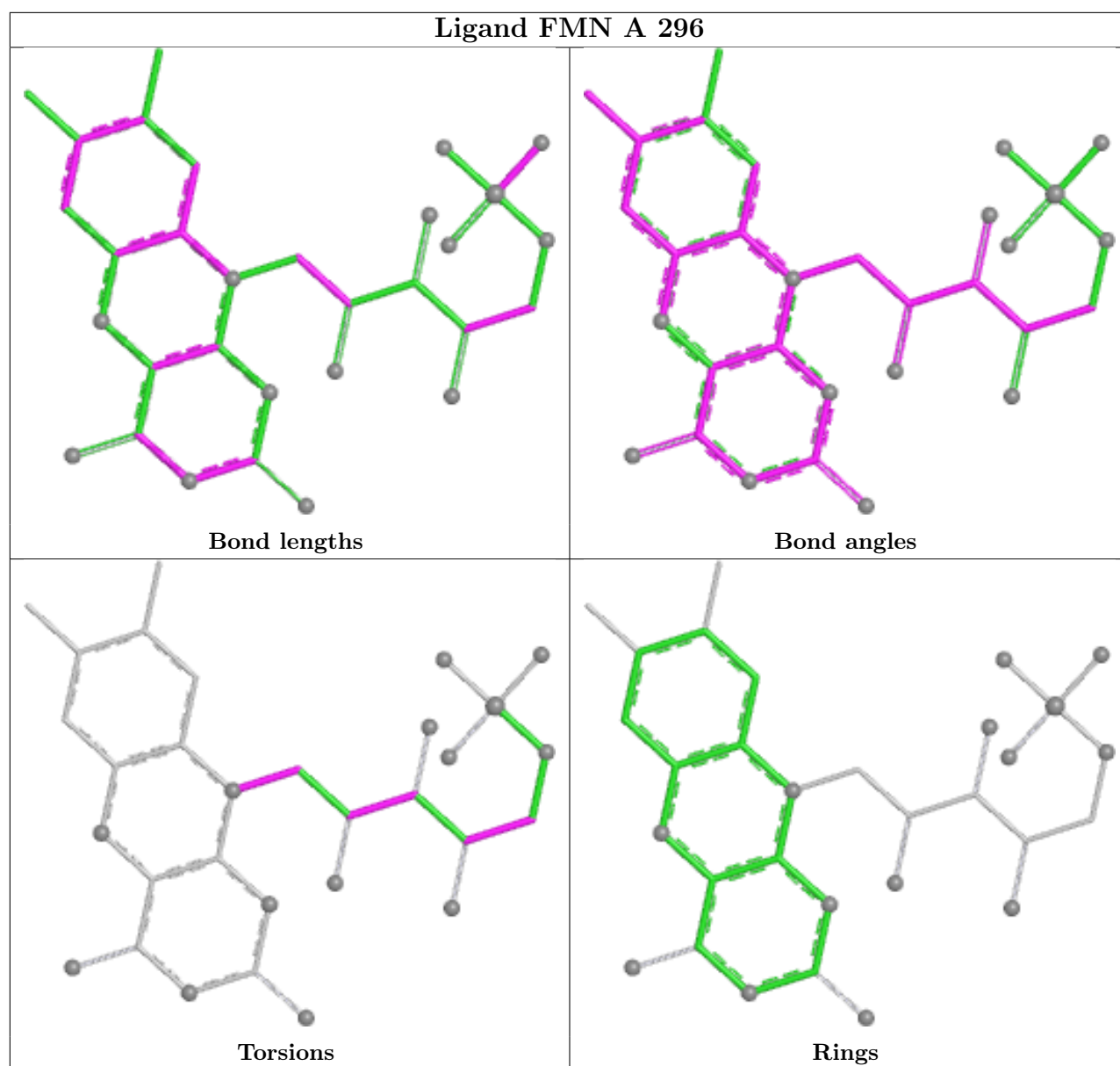
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	295	AMP	4	0
2	B	594	ADP	1	0
2	A	294	ADP	1	0
4	A	296	FMN	1	0
4	B	596	FMN	4	0
3	B	595	AMP	2	0

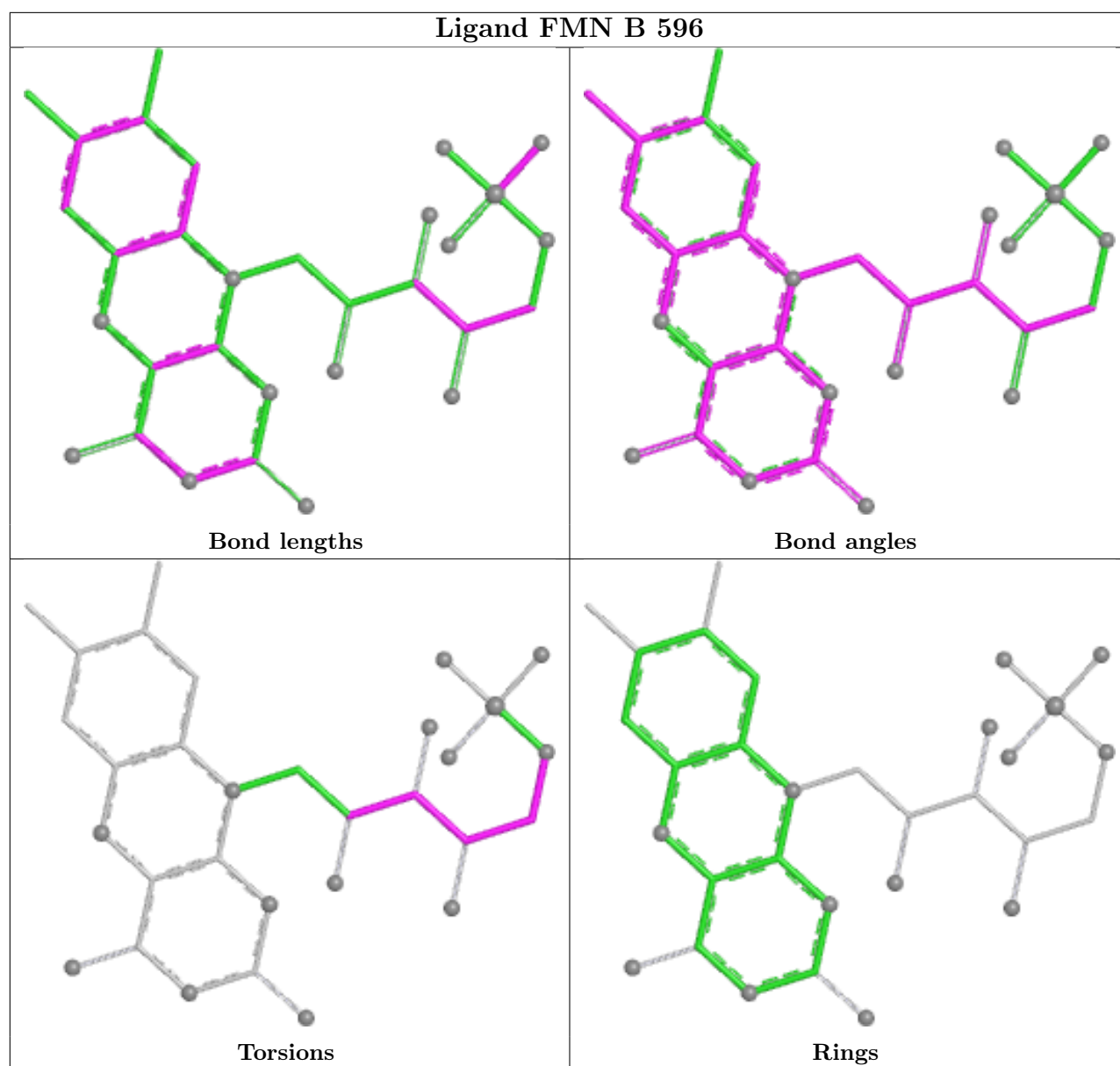
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

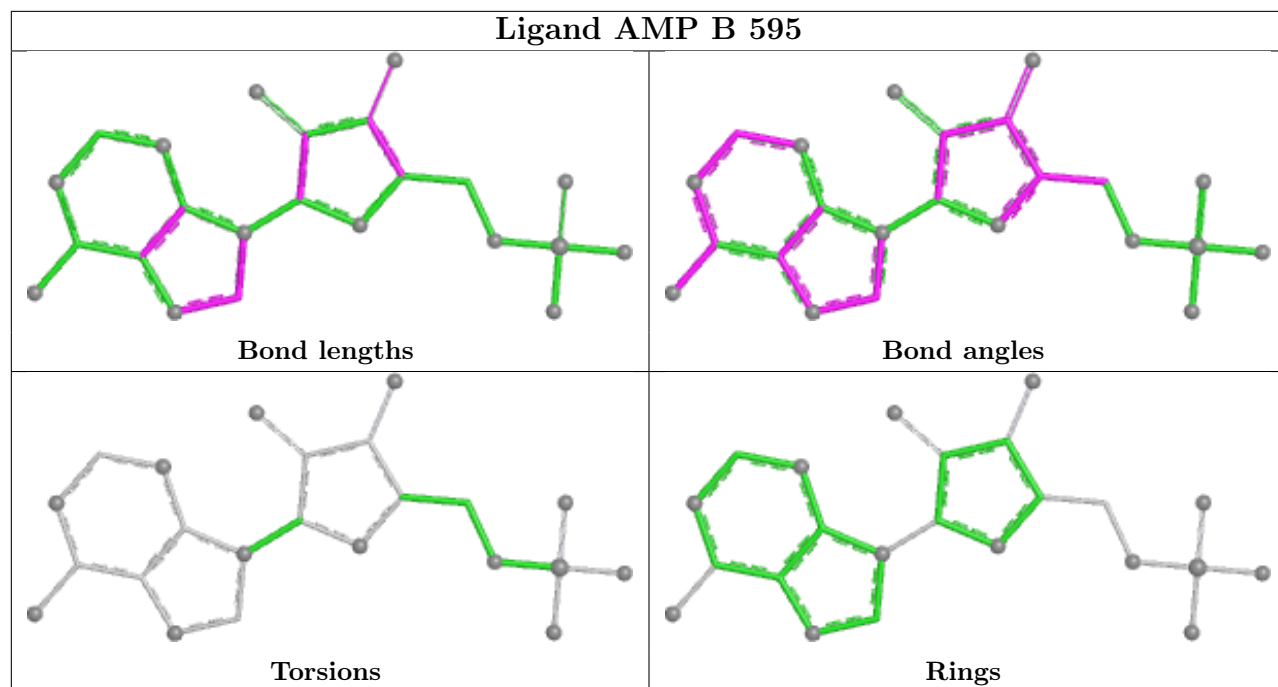
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	268/293 (91%)	-0.33	0 100 100	31, 77, 119, 144	0
1	B	270/293 (92%)	-0.43	0 100 100	42, 74, 116, 141	0
All	All	538/586 (91%)	-0.38	0 100 100	31, 75, 116, 144	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

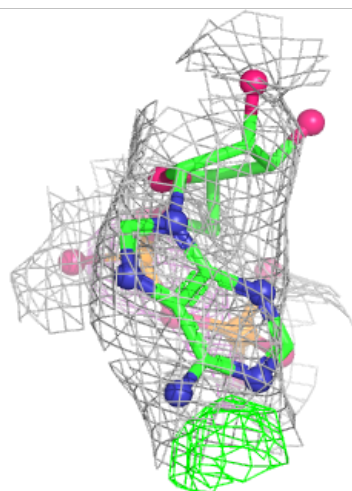
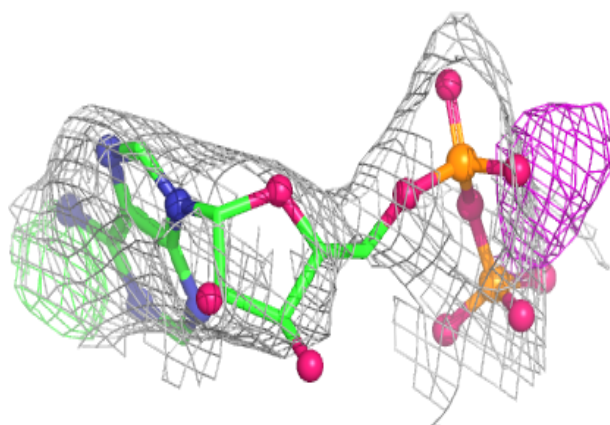
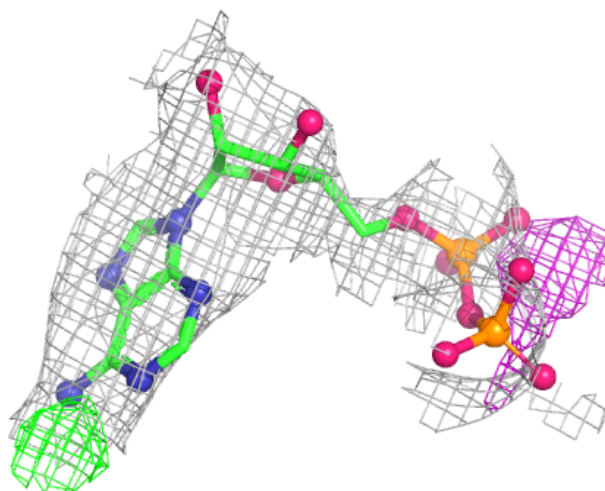
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	A	294	27/27	0.68	0.12	118,126,148,148	0
4	FMN	B	596	31/31	0.81	0.10	59,66,127,128	0
2	ADP	B	594	27/27	0.85	0.08	124,130,138,138	0
4	FMN	A	296	31/31	0.88	0.11	77,85,123,123	0
3	AMP	B	595	23/23	0.89	0.10	76,87,93,93	0
3	AMP	A	295	23/23	0.93	0.09	72,75,86,86	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.

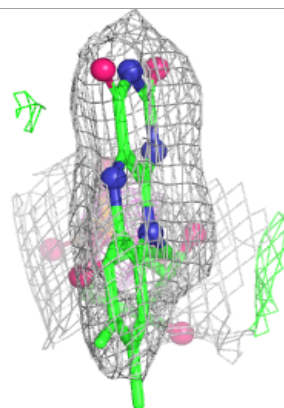
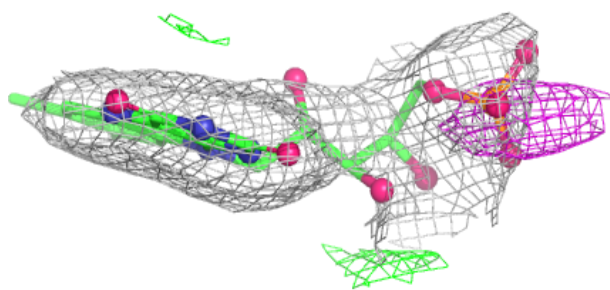
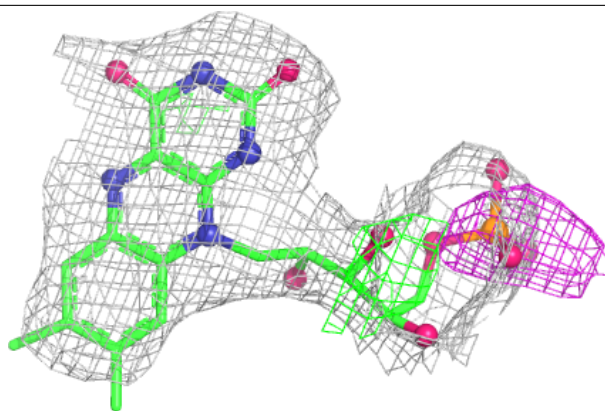
Electron density around ADP A 294:

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

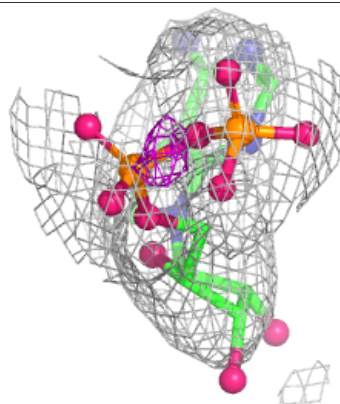
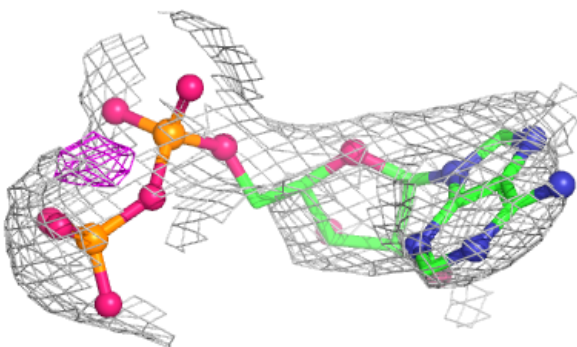
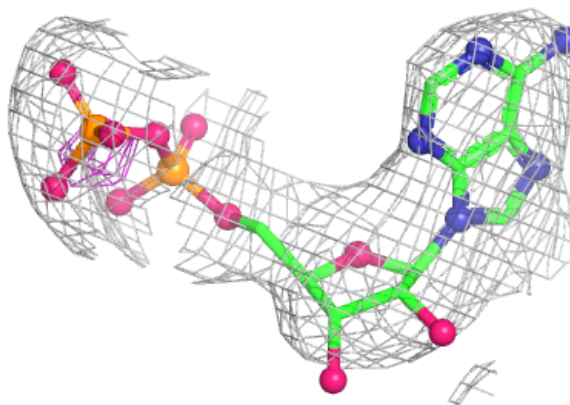


Electron density around FMN B 596:

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

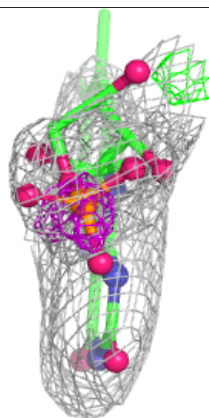
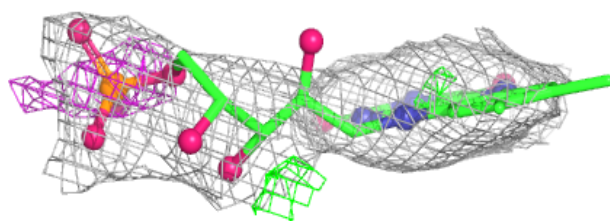
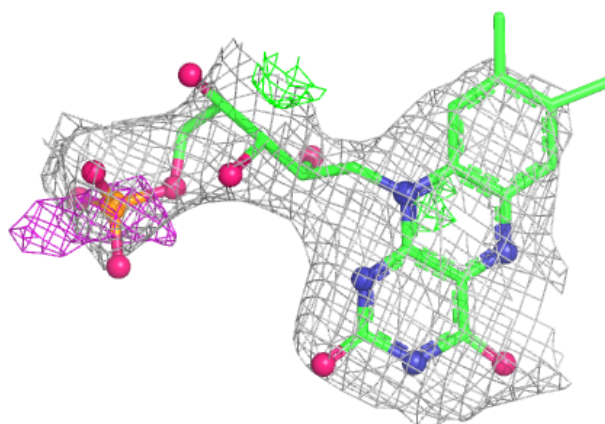
**Electron density around ADP B 594:**

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



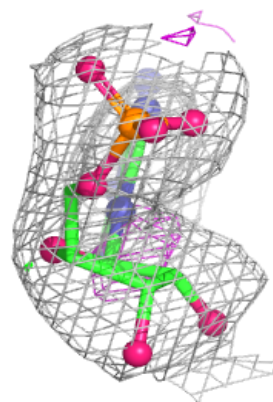
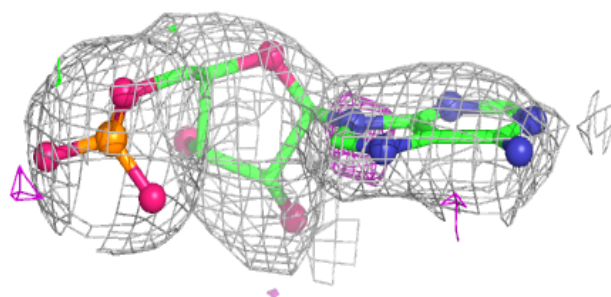
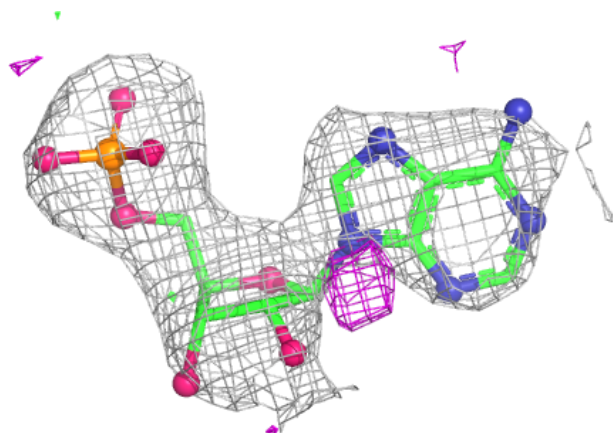
Electron density around FMN A 296:

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



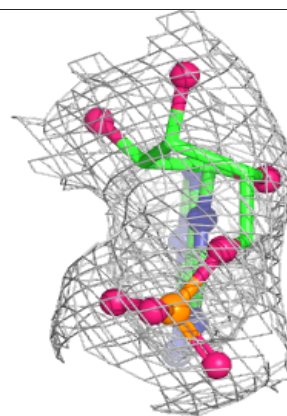
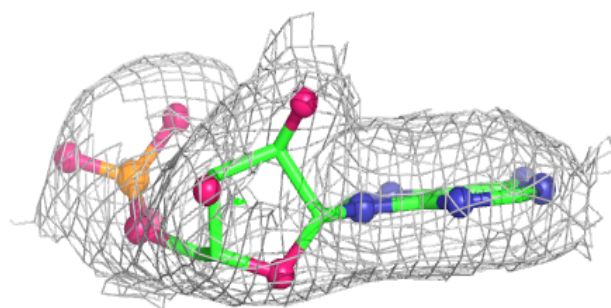
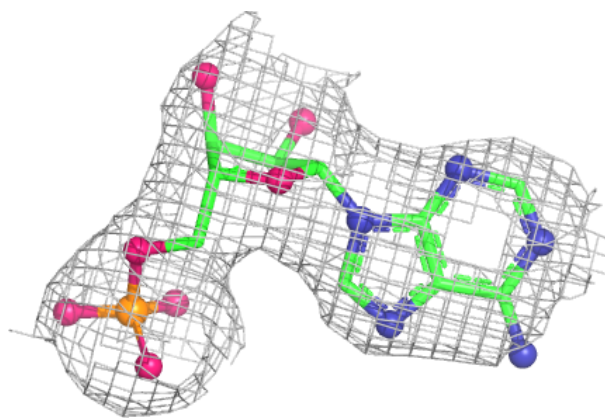
Electron density around AMP B 595:

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



Electron density around AMP A 295:

$2mF_o-DF_c$ (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.