



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:49 AM UTC

PDB ID : 2J4D / pdb_00002j4d
Title : Cryptochrome 3 from Arabidopsis thaliana
Authors : Klar, T.; Pokorny, R.; Batschauer, A.; Essen, L.-O.
Deposited on : 2006-08-28
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

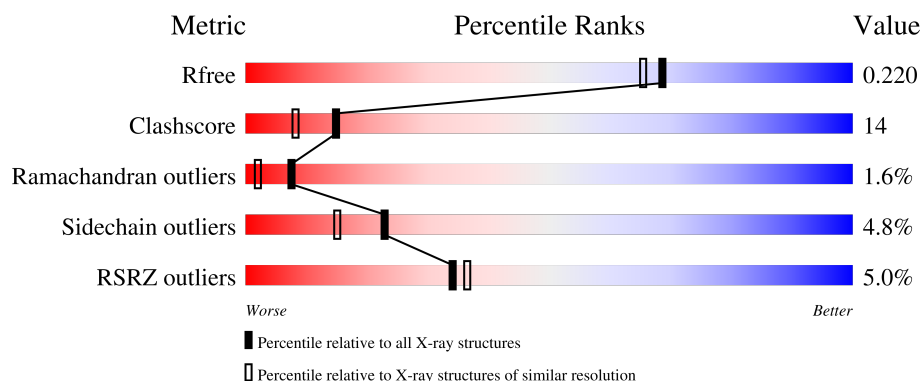
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	525	4% 72% 18% • • 6%
1	B	525	6% 70% 18% 5% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9038 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 CRYPTOCHROME DASH.

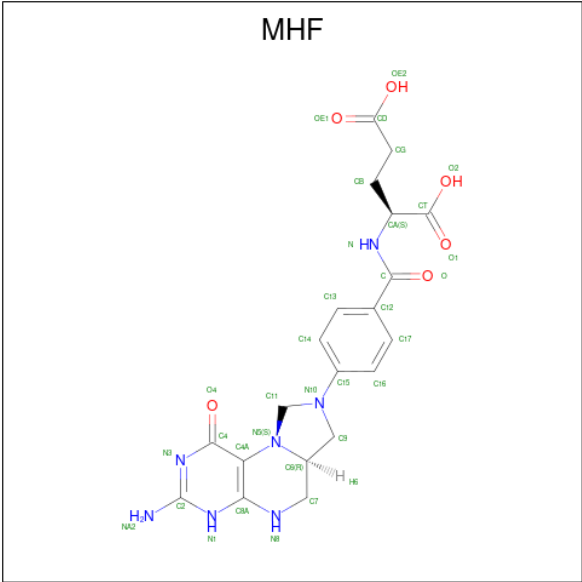
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			4050	2596	702	732	20			
1	B	499	Total	C	N	O	S	9	0	0
			4069	2607	706	736	20			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

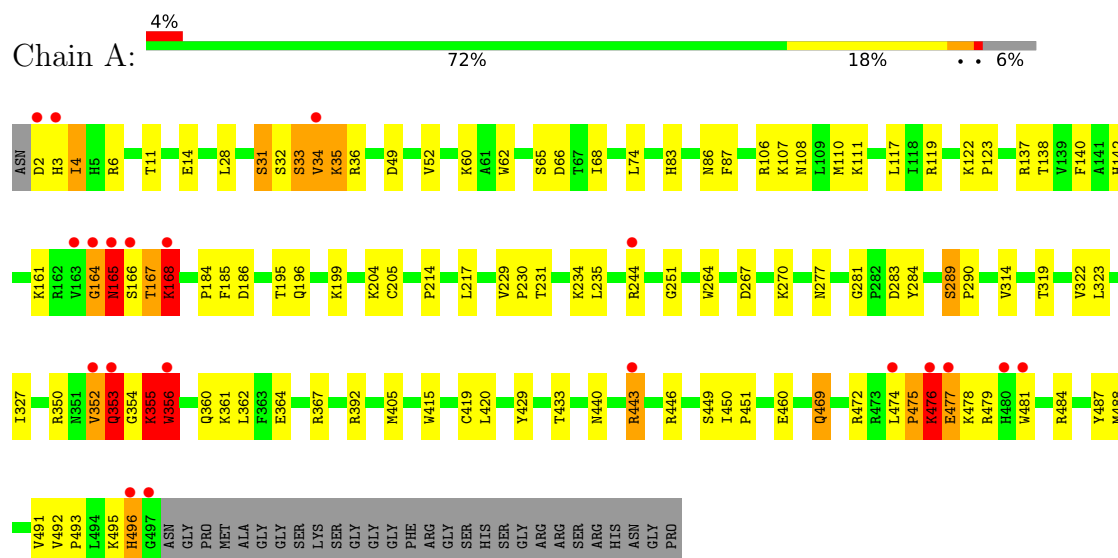
- Molecule 3 is 5,10-METHENYL-6,7,8-TRIHYDROFOLIC ACID (CCD ID: MHF) (formula: $C_{20}H_{23}N_7O_6$).



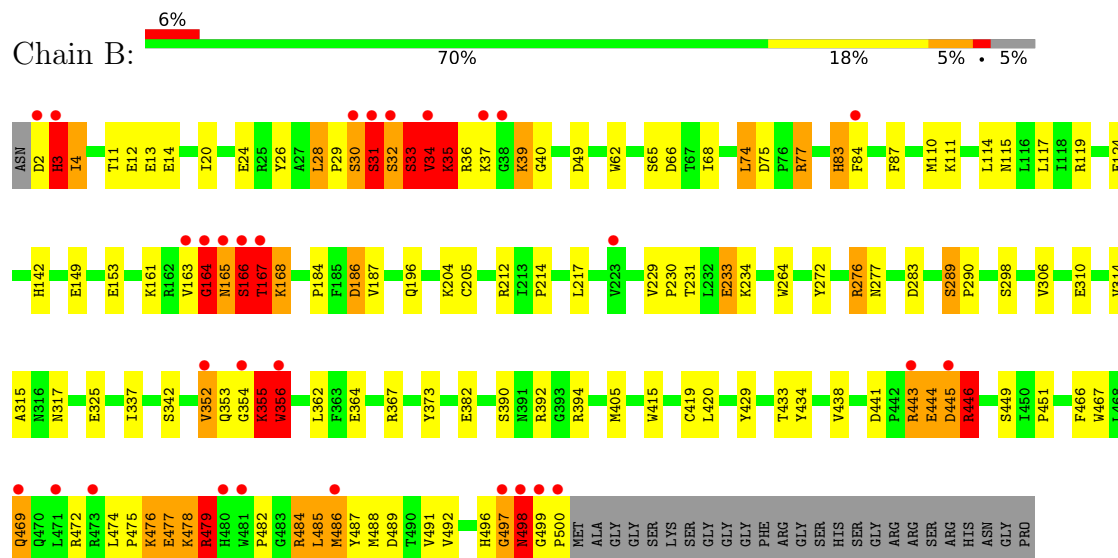
3 Residue-property plots

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: CRYPTOCHROME DASH



• Molecule 1: CRYPTOCHROME DASH



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.30Å 116.78Å 135.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.90) 97.4 (20.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.221 0.189 , 0.220	Depositor DCC
R_{free} test set	1420 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9038	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: FAD, MHF

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	0.51	1/4162 (0.0%)	1.07	35/5631 (0.6%)
1	B	0.80	2/4182 (0.0%)	1.23	50/5659 (0.9%)
All	All	0.67	3/8344 (0.0%)	1.15	85/11290 (0.8%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	GLY	C-N	-41.32	0.79	1.33
1	A	164	GLY	C-N	-17.05	1.09	1.33
1	B	34	VAL	CA-CB	5.47	1.61	1.54

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	GLY	O-C-N	-28.09	86.19	122.70
1	B	39	LYS	N-CA-C	18.60	135.23	112.54
1	B	166	SER	N-CA-C	-14.36	85.29	108.12
1	B	33	SER	N-CA-C	-13.75	81.50	110.80
1	B	32	SER	N-CA-C	-10.96	93.15	110.14
1	A	352	VAL	N-CA-C	10.48	124.01	109.55
1	B	354	GLY	N-CA-C	10.47	124.06	110.45
1	A	419	CYS	N-CA-C	9.84	123.79	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	CYS	N-CA-C	9.67	123.58	111.69
1	B	83	HIS	N-CA-C	9.19	120.90	111.07
1	B	445	ASP	N-CA-C	-9.19	91.24	110.80
1	A	167	THR	CA-C-N	8.95	135.07	122.72
1	A	167	THR	C-N-CA	8.95	135.07	122.72
1	A	356	TRP	N-CA-C	8.77	129.49	110.80
1	B	164	GLY	CA-C-N	-8.69	108.15	122.32
1	B	164	GLY	C-N-CA	-8.69	108.15	122.32
1	A	229	VAL	N-CA-C	-8.36	100.76	108.95
1	B	356	TRP	N-CA-C	8.14	128.14	110.80
1	B	167	THR	O-C-N	-8.12	111.79	122.59
1	A	83	HIS	N-CA-C	8.09	120.89	111.02
1	A	283	ASP	N-CA-C	8.03	120.94	111.71
1	A	87	PHE	N-CA-C	-7.80	101.16	110.13
1	A	355	LYS	N-CA-C	7.60	126.99	110.80
1	B	166	SER	O-C-N	7.53	127.48	120.71
1	B	445	ASP	CB-CA-C	7.50	125.34	110.42
1	B	283	ASP	N-CA-C	7.42	120.42	111.82
1	B	446	ARG	N-CA-C	7.39	126.55	110.80
1	A	165	ASN	N-CA-C	-7.38	95.08	110.80
1	B	31	SER	N-CA-C	7.25	126.24	110.80
1	B	87	PHE	N-CA-C	-7.01	102.07	110.13
1	B	168	LYS	N-CA-C	6.77	121.09	110.32
1	A	496	HIS	N-CA-C	6.57	120.89	107.69
1	B	4	ILE	N-CA-C	6.56	117.56	107.99
1	B	264	TRP	N-CA-C	6.50	119.63	111.24
1	A	481	TRP	CA-C-N	6.49	126.12	119.56
1	A	481	TRP	C-N-CA	6.49	126.12	119.56
1	A	86	ASN	N-CA-C	6.42	120.24	111.39
1	A	420	LEU	N-CA-C	6.29	119.39	109.96
1	A	352	VAL	CB-CA-C	-6.29	102.96	111.63
1	B	276	ARG	N-CA-C	6.07	120.22	112.34
1	B	165	ASN	N-CA-C	-5.90	97.84	108.58
1	B	229	VAL	N-CA-C	-5.90	103.17	108.95
1	B	353	GLN	CA-C-N	-5.88	111.77	121.12
1	B	353	GLN	C-N-CA	-5.88	111.77	121.12
1	B	498	ASN	N-CA-C	-5.81	98.42	110.80
1	B	420	LEU	N-CA-C	5.80	118.60	109.96
1	B	167	THR	CA-C-N	5.79	131.97	122.07
1	B	167	THR	C-N-CA	5.79	131.97	122.07
1	A	289	SER	N-CA-C	5.75	121.45	113.45
1	A	264	TRP	N-CA-C	5.74	120.34	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	GLY	N-CA-C	5.71	119.20	111.72
1	B	40	GLY	N-CA-C	5.70	122.85	112.58
1	A	355	LYS	CA-C-N	5.65	132.34	121.54
1	A	355	LYS	C-N-CA	5.65	132.34	121.54
1	B	298	SER	CA-C-N	5.60	125.27	119.05
1	B	298	SER	C-N-CA	5.60	125.27	119.05
1	B	186	ASP	N-CA-C	-5.53	102.30	110.48
1	A	186	ASP	N-CA-C	-5.52	102.31	110.48
1	B	34	VAL	N-CA-C	-5.51	97.89	109.34
1	A	52	VAL	N-CA-C	-5.48	107.09	111.81
1	A	446	ARG	N-CA-C	5.42	117.43	109.24
1	A	167	THR	O-C-N	-5.40	117.01	123.27
1	A	484	ARG	N-CA-C	5.39	119.11	112.54
1	B	497	GLY	N-CA-C	5.35	120.97	111.02
1	B	443	ARG	CA-C-N	-5.34	115.07	123.13
1	B	443	ARG	C-N-CA	-5.34	115.07	123.13
1	B	355	LYS	CA-C-N	5.29	131.64	121.54
1	B	355	LYS	C-N-CA	5.29	131.64	121.54
1	B	496	HIS	N-CA-C	5.28	117.26	108.02
1	B	66	ASP	N-CA-C	-5.27	106.79	114.12
1	B	204	LYS	N-CA-C	5.22	120.50	113.72
1	A	165	ASN	CB-CA-C	5.17	120.71	110.42
1	B	342	SER	N-CA-C	-5.17	106.81	113.01
1	A	281	GLY	CA-C-N	5.17	124.67	119.19
1	A	281	GLY	C-N-CA	5.17	124.67	119.19
1	A	493	PRO	N-CA-C	-5.14	103.76	111.57
1	A	168	LYS	N-CA-C	5.13	117.61	109.24
1	B	3	HIS	N-CA-CB	-5.11	101.86	110.49
1	B	479	ARG	N-CA-C	5.09	117.56	111.71
1	A	284	TYR	N-CA-C	5.08	118.74	112.54
1	B	289	SER	N-CA-C	5.07	120.47	113.77
1	A	475	PRO	N-CA-C	-5.04	103.61	111.13
1	A	353	GLN	N-CA-C	5.02	121.48	110.80
1	B	373	TYR	CA-C-N	5.01	124.45	119.24
1	B	373	TYR	C-N-CA	5.01	124.45	119.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	164	GLY	Mainchain

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	4050	0	3973	104	0
1	B	4069	0	3989	121	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	33	0	21	0	0
3	B	33	0	21	0	0
4	A	437	0	0	4	0
4	B	310	0	0	6	0
All	All	9038	0	8066	225	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 14.

All (225) 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:B:35:LYS:O	1:B:39:LYS:HE3	1.31	1.30
1:B:32:SER:HA	1:B:34:VAL:CG1	1.63	1.28
1:B:484:ARG:NH1	1:B:489:ASP:OD1	1.78	1.17
1:B:34:VAL:HG22	1:B:35:LYS:H	0.97	1.07
1:B:32:SER:CA	1:B:34:VAL:HG12	1.89	1.01
1:B:32:SER:HA	1:B:34:VAL:HG12	0.97	0.97
1:B:34:VAL:CG2	1:B:35:LYS:H	1.76	0.95
1:B:34:VAL:HG23	1:B:36:ARG:HG3	1.49	0.94
1:B:34:VAL:O	1:B:35:LYS:HB2	1.63	0.94
1:B:34:VAL:HG22	1:B:35:LYS:N	1.77	0.93
1:B:34:VAL:CG2	1:B:36:ARG:HG3	1.99	0.93
1:B:36:ARG:HA	1:B:39:LYS:HD2	1.49	0.92
1:A:355:LYS:HG3	1:A:356:TRP:H	1.36	0.91
1:B:35:LYS:O	1:B:39:LYS:CE	2.19	0.89
1:B:486:MET:HE2	1:B:486:MET:H	1.36	0.89
1:A:495:LYS:HE2	1:A:496:HIS:NE2	1.88	0.88
1:B:498:ASN:HD22	1:B:499:GLY:H	1.19	0.87
1:A:355:LYS:CG	1:A:356:TRP:H	1.83	0.81
1:B:497:GLY:O	1:B:498:ASN:HB2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:HG3	4:A:2175:HOH:O	1.85	0.77
1:B:164:GLY:C	1:B:166:SER:N	2.44	0.75
1:B:34:VAL:CG2	1:B:35:LYS:N	2.38	0.74
1:B:32:SER:O	1:B:33:SER:HB3	1.86	0.73
1:A:49:ASP:OD2	1:A:142:HIS:HD2	1.72	0.72
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.55	0.72
1:B:486:MET:HE2	1:B:486:MET:N	2.05	0.71
1:B:498:ASN:ND2	1:B:499:GLY:H	1.88	0.70
1:A:34:VAL:HG11	1:A:62:TRP:CH2	2.26	0.70
1:B:75:ASP:OD1	1:B:77:ARG:HD2	1.92	0.69
1:B:445:ASP:O	1:B:446:ARG:HB2	1.91	0.69
1:A:476:LYS:HA	1:A:479:ARG:HG3	1.73	0.69
1:B:184:PRO:HD3	1:B:205:CYS:SG	2.32	0.69
1:A:165:ASN:O	1:A:166:SER:HB3	1.93	0.69
1:A:244:ARG:NH1	1:A:469:GLN:HE22	1.90	0.69
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.08	0.69
1:B:39:LYS:HB3	1:B:65:SER:HA	1.75	0.68
1:A:355:LYS:HG3	1:A:356:TRP:N	2.09	0.68
1:B:477:GLU:H	1:B:477:GLU:CD	2.01	0.67
1:B:164:GLY:C	1:B:165:ASN:C	2.37	0.67
1:B:352:VAL:CG1	1:B:438:VAL:HG12	2.25	0.67
1:B:289:SER:OG	1:B:290:PRO:HD3	1.95	0.67
1:B:20:ILE:O	1:B:24:GLU:HG3	1.96	0.66
1:A:74:LEU:HD21	1:A:235:LEU:CD1	2.24	0.66
1:A:352:VAL:CG1	1:A:353:GLN:HB2	2.26	0.65
1:B:498:ASN:HD22	1:B:499:GLY:N	1.93	0.65
1:B:119:ARG:HD2	4:B:2091:HOH:O	1.97	0.64
1:B:352:VAL:HG11	1:B:438:VAL:HG12	1.79	0.64
1:B:484:ARG:HH11	1:B:489:ASP:CG	2.02	0.64
1:A:460:GLU:OE2	1:A:476:LYS:HE3	1.98	0.64
1:B:49:ASP:OD2	1:B:142:HIS:HD2	1.80	0.64
1:B:28:LEU:HD23	1:B:29:PRO:HD2	1.80	0.63
1:B:196:GLN:HG3	4:B:2053:HOH:O	1.99	0.63
1:A:277:ASN:HD21	1:A:392:ARG:HH21	1.47	0.62
1:A:353:GLN:HG3	1:A:354:GLY:H	1.63	0.62
1:A:138:THR:HG22	1:A:168:LYS:CG	2.29	0.62
1:A:196:GLN:HG3	4:A:2075:HOH:O	1.98	0.62
1:A:469:GLN:CD	1:A:469:GLN:H	2.07	0.62
1:B:478:LYS:HE2	1:B:478:LYS:HA	1.82	0.62
1:B:486:MET:H	1:B:486:MET:CE	2.11	0.61
1:A:35:LYS:NZ	1:A:35:LYS:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:HH22	1:A:472:ARG:NH2	1.99	0.60
1:A:352:VAL:CG1	1:A:353:GLN:N	2.64	0.59
1:A:476:LYS:HB2	1:A:477:GLU:OE2	2.02	0.59
1:A:231:THR:HG23	1:A:234:LYS:HE3	1.84	0.59
1:A:277:ASN:ND2	1:A:392:ARG:HH21	2.00	0.59
1:A:35:LYS:O	1:A:35:LYS:HG2	2.02	0.58
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.15	0.58
1:B:231:THR:OG1	1:B:234:LYS:HG3	2.02	0.58
1:B:231:THR:HG23	1:B:234:LYS:HE3	1.83	0.58
1:B:434:TYR:HE2	1:B:444:GLU:OE2	1.85	0.58
1:B:485:LEU:CD1	1:B:485:LEU:C	2.77	0.58
1:A:62:TRP:HA	1:A:68:ILE:HD11	1.86	0.57
1:A:352:VAL:HG12	1:A:353:GLN:CB	2.34	0.57
1:B:77:ARG:NH2	1:B:124:GLU:OE2	2.36	0.57
1:B:485:LEU:HB3	1:B:486:MET:HE2	1.85	0.57
1:A:184:PRO:HD3	1:A:205:CYS:SG	2.45	0.56
1:A:450:ILE:N	1:A:451:PRO:HD2	2.20	0.56
1:B:2:ASP:HB3	1:B:466:PHE:HE2	1.70	0.56
1:A:353:GLN:CG	1:A:354:GLY:H	2.18	0.56
1:B:32:SER:CA	1:B:34:VAL:CG1	2.59	0.56
1:A:350:ARG:HB3	1:A:352:VAL:HG23	1.87	0.56
1:B:11:THR:OG1	1:B:14:GLU:HG3	2.05	0.56
1:B:485:LEU:C	1:B:485:LEU:HD13	2.31	0.56
1:B:32:SER:HA	1:B:34:VAL:HG13	1.76	0.56
1:A:214:PRO:HG2	1:A:217:LEU:CD2	2.37	0.56
1:A:495:LYS:CE	1:A:496:HIS:NE2	2.66	0.55
1:A:60:LYS:HG3	1:A:140:PHE:CE1	2.41	0.55
1:B:367:ARG:HG3	1:B:415:TRP:CE2	2.42	0.54
1:A:74:LEU:CD2	1:A:235:LEU:HD21	2.36	0.54
1:B:445:ASP:O	1:B:446:ARG:CB	2.52	0.54
1:A:475:PRO:O	1:A:479:ARG:HG2	2.08	0.54
1:A:74:LEU:HD21	1:A:235:LEU:HD11	1.88	0.54
1:A:138:THR:HG22	1:A:168:LYS:HG3	1.90	0.54
1:B:74:LEU:HD13	1:B:230:PRO:HG3	1.89	0.54
1:A:429:TYR:O	1:A:433:THR:HG23	2.07	0.54
1:B:36:ARG:HA	1:B:39:LYS:CD	2.30	0.53
1:A:360:GLN:O	1:A:364:GLU:HG3	2.08	0.53
1:A:352:VAL:HG13	1:A:353:GLN:HB2	1.90	0.53
1:A:138:THR:HG22	1:A:168:LYS:HG2	1.91	0.53
1:B:26:TYR:O	1:B:212:ARG:HD2	2.09	0.53
1:B:34:VAL:HG23	1:B:36:ARG:CG	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:SER:HB3	2:B:1501:FAD:H5'2	1.90	0.53
1:A:74:LEU:HD22	1:A:230:PRO:HG3	1.90	0.52
1:B:434:TYR:CE2	1:B:444:GLU:OE2	2.63	0.52
1:A:475:PRO:C	1:A:476:LYS:O	2.47	0.52
1:B:487:TYR:CZ	1:B:488:MET:HE3	2.45	0.52
1:A:108:ASN:HA	1:A:111:LYS:HE2	1.92	0.52
1:B:75:ASP:OD1	1:B:77:ARG:CD	2.58	0.52
1:A:11:THR:OG1	1:A:14:GLU:HG3	2.10	0.51
1:B:382:GLU:HG3	1:B:467:TRP:CZ2	2.45	0.51
1:B:364:GLU:HG2	1:B:367:ARG:NH2	2.25	0.51
1:A:214:PRO:HG2	1:A:217:LEU:HD23	1.92	0.51
1:B:29:PRO:O	1:B:30:SER:C	2.52	0.51
1:B:36:ARG:HB3	1:B:65:SER:O	2.10	0.51
1:A:350:ARG:HD2	1:A:352:VAL:CG2	2.40	0.51
1:A:164:GLY:C	1:A:165:ASN:O	2.39	0.51
1:B:277:ASN:ND2	4:B:2199:HOH:O	2.43	0.51
1:A:34:VAL:HA	1:A:35:LYS:NZ	2.26	0.51
1:A:34:VAL:HA	1:A:35:LYS:HZ2	1.76	0.50
1:B:29:PRO:O	1:B:30:SER:O	2.30	0.50
1:B:355:LYS:C	1:B:356:TRP:CD1	2.89	0.50
1:B:2:ASP:CG	1:B:3:HIS:H	2.20	0.50
1:B:111:LYS:NZ	4:B:2085:HOH:O	2.45	0.50
1:B:39:LYS:CB	1:B:65:SER:HA	2.42	0.50
1:A:35:LYS:H	1:A:35:LYS:HZ3	1.60	0.49
1:A:289:SER:HB3	2:A:1498:FAD:H5'2	1.93	0.49
1:A:319:THR:O	1:A:322:VAL:HG12	2.12	0.49
1:B:164:GLY:C	1:B:166:SER:H	2.19	0.49
1:B:276:ARG:HD3	4:B:2193:HOH:O	2.13	0.49
1:B:352:VAL:HG13	1:B:438:VAL:HG12	1.95	0.49
1:B:187:VAL:HG21	1:B:337:ILE:HG21	1.95	0.49
1:A:244:ARG:NH2	1:A:472:ARG:HH22	2.11	0.49
1:A:352:VAL:HG12	1:A:353:GLN:HB2	1.94	0.48
1:B:362:LEU:HD22	1:B:405:MET:HE2	1.96	0.48
1:A:195:THR:CG2	1:A:199:LYS:HE2	2.44	0.48
1:A:267:ASP:OD2	1:A:270:LYS:HE3	2.14	0.48
1:B:478:LYS:HE2	1:B:478:LYS:CA	2.42	0.48
1:A:476:LYS:O	1:A:477:GLU:HB2	2.14	0.48
1:B:30:SER:OG	1:B:31:SER:N	2.46	0.48
1:A:362:LEU:O	1:A:405:MET:HE1	2.13	0.48
1:A:367:ARG:HG3	1:A:415:TRP:CE2	2.49	0.48
1:B:83:HIS:CD2	1:B:84:PHE:CZ	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LYS:HG2	1:B:477:GLU:N	2.28	0.47
1:B:28:LEU:CD2	1:B:29:PRO:HD2	2.45	0.47
1:B:110:MET:HA	1:B:114:LEU:O	2.15	0.47
1:A:195:THR:HG22	1:A:199:LYS:HE2	1.97	0.47
1:A:491:VAL:HG13	1:A:492:VAL:HG22	1.96	0.47
1:B:364:GLU:HG2	1:B:367:ARG:CZ	2.45	0.47
1:A:165:ASN:O	1:A:166:SER:CB	2.57	0.47
1:A:476:LYS:O	1:A:477:GLU:CB	2.61	0.47
1:B:83:HIS:HD2	1:B:84:PHE:CE2	2.33	0.46
1:B:272:TYR:OH	1:B:325:GLU:HG3	2.15	0.46
1:B:485:LEU:HD13	1:B:485:LEU:O	2.15	0.46
1:A:244:ARG:NH1	1:A:469:GLN:NE2	2.61	0.46
1:A:244:ARG:NH2	1:A:472:ARG:NH2	2.62	0.46
1:B:3:HIS:HB3	1:B:4:ILE:H	1.41	0.46
1:A:74:LEU:HD21	1:A:235:LEU:HD13	1.97	0.46
1:B:36:ARG:CA	1:B:39:LYS:HD2	2.34	0.46
1:B:33:SER:O	1:B:34:VAL:O	2.33	0.46
1:B:474:LEU:O	1:B:479:ARG:HD3	2.15	0.46
1:B:482:PRO:HG2	1:B:487:TYR:HB2	1.98	0.46
1:A:4:ILE:H	1:A:4:ILE:HG12	1.61	0.45
1:A:478:LYS:HD2	1:A:478:LYS:HA	1.72	0.45
1:B:497:GLY:O	1:B:498:ASN:CB	2.56	0.45
1:A:36:ARG:O	1:A:66:ASP:HB3	2.16	0.45
1:B:166:SER:HB2	1:B:167:THR:H	1.14	0.45
1:A:289:SER:OG	1:A:290:PRO:HD3	2.17	0.45
1:A:107:LYS:O	1:A:111:LYS:HG3	2.16	0.44
1:B:168:LYS:H	1:B:168:LYS:HG2	1.54	0.44
1:A:231:THR:HG23	1:A:234:LYS:CE	2.47	0.44
1:B:306:VAL:O	1:B:310:GLU:HG3	2.17	0.44
1:B:163:VAL:O	1:B:163:VAL:HG12	2.17	0.44
1:B:277:ASN:HD21	1:B:392:ARG:HH21	1.65	0.44
1:A:137:ARG:O	1:A:168:LYS:HE3	2.17	0.44
1:A:204:LYS:NZ	4:A:2233:HOH:O	2.51	0.44
1:A:352:VAL:HG13	1:A:353:GLN:N	2.32	0.44
1:A:477:GLU:N	1:A:477:GLU:CD	2.76	0.44
1:B:469:GLN:HB3	1:B:472:ARG:CZ	2.48	0.44
1:A:117:LEU:HD11	1:A:119:ARG:CZ	2.48	0.44
1:B:484:ARG:HD3	1:B:489:ASP:OD2	2.18	0.44
1:A:74:LEU:HD23	1:A:235:LEU:HD21	2.00	0.44
1:B:62:TRP:HA	1:B:68:ILE:HD11	2.00	0.44
1:B:429:TYR:O	1:B:433:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:TYR:CZ	1:A:488:MET:HE3	2.52	0.44
1:B:475:PRO:O	1:B:479:ARG:HG2	2.18	0.44
1:A:74:LEU:CD2	1:A:235:LEU:CD2	2.95	0.43
1:A:474:LEU:O	1:A:479:ARG:HD3	2.18	0.43
1:B:149:GLU:O	1:B:153:GLU:HG3	2.18	0.43
1:B:477:GLU:N	1:B:477:GLU:OE1	2.46	0.43
1:B:491:VAL:HG23	1:B:492:VAL:HG13	1.99	0.43
1:A:350:ARG:HA	1:A:440:ASN:HD21	1.83	0.43
1:B:390:SER:O	1:B:394:ARG:HG3	2.18	0.43
1:B:117:LEU:HD11	1:B:119:ARG:NH2	2.33	0.43
1:B:277:ASN:ND2	1:B:392:ARG:HH21	2.17	0.43
1:A:476:LYS:H	1:A:476:LYS:HD3	1.83	0.43
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.87	0.43
1:B:314:VAL:HG22	1:B:315:ALA:N	2.33	0.42
1:A:31:SER:O	1:A:32:SER:C	2.62	0.42
1:B:310:GLU:HB3	1:B:315:ALA:HB2	2.02	0.42
1:B:34:VAL:HG21	1:B:36:ARG:HG3	1.96	0.42
1:B:110:MET:HE3	1:B:115:ASN:ND2	2.35	0.42
1:B:163:VAL:O	1:B:163:VAL:CG1	2.68	0.42
1:B:161:LYS:HE3	1:B:161:LYS:HB2	1.92	0.42
1:A:6:ARG:NH1	4:A:2003:HOH:O	2.53	0.42
1:B:186:ASP:HB3	4:B:2143:HOH:O	2.19	0.42
1:B:214:PRO:HD2	1:B:217:LEU:HD21	2.02	0.42
1:A:449:SER:OG	1:A:451:PRO:HG2	2.21	0.41
1:B:486:MET:HE3	1:B:486:MET:HB2	1.77	0.41
1:A:460:GLU:HB3	1:A:476:LYS:NZ	2.35	0.41
1:A:32:SER:OG	1:A:33:SER:N	2.52	0.41
1:B:449:SER:OG	1:B:451:PRO:HD2	2.21	0.41
1:A:49:ASP:OD2	1:A:142:HIS:CD2	2.63	0.41
1:A:106:ARG:O	1:A:110:MET:HG3	2.21	0.41
1:A:350:ARG:HD2	1:A:352:VAL:HG21	2.02	0.41
1:A:475:PRO:O	1:A:476:LYS:O	2.39	0.41
1:A:122:LYS:HA	1:A:123:PRO:HD3	1.97	0.40
1:A:36:ARG:HB3	1:A:65:SER:O	2.20	0.40
1:B:441:ASP:OD1	1:B:441:ASP:C	2.63	0.40
1:A:2:ASP:CG	1:A:3:HIS:H	2.30	0.40
1:A:165:ASN:O	1:A:167:THR:N	2.55	0.40
1:A:323:LEU:O	1:A:327:ILE:HG13	2.22	0.40
1:B:34:VAL:O	1:B:35:LYS:CB	2.48	0.40
1:B:83:HIS:HD2	1:B:84:PHE:CD2	2.40	0.40
1:A:353:GLN:CG	1:A:354:GLY:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:H	1:B:233:GLU:HG2	1.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/525 (94%)	465 (94%)	24 (5%)	5 (1%)	12	5
1	B	497/525 (95%)	458 (92%)	28 (6%)	11 (2%)	5	1
All	All	991/1050 (94%)	923 (93%)	52 (5%)	16 (2%)	7	2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	355	LYS
1	B	30	SER
1	B	33	SER
1	B	34	VAL
1	B	35	LYS
1	B	355	LYS
1	B	498	ASN
1	A	356	TRP
1	B	356	TRP
1	A	476	LYS
1	B	3	HIS
1	B	167	THR
1	A	165	ASN
1	B	31	SER
1	B	446	ARG

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	439/458 (96%)	424 (97%)	15 (3%)	32	25
1	B	441/458 (96%)	414 (94%)	27 (6%)	17	9
All	All	880/916 (96%)	838 (95%)	42 (5%)	23	15

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	28	LEU
1	A	31	SER
1	A	33	SER
1	A	34	VAL
1	A	35	LYS
1	A	168	LYS
1	A	185	PHE
1	A	314	VAL
1	A	353	GLN
1	A	361	LYS
1	A	443	ARG
1	A	469	GLN
1	A	476	LYS
1	A	477	GLU
1	B	3	HIS
1	B	12	GLU
1	B	13	GLU
1	B	28	LEU
1	B	34	VAL
1	B	35	LYS
1	B	37	LYS
1	B	74	LEU
1	B	77	ARG
1	B	166	SER
1	B	167	THR
1	B	233	GLU

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Mol	Chain	Res	Type
1	B	317	ASN
1	B	352	VAL
1	B	356	TRP
1	B	443	ARG
1	B	444	GLU
1	B	446	ARG
1	B	469	GLN
1	B	476	LYS
1	B	477	GLU
1	B	478	LYS
1	B	479	ARG
1	B	484	ARG
1	B	485	LEU
1	B	486	MET
1	B	500	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	142	HIS
1	A	277	ASN
1	A	353	GLN
1	A	428	ASN
1	A	440	ASN
1	A	469	GLN
1	B	83	HIS
1	B	142	HIS
1	B	277	ASN
1	B	353	GLN
1	B	428	ASN
1	B	440	ASN
1	B	496	HIS
1	B	498	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MHF	B	1502	-	35,36,36	2.10	8 (22%)	37,52,52	1.52	5 (13%)
2	FAD	A	1498	-	58,58,58	1.21	7 (12%)	85,89,89	0.95	4 (4%)
2	FAD	B	1501	-	58,58,58	1.25	5 (8%)	85,89,89	1.01	6 (7%)
3	MHF	A	1499	-	35,36,36	2.08	7 (20%)	37,52,52	1.37	4 (10%)

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	MHF	B	1502	-	-	4/21/42/42	0/4/4/4
2	FAD	A	1498	-	-	3/34/50/50	0/6/6/6
2	FAD	B	1501	-	-	4/34/50/50	0/6/6/6
3	MHF	A	1499	-	-	4/21/42/42	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1499	MHF	C8A-N8	8.16	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1502	MHF	C8A-N8	7.69	1.40	1.32
2	A	1498	FAD	C4X-N5	4.66	1.40	1.30
2	B	1501	FAD	C4X-N5	4.49	1.40	1.30
3	A	1499	MHF	C7-N8	4.04	1.50	1.46
3	B	1502	MHF	C7-N8	3.90	1.50	1.46
3	B	1502	MHF	C16-C15	3.52	1.45	1.39
3	A	1499	MHF	C16-C15	3.33	1.45	1.39
3	B	1502	MHF	C17-C12	3.10	1.44	1.39
2	B	1501	FAD	PA-O3P	3.08	1.62	1.59
2	A	1498	FAD	C10-N1	2.72	1.38	1.33
3	B	1502	MHF	C15-N10	2.55	1.45	1.38
2	B	1501	FAD	C2A-N1A	2.55	1.38	1.33
3	A	1499	MHF	C7-C6	2.52	1.55	1.52
3	A	1499	MHF	C13-C12	2.51	1.43	1.39
2	B	1501	FAD	C9A-C5X	2.47	1.45	1.41
3	B	1502	MHF	C7-C6	2.47	1.54	1.52
3	A	1499	MHF	C15-N10	2.42	1.45	1.38
3	B	1502	MHF	C13-C12	2.36	1.43	1.39
3	A	1499	MHF	C17-C12	2.26	1.42	1.39
2	A	1498	FAD	C2A-N1A	2.21	1.37	1.33
2	A	1498	FAD	C9-C9A	2.17	1.43	1.39
2	A	1498	FAD	PA-O3P	2.14	1.61	1.59
3	B	1502	MHF	C17-C16	2.13	1.42	1.38
2	B	1501	FAD	C10-N1	2.11	1.37	1.33
2	A	1498	FAD	C9A-C5X	2.07	1.44	1.41
2	A	1498	FAD	C10-N10	2.02	1.41	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1502	MHF	C9-N10-C15	-6.10	113.60	122.71
3	A	1499	MHF	C9-N10-C15	-5.35	114.71	122.71
3	B	1502	MHF	C9-C6-N5	2.81	106.45	101.70
2	B	1501	FAD	C9A-C5X-N5	-2.74	119.55	122.45
2	A	1498	FAD	C9A-C5X-N5	-2.72	119.57	122.45
3	A	1499	MHF	C9-C6-N5	2.65	106.19	101.70
3	B	1502	MHF	C12-C-N	2.39	121.47	117.04
2	B	1501	FAD	C4-C4X-N5	2.39	121.50	118.21
3	B	1502	MHF	C14-C15-N10	-2.36	118.12	121.39
3	A	1499	MHF	C12-C-N	2.28	121.27	117.04
3	A	1499	MHF	N1-C8A-N8	2.28	121.56	117.28
3	B	1502	MHF	N1-C8A-N8	2.28	121.56	117.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1498	FAD	C4-C4X-N5	2.24	121.30	118.21
2	B	1501	FAD	O3P-PA-O1A	-2.16	104.21	110.70
2	A	1498	FAD	C10-C4X-N5	-2.10	120.51	124.81
2	B	1501	FAD	C10-C4X-N5	-2.10	120.52	124.81
2	B	1501	FAD	N3A-C2A-N1A	-2.08	125.43	128.58
2	A	1498	FAD	N3A-C2A-N1A	-2.06	125.46	128.58
2	B	1501	FAD	O3P-P-O1P	2.02	116.78	110.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1498	FAD	C5B-O5B-PA-O1A
2	B	1501	FAD	C5B-O5B-PA-O1A
3	A	1499	MHF	C14-C15-N10-C9
3	A	1499	MHF	C16-C15-N10-C9
3	B	1502	MHF	C14-C15-N10-C9
3	B	1502	MHF	C16-C15-N10-C9
2	A	1498	FAD	C4'-C5'-O5'-P
2	B	1501	FAD	C4'-C5'-O5'-P
3	B	1502	MHF	OE2-CD-CG-CB
3	A	1499	MHF	OE2-CD-CG-CB
3	B	1502	MHF	OE1-CD-CG-CB
3	A	1499	MHF	OE1-CD-CG-CB
2	B	1501	FAD	P-O3P-PA-O1A
2	B	1501	FAD	P-O3P-PA-O2A
2	A	1498	FAD	P-O3P-PA-O2A

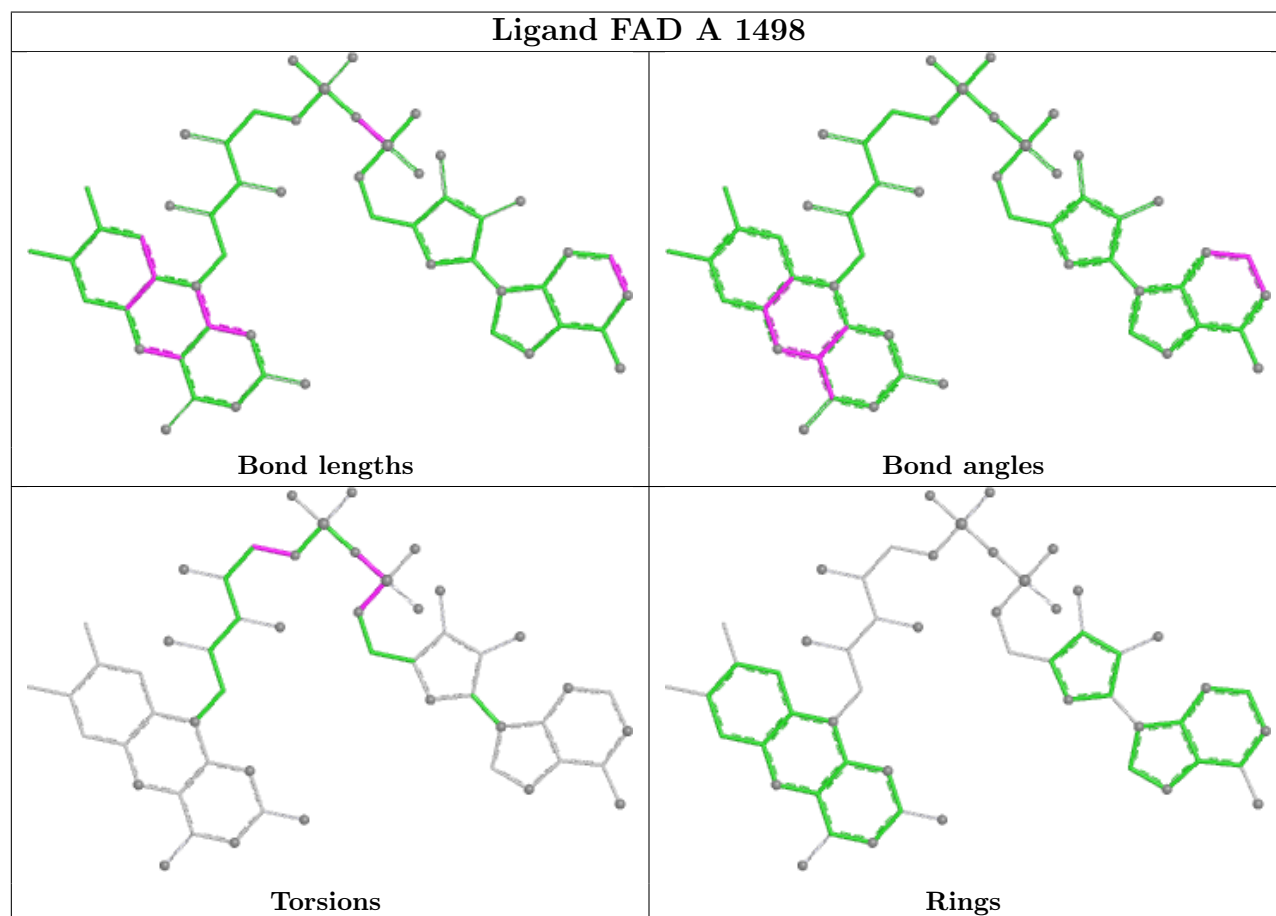
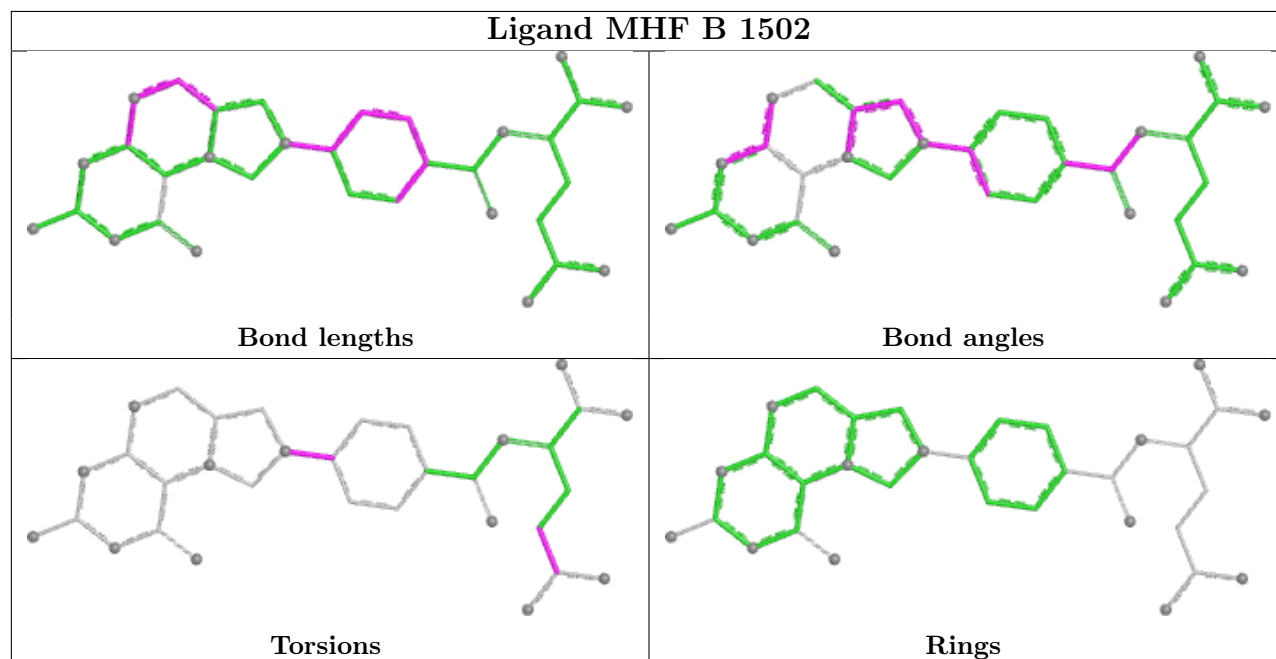
There are no ring outliers.

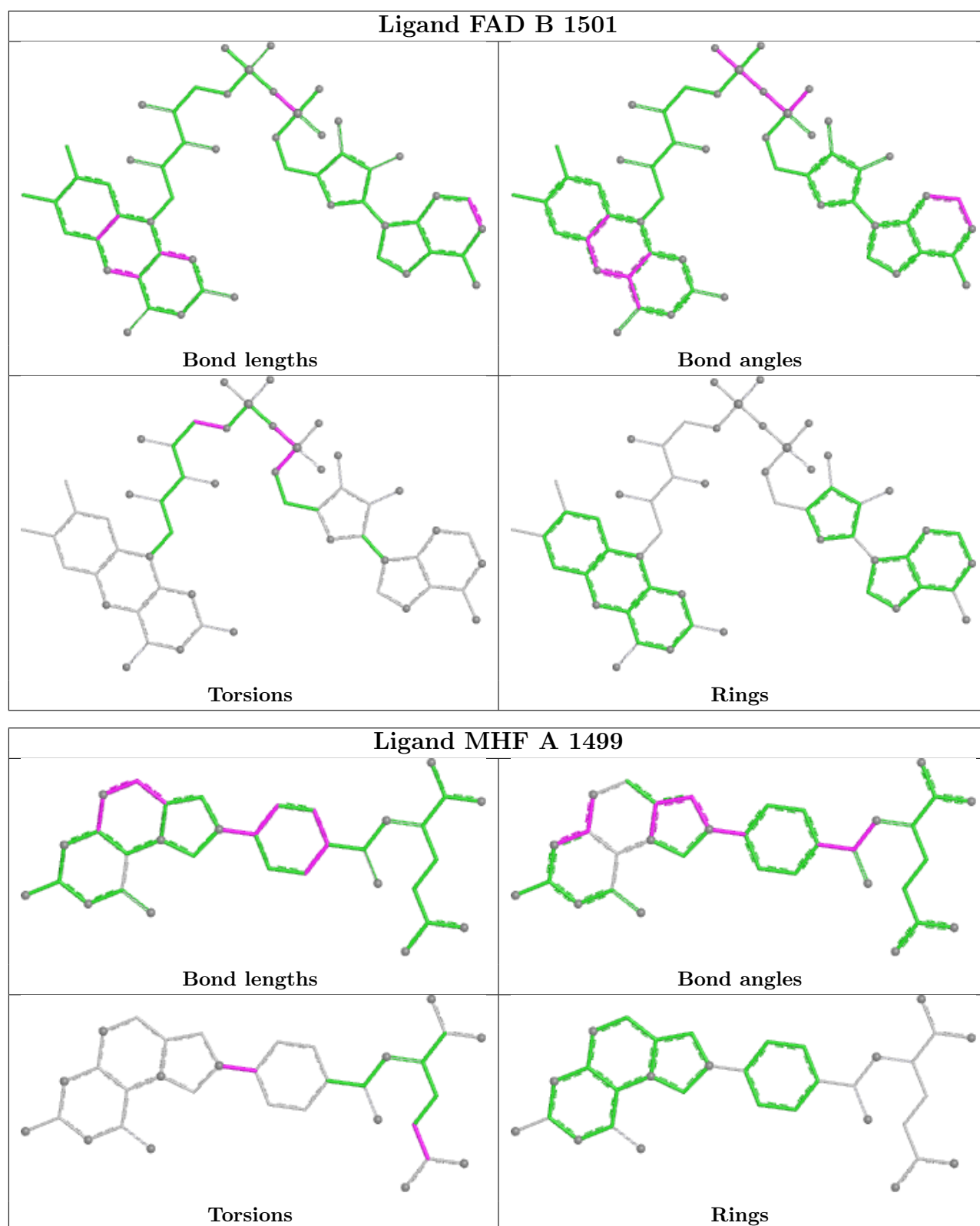
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1498	FAD	1	0
2	B	1501	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	164:GLY	C	165:ASN	N	1.09
1	B	164:GLY	C	165:ASN	N	0.79

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	496/525 (94%)	-0.13	20 (4%) 42 45	15, 26, 54, 69	0
1	B	499/525 (95%)	0.36	30 (6%) 27 29	18, 34, 66, 90	1 (0%)
All	All	995/1050 (94%)	0.11	50 (5%) 34 36	15, 30, 62, 90	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	TRP	5.0
1	B	165	ASN	4.7
1	A	481	TRP	4.6
1	B	164	GLY	4.5
1	B	480	HIS	4.2
1	A	166	SER	4.2
1	B	356	TRP	4.2
1	B	166	SER	4.1
1	B	34	VAL	4.0
1	B	84	PHE	3.9
1	B	30	SER	3.9
1	B	31	SER	3.6
1	A	2	ASP	3.4
1	B	499	GLY	3.4
1	A	353	GLN	3.4
1	B	500	PRO	3.3
1	B	443	ARG	3.3
1	A	164	GLY	3.2
1	A	477	GLU	3.2
1	B	354	GLY	3.2
1	A	497	GLY	3.1
1	B	32	SER	3.1
1	A	356	TRP	3.0
1	A	163	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	486	MET	2.9
1	B	167	THR	2.8
1	A	165	ASN	2.8
1	B	3	HIS	2.8
1	B	469	GLN	2.7
1	A	480	HIS	2.7
1	A	3	HIS	2.6
1	B	498	ASN	2.5
1	A	476	LYS	2.5
1	B	497	GLY	2.5
1	A	443	ARG	2.5
1	A	352	VAL	2.4
1	A	474	LEU	2.4
1	B	473	ARG	2.3
1	B	163	VAL	2.3
1	A	168	LYS	2.2
1	B	37	LYS	2.2
1	B	38	GLY	2.2
1	A	34	VAL	2.2
1	B	471	LEU	2.2
1	B	2	ASP	2.2
1	A	496	HIS	2.2
1	B	445	ASP	2.2
1	A	244	ARG	2.1
1	B	223	VAL	2.1
1	B	352	VAL	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](#)

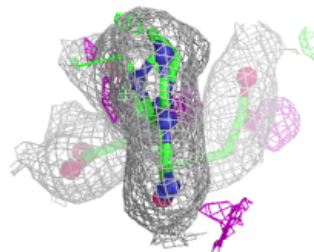
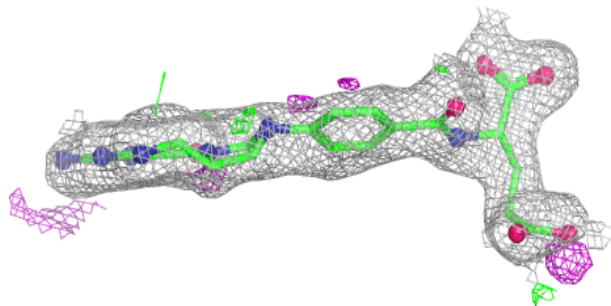
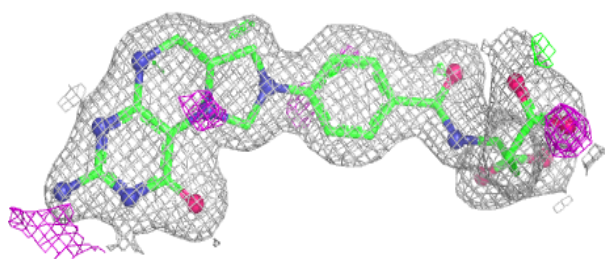
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MHF	B	1502	33/33	0.91	0.09	24,27,45,49	0
3	MHF	A	1499	33/33	0.93	0.08	16,21,38,47	0
2	FAD	A	1498	53/53	0.98	0.04	15,18,21,22	0
2	FAD	B	1501	53/53	0.98	0.05	18,22,24,25	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.

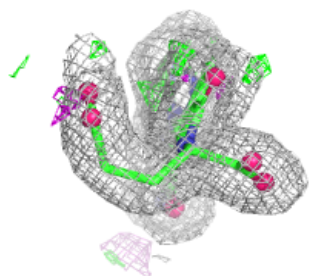
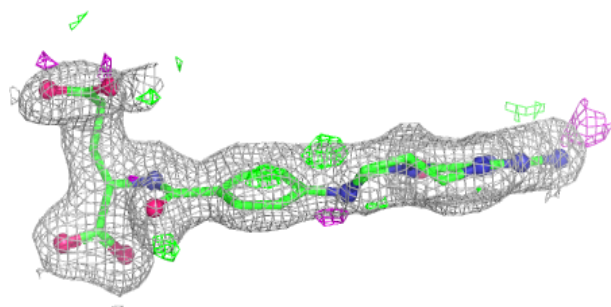
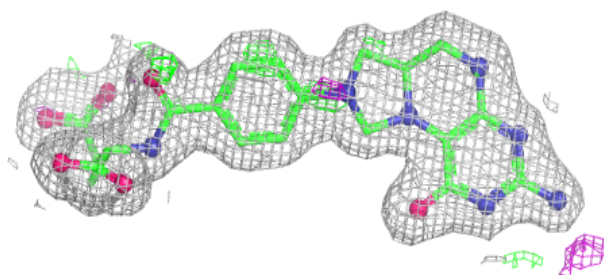
Electron density around MHF B 1502:

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

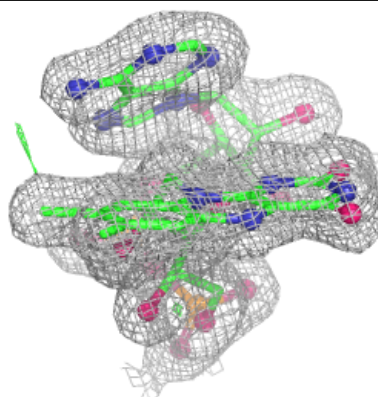
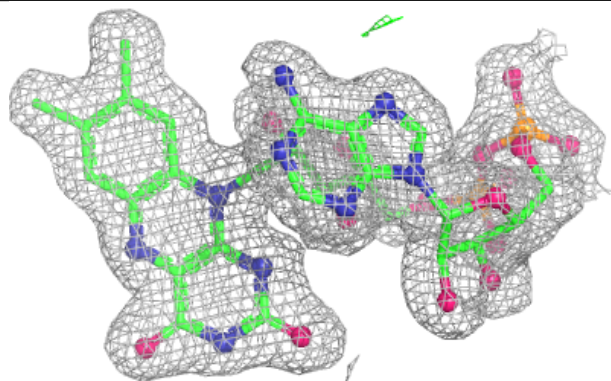
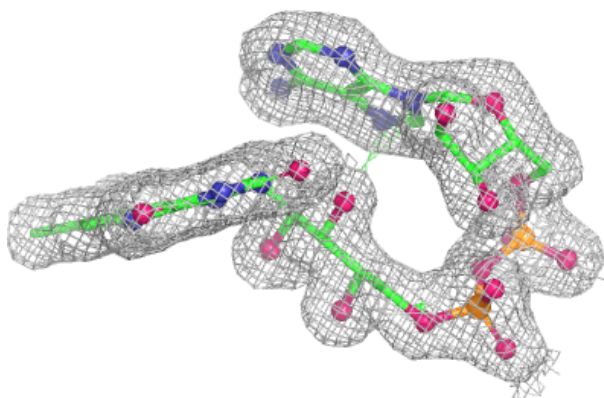


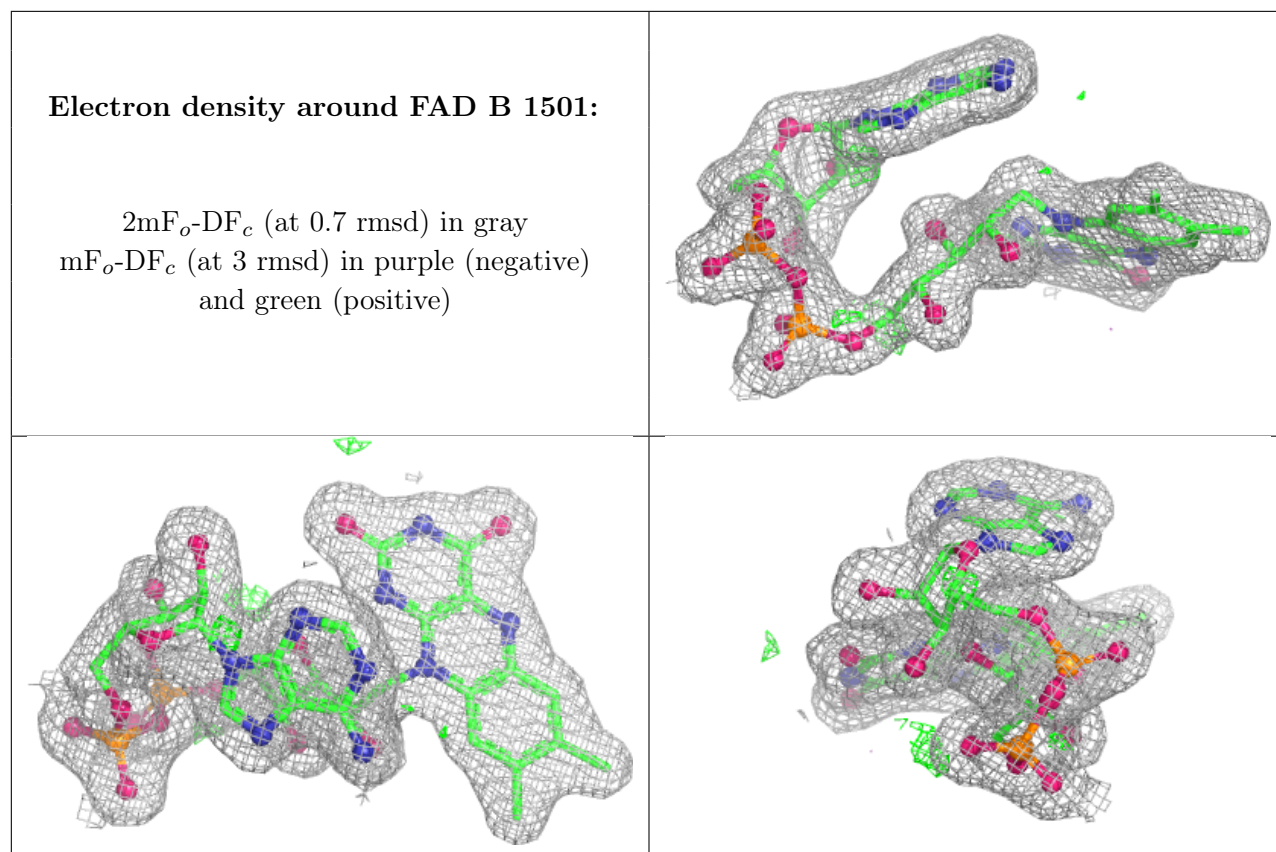
Electron density around MHF A 1499:

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

**Electron density around FAD A 1498:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.