



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:52 PM UTC

PDB ID : 2GV8 / pdb_00002gv8
Title : Crystal structure of flavin-containing monooxygenase (FMO) from *S.pombe* and NADPH cofactor complex
Authors : Eswaramoorthy, S.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-05-02
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

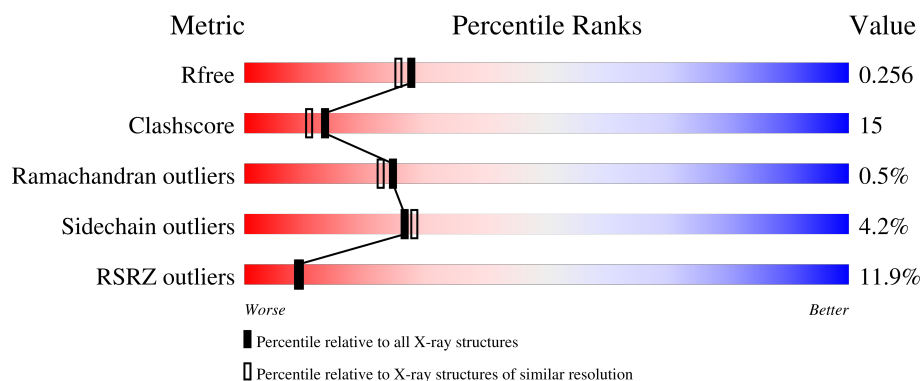
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	8% 70% 25% ..
1	B	447	16% 69% 26% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7618 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 monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			
1	B	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			

There are 10 discrepancies between the modelled and reference sequences:

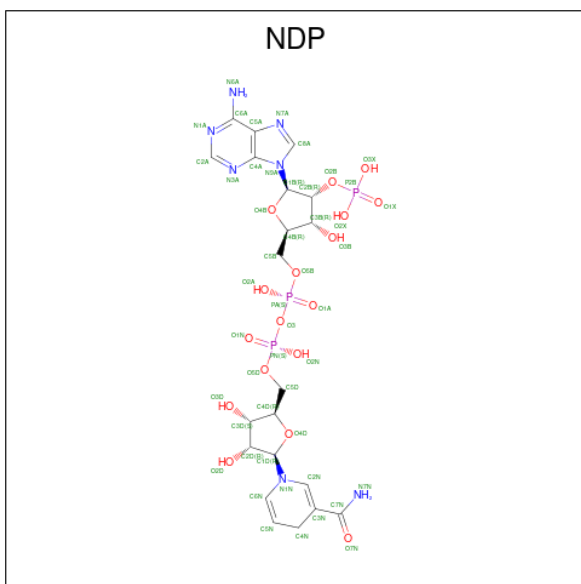
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9HFE4
A	97	MSE	MET	modified residue	UNP Q9HFE4
A	377	MSE	MET	modified residue	UNP Q9HFE4
A	386	MSE	MET	modified residue	UNP Q9HFE4
A	433	MSE	MET	modified residue	UNP Q9HFE4
B	1	MSE	MET	modified residue	UNP Q9HFE4
B	97	MSE	MET	modified residue	UNP Q9HFE4
B	377	MSE	MET	modified residue	UNP Q9HFE4
B	386	MSE	MET	modified residue	UNP Q9HFE4
B	433	MSE	MET	modified residue	UNP Q9HFE4

- 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 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

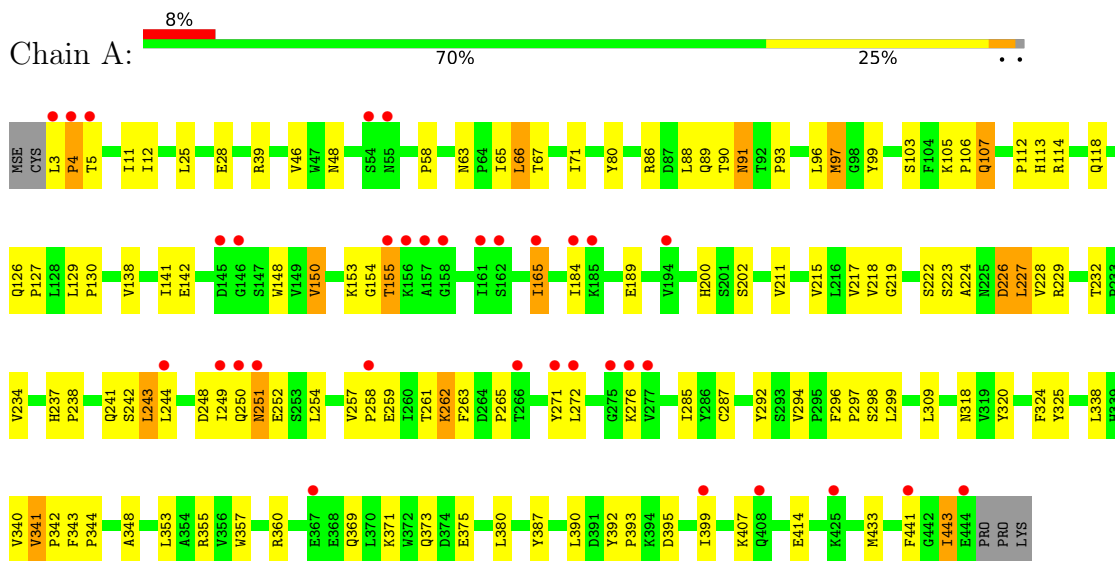
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	231	Total	O	0	0
			231	231		
5	B	201	Total	O	0	0
			201	201		

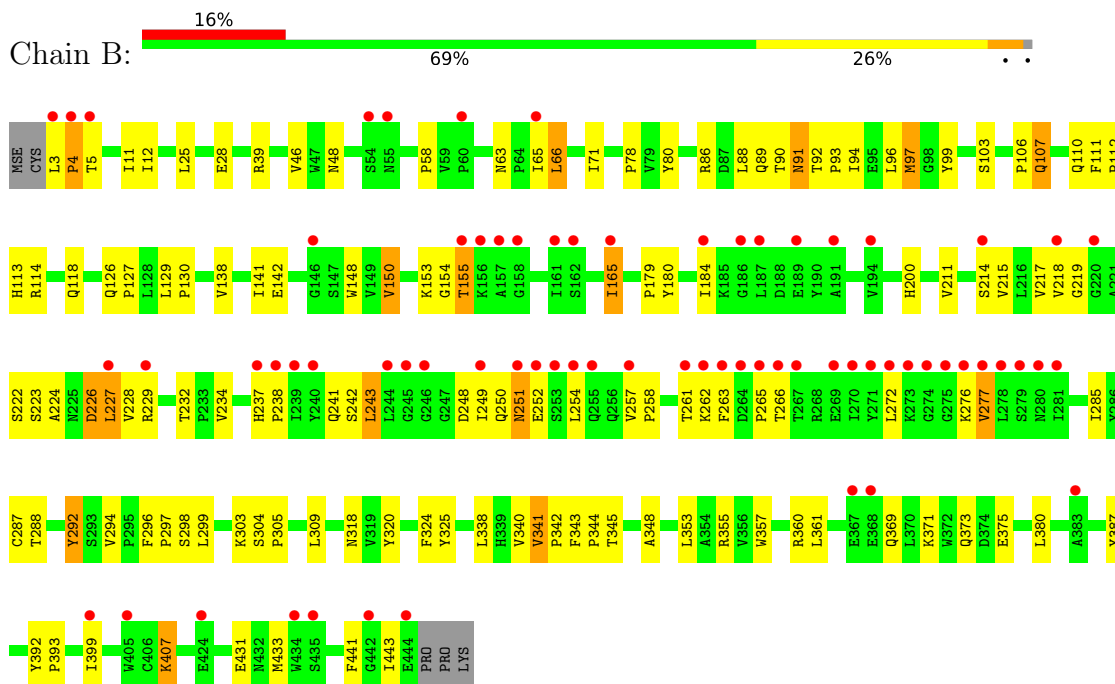
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: monooxygenase



• Molecule 1: monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.31Å 72.53Å 80.37Å 98.59° 107.40° 101.72°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 89.0 (50.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.259 0.231 , 0.256	Depositor DCC
R_{free} test set	2070 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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, NDP, GOL

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	0.44	1/3583 (0.0%)	0.98	15/4880 (0.3%)
1	B	0.43	0/3583	0.98	17/4880 (0.3%)
All	All	0.44	1/7166 (0.0%)	0.98	32/9760 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLN	CA-C	-5.15	1.46	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	A	97	MSE	N-CA-C	9.16	123.71	112.54
1	B	97	MSE	N-CA-C	9.15	123.70	112.54
1	A	107	GLN	CA-CB-CG	-8.31	97.48	114.10
1	A	107	GLN	CB-CG-CD	7.64	125.59	112.60
1	B	86	ARG	N-CA-C	7.33	119.91	111.11
1	A	86	ARG	N-CA-C	7.19	119.74	111.11
1	A	341	VAL	CA-C-N	6.66	128.17	119.84
1	A	341	VAL	C-N-CA	6.66	128.17	119.84
1	B	107	GLN	CG-CD-NE2	6.63	126.35	116.40
1	B	341	VAL	CA-C-N	6.58	128.07	119.84
1	B	341	VAL	C-N-CA	6.58	128.07	119.84
1	B	324	PHE	N-CA-C	5.95	118.35	109.25
1	A	324	PHE	N-CA-C	5.93	118.32	109.25
1	B	294	VAL	CA-C-N	5.68	126.94	119.84
1	B	294	VAL	C-N-CA	5.68	126.94	119.84
1	B	215	VAL	N-CA-C	5.67	117.58	108.85
1	A	215	VAL	N-CA-C	5.65	117.56	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	VAL	CA-C-N	5.64	126.89	119.84
1	A	294	VAL	C-N-CA	5.64	126.89	119.84
1	B	277	VAL	N-CA-C	5.54	115.86	108.11
1	A	296	PHE	CA-C-N	5.43	126.63	119.84
1	A	296	PHE	C-N-CA	5.43	126.63	119.84
1	B	99	TYR	N-CA-C	-5.35	102.95	110.50
1	A	99	TYR	N-CA-C	-5.33	102.98	110.50
1	A	443	ILE	N-CA-C	5.26	115.24	108.82
1	B	296	PHE	CA-C-N	5.26	126.42	119.84
1	B	296	PHE	C-N-CA	5.26	126.42	119.84
1	B	292	TYR	N-CA-C	-5.15	103.24	110.50
1	B	111	PHE	CA-C-N	5.08	125.36	119.92
1	B	111	PHE	C-N-CA	5.08	125.36	119.92
1	A	341	VAL	N-CA-C	-5.03	98.01	108.88

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	3486	0	3483	110	0
1	B	3486	0	3483	103	0
2	A	53	0	31	3	0
2	B	53	0	31	3	0
3	A	48	0	26	4	0
3	B	48	0	26	4	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	231	0	0	13	0
5	B	201	0	0	5	0
All	All	7618	0	7096	212	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 15.

All (212) 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:114:ARG:HH11	1:A:118:GLN:HE22	1.13	0.95
1:A:244:LEU:HD23	1:A:259:GLU:OE1	1.69	0.93
1:B:114:ARG:HH11	1:B:118:GLN:HE22	1.11	0.92
1:A:262:LYS:HE2	1:A:271:TYR:CG	2.06	0.91
1:A:259:GLU:HG2	5:A:646:HOH:O	1.82	0.79
1:A:407:LYS:HD3	5:A:730:HOH:O	1.85	0.76
1:B:241:GLN:HG2	1:B:243:LEU:CD2	2.17	0.75
1:B:93:PRO:HD2	1:B:433:MSE:HE2	1.68	0.75
1:A:262:LYS:HD3	1:A:271:TYR:HB2	1.67	0.74
1:A:93:PRO:HD2	1:A:433:MSE:HE2	1.69	0.73
1:A:106:PRO:HG2	1:B:106:PRO:HG2	1.68	0.73
1:A:262:LYS:CD	1:A:271:TYR:HB2	2.19	0.72
1:A:241:GLN:HG2	1:A:243:LEU:CD2	2.20	0.71
1:B:238:PRO:HB3	1:B:252:GLU:O	1.91	0.70
1:A:414:GLU:HG2	5:A:727:HOH:O	1.92	0.69
1:A:155:THR:HG21	5:A:561:HOH:O	1.92	0.68
1:B:63:ASN:OD1	1:B:65:ILE:HG22	1.93	0.68
1:B:114:ARG:NH1	1:B:118:GLN:HE22	1.89	0.67
1:A:238:PRO:HB3	1:A:252:GLU:O	1.95	0.67
1:A:63:ASN:OD1	1:A:65:ILE:HG22	1.95	0.66
1:B:249:ILE:HG21	1:B:254:LEU:HD23	1.78	0.66
1:B:249:ILE:HG23	1:B:251:ASN:OD1	1.97	0.65
1:A:67:THR:HG23	5:A:713:HOH:O	1.96	0.65
1:A:249:ILE:HG21	1:A:254:LEU:HD23	1.78	0.65
1:B:222:SER:OG	3:B:501:NDP:H2D	1.97	0.64
1:B:227:LEU:HD21	1:B:285:ILE:HG21	1.80	0.64
1:B:407:LYS:HD3	5:B:581:HOH:O	1.97	0.64
1:A:222:SER:OG	3:A:501:NDP:H2D	1.98	0.63
1:A:227:LEU:HD21	1:A:285:ILE:HG21	1.79	0.63
1:A:142:GLU:HB3	1:A:298:SER:CB	2.28	0.63
1:A:249:ILE:HG23	1:A:251:ASN:OD1	1.98	0.63
1:B:142:GLU:HB3	1:B:298:SER:CB	2.28	0.63
1:B:91:ASN:C	1:B:91:ASN:HD22	2.06	0.63
1:B:114:ARG:HH11	1:B:118:GLN:NE2	1.92	0.63
1:A:262:LYS:HE2	1:A:271:TYR:CD2	2.35	0.62
1:A:232:THR:O	1:A:237:HIS:HE1	1.83	0.61
1:B:272:LEU:HD12	1:B:276:LYS:HG3	1.83	0.61
1:A:91:ASN:C	1:A:91:ASN:HD22	2.09	0.61
1:B:232:THR:O	1:B:237:HIS:HE1	1.84	0.60
1:B:106:PRO:O	1:B:107:GLN:HB2	1.99	0.60
1:B:263:PHE:O	1:B:265:PRO:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH1	1:A:118:GLN:HE22	1.92	0.60
1:A:262:LYS:CE	1:A:271:TYR:CG	2.82	0.60
1:B:251:ASN:OD1	1:B:251:ASN:N	2.35	0.60
1:A:251:ASN:OD1	1:A:251:ASN:N	2.34	0.60
1:B:155:THR:HG21	5:B:527:HOH:O	2.01	0.60
1:A:39:ARG:HD2	5:A:627:HOH:O	2.02	0.59
1:B:93:PRO:CD	1:B:433:MSE:HE2	2.32	0.59
1:B:165:ILE:HG12	1:B:165:ILE:O	2.01	0.59
1:A:262:LYS:HE2	1:A:271:TYR:CD1	2.38	0.59
1:A:318:ASN:H	1:A:373:GLN:HE22	1.51	0.58
1:A:272:LEU:HD12	1:A:276:LYS:HG3	1.84	0.58
1:B:318:ASN:H	1:B:373:GLN:HE22	1.51	0.58
1:B:88:LEU:HD11	2:B:500:FAD:H6	1.86	0.58
1:B:58:PRO:HG3	1:B:66:LEU:CD2	2.34	0.58
1:A:414:GLU:CG	5:A:727:HOH:O	2.52	0.57
1:A:441:PHE:O	1:A:443:ILE:HG23	2.05	0.57
1:B:241:GLN:HG2	1:B:243:LEU:HD21	1.84	0.57
1:A:165:ILE:HG12	1:A:165:ILE:O	2.03	0.57
1:A:93:PRO:CD	1:A:433:MSE:HE2	2.33	0.57
1:A:371:LYS:HE3	1:A:375:GLU:OE1	2.05	0.57
1:A:88:LEU:HD11	2:A:500:FAD:H6	1.86	0.57
1:A:241:GLN:HG2	1:A:243:LEU:HD21	1.85	0.57
1:B:441:PHE:O	1:B:443:ILE:HG23	2.05	0.57
1:B:371:LYS:HE3	1:B:375:GLU:OE1	2.05	0.56
1:A:58:PRO:HG3	1:A:66:LEU:CD2	2.35	0.55
1:B:58:PRO:HG3	1:B:66:LEU:HD21	1.88	0.55
1:B:343:PHE:HB2	1:B:344:PRO:HD3	1.88	0.55
1:A:222:SER:HB2	5:A:562:HOH:O	2.07	0.55
1:A:299:LEU:HB3	1:A:309:LEU:HD12	1.90	0.54
1:A:263:PHE:O	1:A:265:PRO:HD3	2.08	0.54
1:B:241:GLN:HG2	1:B:243:LEU:HD23	1.89	0.54
1:A:114:ARG:HH11	1:A:118:GLN:NE2	1.95	0.54
1:B:71:ILE:N	1:B:71:ILE:HD12	2.23	0.54
1:A:5:THR:HG23	5:A:699:HOH:O	2.07	0.53
1:A:58:PRO:HG3	1:A:66:LEU:HD21	1.90	0.53
1:A:343:PHE:HB2	1:A:344:PRO:HD3	1.90	0.53
1:B:179:PRO:HB3	1:B:200:HIS:CE1	2.43	0.53
1:A:71:ILE:N	1:A:71:ILE:HD12	2.24	0.53
1:A:200:HIS:CD2	1:A:202:SER:H	2.26	0.53
1:A:392:TYR:CD1	1:A:393:PRO:HA	2.44	0.53
1:B:299:LEU:HB3	1:B:309:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:O	1:B:342:PRO:HD3	2.10	0.52
1:B:341:VAL:O	1:B:344:PRO:HD2	2.09	0.52
1:A:224:ALA:O	1:A:228:VAL:HG23	2.10	0.52
1:A:341:VAL:O	1:A:344:PRO:HD2	2.10	0.52
1:B:224:ALA:O	1:B:228:VAL:HG23	2.10	0.51
1:B:392:TYR:CD1	1:B:393:PRO:HA	2.45	0.51
1:A:39:ARG:HD3	1:A:80:TYR:CE1	2.46	0.51
1:B:218:VAL:HG22	1:B:242:SER:HB3	1.93	0.51
1:A:218:VAL:HG22	1:A:242:SER:HB3	1.91	0.51
1:B:217:VAL:O	1:B:241:GLN:HA	2.11	0.51
1:B:223:SER:HA	3:B:501:NDP:H5N	1.92	0.50
1:A:243:LEU:HD23	1:A:243:LEU:N	2.27	0.50
1:A:241:GLN:HG2	1:A:243:LEU:HD23	1.93	0.50
1:A:249:ILE:CG2	1:A:251:ASN:OD1	2.59	0.50
1:B:249:ILE:CG2	1:B:251:ASN:OD1	2.60	0.50
1:A:67:THR:HA	5:A:713:HOH:O	2.11	0.50
1:A:223:SER:HA	3:A:501:NDP:H5N	1.93	0.50
1:B:242:SER:O	3:B:501:NDP:H2A	2.11	0.50
1:A:340:VAL:O	1:A:342:PRO:HD3	2.12	0.50
1:B:211:VAL:HG12	1:B:234:VAL:HB	1.94	0.49
1:A:97:MSE:HE1	1:A:112:PRO:HD2	1.94	0.49
1:A:211:VAL:HG12	1:A:234:VAL:HB	1.94	0.49
1:A:217:VAL:O	1:A:241:GLN:HA	2.13	0.49
1:B:11:ILE:HD11	1:B:25:LEU:HD12	1.94	0.49
1:B:237:HIS:HD2	1:B:252:GLU:OE2	1.96	0.49
1:B:39:ARG:HD3	1:B:80:TYR:CE1	2.47	0.49
1:B:97:MSE:O	1:B:343:PHE:HB2	2.12	0.49
1:B:141:ILE:O	1:B:298:SER:HB2	2.13	0.49
1:B:292:TYR:OH	1:B:338:LEU:HD13	2.12	0.49
1:A:141:ILE:O	1:A:298:SER:HB2	2.13	0.48
1:A:248:ASP:O	1:A:250:GLN:HG2	2.13	0.48
1:A:226:ASP:OD1	1:A:229:ARG:NH2	2.46	0.48
1:B:257:VAL:HB	1:B:258:PRO:HD2	1.96	0.48
1:B:226:ASP:OD1	1:B:229:ARG:NH2	2.46	0.48
1:B:248:ASP:O	1:B:250:GLN:HG2	2.12	0.48
1:B:380:LEU:HD11	1:B:387:TYR:HA	1.95	0.48
1:A:106:PRO:O	1:A:107:GLN:HB2	2.13	0.48
1:A:242:SER:O	3:A:501:NDP:H2A	2.13	0.48
1:B:39:ARG:HG2	2:B:500:FAD:N3A	2.28	0.48
1:B:97:MSE:HE1	1:B:112:PRO:HD2	1.96	0.48
1:B:243:LEU:HD23	1:B:243:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:O	1:A:5:THR:N	2.47	0.47
1:A:237:HIS:HD2	1:A:252:GLU:OE2	1.97	0.47
1:B:3:LEU:O	1:B:5:THR:N	2.47	0.47
1:A:39:ARG:HG2	2:A:500:FAD:N3A	2.29	0.47
1:B:39:ARG:HD2	5:B:570:HOH:O	2.14	0.47
1:B:91:ASN:C	1:B:91:ASN:ND2	2.69	0.47
1:B:106:PRO:O	1:B:107:GLN:CB	2.63	0.47
1:A:257:VAL:HB	1:A:258:PRO:HD2	1.97	0.46
1:A:355:ARG:HG3	1:A:355:ARG:HH11	1.79	0.46
1:A:97:MSE:O	1:A:343:PHE:HB2	2.15	0.46
1:B:214:SER:HA	5:B:649:HOH:O	2.15	0.46
1:A:11:ILE:HD11	1:A:25:LEU:HD12	1.96	0.46
1:A:5:THR:HA	5:A:699:HOH:O	2.15	0.46
1:A:219:GLY:HA2	3:A:501:NDP:N3A	2.31	0.46
1:A:292:TYR:OH	1:A:338:LEU:HD13	2.15	0.46
1:B:39:ARG:HD3	1:B:80:TYR:CD1	2.51	0.46
1:B:320:TYR:CG	1:B:369:GLN:HG2	2.50	0.46
1:A:309:LEU:HD21	1:A:325:TYR:CD1	2.51	0.46
1:B:348:ALA:HB2	1:B:399:ILE:HG23	1.98	0.45
1:A:320:TYR:CG	1:A:369:GLN:HG2	2.51	0.45
1:A:380:LEU:HD11	1:A:387:TYR:HA	1.98	0.45
1:B:222:SER:O	1:B:226:ASP:HB2	2.17	0.45
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.80	0.45
1:B:148:TRP:O	1:B:165:ILE:HA	2.17	0.45
1:A:39:ARG:HD3	1:A:80:TYR:CD1	2.52	0.45
1:B:71:ILE:N	1:B:71:ILE:CD1	2.80	0.45
1:A:89:GLN:HG2	1:A:113:HIS:HA	1.99	0.45
1:B:237:HIS:CD2	1:B:252:GLU:OE2	2.69	0.45
1:A:237:HIS:CD2	1:A:252:GLU:OE2	2.70	0.44
1:A:343:PHE:N	1:A:343:PHE:CD1	2.85	0.44
1:A:348:ALA:HB2	1:A:399:ILE:HG23	1.99	0.44
1:B:353:LEU:HD11	1:B:357:TRP:CE2	2.52	0.44
1:A:227:LEU:CD2	1:A:285:ILE:HG21	2.47	0.44
1:B:227:LEU:HD22	1:B:287:CYS:SG	2.58	0.44
1:A:371:LYS:O	1:A:375:GLU:HG3	2.17	0.44
1:B:28:GLU:OE1	1:B:360:ARG:HD3	2.17	0.44
1:B:343:PHE:CD1	1:B:343:PHE:N	2.84	0.44
1:A:251:ASN:HB2	1:A:252:GLU:H	1.56	0.44
1:B:219:GLY:HA2	3:B:501:NDP:N3A	2.31	0.44
1:A:222:SER:O	1:A:226:ASP:HB2	2.17	0.44
1:B:90:THR:HA	2:B:500:FAD:O4	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:VAL:CG2	1:B:272:LEU:HD13	2.47	0.44
1:B:345:THR:HB	5:B:536:HOH:O	2.17	0.44
1:A:90:THR:HA	2:A:500:FAD:O4	2.17	0.44
1:A:360:ARG:NH1	5:A:656:HOH:O	2.26	0.44
1:A:148:TRP:O	1:A:165:ILE:HA	2.18	0.43
1:A:189:GLU:CD	5:A:662:HOH:O	2.60	0.43
1:A:257:VAL:CG2	1:A:272:LEU:HD13	2.48	0.43
1:B:309:LEU:HD21	1:B:325:TYR:CD1	2.53	0.43
1:B:407:LYS:HA	1:B:407:LYS:HD2	1.79	0.43
1:A:355:ARG:HG3	1:A:355:ARG:NH1	2.33	0.43
1:A:91:ASN:C	1:A:91:ASN:ND2	2.72	0.43
1:A:227:LEU:HD22	1:A:287:CYS:SG	2.59	0.43
1:B:371:LYS:O	1:B:375:GLU:HG3	2.18	0.43
1:A:126:GLN:HB3	1:A:127:PRO:CD	2.49	0.43
1:B:180:TYR:O	1:B:288:THR:OG1	2.34	0.43
1:B:355:ARG:HG3	1:B:355:ARG:NH1	2.34	0.43
1:B:126:GLN:HB3	1:B:127:PRO:CD	2.49	0.43
1:A:97:MSE:HA	1:A:341:VAL:CG1	2.49	0.43
1:A:153:LYS:O	1:A:154:GLY:C	2.62	0.43
1:A:184:ILE:HG22	1:A:262:LYS:HA	2.01	0.43
1:B:89:GLN:HG2	1:B:113:HIS:HA	2.00	0.43
1:A:46:VAL:C	1:A:48:ASN:H	2.27	0.42
1:A:28:GLU:OE1	1:A:360:ARG:HD3	2.19	0.42
1:A:71:ILE:N	1:A:71:ILE:CD1	2.82	0.42
1:B:179:PRO:HB3	1:B:200:HIS:ND1	2.34	0.42
1:B:392:TYR:CE2	1:B:431:GLU:HG3	2.54	0.42
1:B:12:ILE:HD12	1:B:138:VAL:HG21	2.01	0.42
1:B:251:ASN:HB2	1:B:252:GLU:H	1.56	0.42
1:B:94:ILE:HG12	1:B:110:GLN:HA	2.01	0.42
1:A:353:LEU:HD11	1:A:357:TRP:CE2	2.54	0.42
1:B:92:THR:O	1:B:97:MSE:HE2	2.20	0.42
1:A:138:VAL:HG13	1:A:150:VAL:HG23	2.02	0.41
1:A:390:LEU:O	1:A:395:ASP:HB3	2.20	0.41
1:B:107:GLN:OE1	1:B:107:GLN:HA	2.19	0.41
1:B:304:SER:HA	1:B:305:PRO:HD3	1.96	0.41
1:B:88:LEU:C	1:B:88:LEU:HD23	2.45	0.41
1:B:46:VAL:C	1:B:48:ASN:H	2.28	0.41
1:B:138:VAL:HG13	1:B:150:VAL:HG23	2.03	0.41
1:A:200:HIS:HD2	1:A:202:SER:OG	2.03	0.41
1:B:184:ILE:CG2	1:B:262:LYS:HA	2.51	0.41
1:A:129:LEU:N	1:A:130:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASN:ND2	1:B:92:THR:HG23	2.36	0.41
1:B:129:LEU:N	1:B:130:PRO:HD2	2.36	0.41
1:A:65:ILE:O	1:A:66:LEU:C	2.64	0.40
1:A:12:ILE:HD12	1:A:138:VAL:HG21	2.02	0.40
1:B:153:LYS:O	1:B:154:GLY:C	2.64	0.40
1:B:361:LEU:HD23	1:B:361:LEU:HA	1.96	0.40
1:B:78:PRO:HD2	1:B:155:THR:CG2	2.51	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	440/447 (98%)	414 (94%)	24 (6%)	2 (0%)	24	22
1	B	440/447 (98%)	415 (94%)	23 (5%)	2 (0%)	24	22
All	All	880/894 (98%)	829 (94%)	47 (5%)	4 (0%)	24	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	B	4	PRO
1	A	66	LEU
1	B	66	LEU

5.3.2 Protein sidechains [i](#)

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	384/385 (100%)	369 (96%)	15 (4%)	28	31
1	B	384/385 (100%)	367 (96%)	17 (4%)	25	26
All	All	768/770 (100%)	736 (96%)	32 (4%)	26	28

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	91	ASN
1	A	96	LEU
1	A	103	SER
1	A	105	LYS
1	A	150	VAL
1	A	155	THR
1	A	165	ILE
1	A	226	ASP
1	A	227	LEU
1	A	243	LEU
1	A	251	ASN
1	A	261	THR
1	A	262	LYS
1	A	297	PRO
1	B	4	PRO
1	B	91	ASN
1	B	96	LEU
1	B	103	SER
1	B	150	VAL
1	B	155	THR
1	B	165	ILE
1	B	226	ASP
1	B	227	LEU
1	B	243	LEU
1	B	251	ASN
1	B	261	THR
1	B	266	THR
1	B	277	VAL
1	B	297	PRO
1	B	303	LYS
1	B	407	LYS

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	48	ASN
1	A	89	GLN
1	A	91	ASN
1	A	102	GLN
1	A	118	GLN
1	A	121	GLN
1	A	200	HIS
1	A	237	HIS
1	A	373	GLN
1	B	91	ASN
1	B	102	GLN
1	B	118	GLN
1	B	121	GLN
1	B	237	HIS
1	B	373	GLN

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
2	FAD	A	500	-	58,58,58	2.10	15 (25%)	85,89,89	1.64	14 (16%)
3	NDP	A	501	-	51,52,52	1.57	9 (17%)	71,80,80	1.40	9 (12%)
4	GOL	B	502	-	5,5,5	0.45	0	5,5,5	0.60	0
2	FAD	B	500	-	58,58,58	2.15	16 (27%)	85,89,89	1.66	15 (17%)
3	NDP	B	501	-	51,52,52	1.57	10 (19%)	71,80,80	1.44	10 (14%)
4	GOL	A	502	-	5,5,5	0.45	0	5,5,5	0.64	0

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	FAD	A	500	-	-	12/34/50/50	0/6/6/6
3	NDP	A	501	-	-	13/34/77/77	0/5/5/5
4	GOL	B	502	-	-	2/4/4/4	-
2	FAD	B	500	-	-	12/34/50/50	0/6/6/6
3	NDP	B	501	-	-	13/34/77/77	0/5/5/5
4	GOL	A	502	-	-	2/4/4/4	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C4X-N5	6.29	1.44	1.30
2	A	500	FAD	C4X-N5	6.04	1.43	1.30
2	A	500	FAD	P-O5'	5.51	1.81	1.59
2	B	500	FAD	P-O5'	5.26	1.80	1.59
2	B	500	FAD	C4A-N3A	5.06	1.43	1.34
2	A	500	FAD	C4A-N3A	5.02	1.43	1.34
3	A	501	NDP	C4N-C3N	-4.57	1.41	1.50
2	B	500	FAD	C9A-N10	4.43	1.48	1.41
2	B	500	FAD	C2A-N3A	4.38	1.41	1.33
3	B	501	NDP	C4N-C3N	-4.37	1.41	1.50
2	A	500	FAD	C9A-N10	4.37	1.48	1.41
3	B	501	NDP	C4N-C5N	-4.18	1.38	1.49
2	A	500	FAD	C2A-N3A	4.10	1.41	1.33
2	B	500	FAD	C9A-C5X	4.05	1.47	1.41
2	A	500	FAD	C9A-C5X	4.02	1.47	1.41
3	A	501	NDP	C4N-C5N	-3.91	1.38	1.49
2	B	500	FAD	C5A-C4A	-3.86	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C5A-C4A	-3.81	1.32	1.39
3	B	501	NDP	C8A-N9A	3.45	1.43	1.37
3	A	501	NDP	C8A-N9A	3.38	1.43	1.37
2	B	500	FAD	C8A-N9A	3.20	1.43	1.37
2	A	500	FAD	C10-N1	2.95	1.39	1.33
2	B	500	FAD	C6-C7	2.87	1.43	1.39
3	B	501	NDP	P2B-O2B	-2.84	1.54	1.59
2	B	500	FAD	C10-N1	2.84	1.39	1.33
2	B	500	FAD	C5'-C4'	-2.81	1.48	1.51
3	A	501	NDP	P2B-O2B	-2.71	1.54	1.59
3	A	501	NDP	PA-O3	-2.66	1.56	1.59
2	A	500	FAD	C6-C7	2.66	1.43	1.39
3	B	501	NDP	C2N-C3N	2.60	1.42	1.35
3	A	501	NDP	C2N-C3N	2.56	1.42	1.35
2	B	500	FAD	C2B-C3B	-2.53	1.46	1.53
2	A	500	FAD	C8A-N9A	2.49	1.41	1.37
3	B	501	NDP	C4A-N3A	2.47	1.39	1.34
2	A	500	FAD	C1'-C2'	-2.40	1.49	1.52
2	A	500	FAD	C2B-C3B	-2.40	1.46	1.53
3	A	501	NDP	C6N-C5N	2.33	1.40	1.33
2	B	500	FAD	C1'-C2'	-2.33	1.49	1.52
3	B	501	NDP	C6N-C5N	2.30	1.40	1.33
2	A	500	FAD	C4A-N9A	2.20	1.42	1.37
2	A	500	FAD	C5'-C4'	-2.19	1.48	1.51
3	B	501	NDP	C6N-N1N	2.11	1.42	1.37
2	B	500	FAD	C4A-N9A	2.10	1.42	1.37
3	B	501	NDP	C5D-C4D	2.10	1.57	1.51
2	B	500	FAD	C1'-N10	-2.08	1.42	1.47
2	B	500	FAD	C5X-N5	2.07	1.43	1.39
3	B	501	NDP	C2B-C1B	-2.06	1.48	1.53
2	A	500	FAD	C5X-N5	2.05	1.43	1.39
3	A	501	NDP	PA-O1A	-2.01	1.43	1.50
3	A	501	NDP	C5D-C4D	2.00	1.57	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	C4A-N9A-C8A	-5.72	99.74	105.74
2	A	500	FAD	C4A-N9A-C8A	-5.54	99.92	105.74
2	B	500	FAD	C5A-C4A-N9A	4.97	111.23	105.81
2	A	500	FAD	C5A-C4A-N9A	4.93	111.18	105.81
3	A	501	NDP	C1D-N1N-C2N	-4.50	113.72	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NDP	C1D-N1N-C2N	-4.50	113.72	121.14
2	B	500	FAD	N3A-C4A-N9A	-4.44	119.62	127.17
2	A	500	FAD	P-O5'-C5'	4.25	145.70	121.35
2	A	500	FAD	N3A-C4A-N9A	-4.23	119.97	127.17
2	B	500	FAD	P-O5'-C5'	4.17	145.23	121.35
3	B	501	NDP	C3N-C2N-N1N	-4.05	117.25	123.20
3	A	501	NDP	C3N-C2N-N1N	-3.93	117.44	123.20
2	B	500	FAD	C5X-C9A-N10	-3.76	114.57	117.97
2	A	500	FAD	C5X-C9A-N10	-3.75	114.57	117.97
2	B	500	FAD	O3'-C3'-C4'	-3.10	101.89	108.93
2	A	500	FAD	O3'-C3'-C4'	-3.04	102.03	108.93
2	A	500	FAD	O5'-P-O1P	2.94	120.59	108.94
2	B	500	FAD	O5'-P-O1P	2.93	120.56	108.94
3	A	501	NDP	C6N-N1N-C2N	2.85	122.37	119.32
3	B	501	NDP	C6N-N1N-C2N	2.80	122.31	119.32
3	B	501	NDP	O7N-C7N-N7N	-2.67	116.90	122.89
2	A	500	FAD	O2B-C2B-C3B	2.60	120.16	111.82
2	A	500	FAD	C9-C9A-N10	2.59	125.33	121.85
2	B	500	FAD	C9-C9A-N10	2.58	125.33	121.85
2	B	500	FAD	C2'-C1'-N10	2.58	122.38	110.20
2	B	500	FAD	O2B-C2B-C3B	2.56	120.01	111.82
3	A	501	NDP	O7N-C7N-N7N	-2.51	117.27	122.89
2	A	500	FAD	C2'-C1'-N10	2.49	121.98	110.20
2	A	500	FAD	C4'-C3'-C2'	2.46	117.67	113.57
3	B	501	NDP	O5B-C5B-C4B	-2.45	100.66	108.99
2	B	500	FAD	C4'-C3'-C2'	2.43	117.61	113.57
2	B	500	FAD	N3A-C2A-N1A	-2.40	124.95	128.58
2	A	500	FAD	C4X-C10-N10	2.36	119.87	116.48
3	A	501	NDP	O5B-C5B-C4B	-2.36	100.95	108.99
2	B	500	FAD	C4X-C10-N10	2.35	119.84	116.48
3	B	501	NDP	O2A-PA-O1A	2.29	123.11	112.44
2	A	500	FAD	C8M-C8-C9	-2.29	115.54	119.57
3	B	501	NDP	N3A-C2A-N1A	-2.21	125.24	128.58
2	A	500	FAD	N3A-C2A-N1A	-2.20	125.25	128.58
3	B	501	NDP	N9A-C8A-N7A	-2.19	110.83	113.94
2	B	500	FAD	C8M-C8-C9	-2.16	115.76	119.57
3	B	501	NDP	O4B-C1B-N9A	2.12	112.16	108.09
3	A	501	NDP	N9A-C8A-N7A	-2.11	110.95	113.94
3	A	501	NDP	O2A-PA-O1A	2.09	122.18	112.44
3	A	501	NDP	O2B-P2B-O1X	-2.09	101.89	109.33
3	B	501	NDP	O2B-C2B-C3B	2.03	118.97	111.68
3	A	501	NDP	O2B-C2B-C3B	2.03	118.96	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	O3'-C3'-C2'	2.01	113.49	108.93

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FAD	N10-C1'-C2'-O2'
2	A	500	FAD	N10-C1'-C2'-C3'
2	A	500	FAD	C2'-C3'-C4'-C5'
2	A	500	FAD	O3'-C3'-C4'-O4'
2	A	500	FAD	O4'-C4'-C5'-O5'
2	A	500	FAD	C5'-O5'-P-O1P
2	A	500	FAD	C5'-O5'-P-O3P
2	B	500	FAD	N10-C1'-C2'-O2'
2	B	500	FAD	N10-C1'-C2'-C3'
2	B	500	FAD	C2'-C3'-C4'-C5'
2	B	500	FAD	O3'-C3'-C4'-O4'
2	B	500	FAD	O4'-C4'-C5'-O5'
2	B	500	FAD	C5'-O5'-P-O1P
2	B	500	FAD	C5'-O5'-P-O2P
2	B	500	FAD	C5'-O5'-P-O3P
3	A	501	NDP	C5B-O5B-PA-O1A
3	A	501	NDP	C5B-O5B-PA-O2A
3	A	501	NDP	C5B-O5B-PA-O3
3	A	501	NDP	PN-O3-PA-O5B
3	A	501	NDP	O4D-C1D-N1N-C2N
3	B	501	NDP	C5B-O5B-PA-O1A
3	B	501	NDP	C5B-O5B-PA-O2A
3	B	501	NDP	C5B-O5B-PA-O3
3	B	501	NDP	PN-O3-PA-O5B
3	B	501	NDP	O4D-C1D-N1N-C2N
2	A	500	FAD	C2'-C3'-C4'-O4'
2	B	500	FAD	C2'-C3'-C4'-O4'
3	A	501	NDP	O4B-C4B-C5B-O5B
3	B	501	NDP	O4B-C4B-C5B-O5B
2	A	500	FAD	O3'-C3'-C4'-C5'
2	B	500	FAD	O3'-C3'-C4'-C5'
3	A	501	NDP	C3B-C2B-O2B-P2B
3	A	501	NDP	C3B-C4B-C5B-O5B
3	B	501	NDP	C3B-C4B-C5B-O5B
3	A	501	NDP	C1B-C2B-O2B-P2B
3	B	501	NDP	C1B-C2B-O2B-P2B

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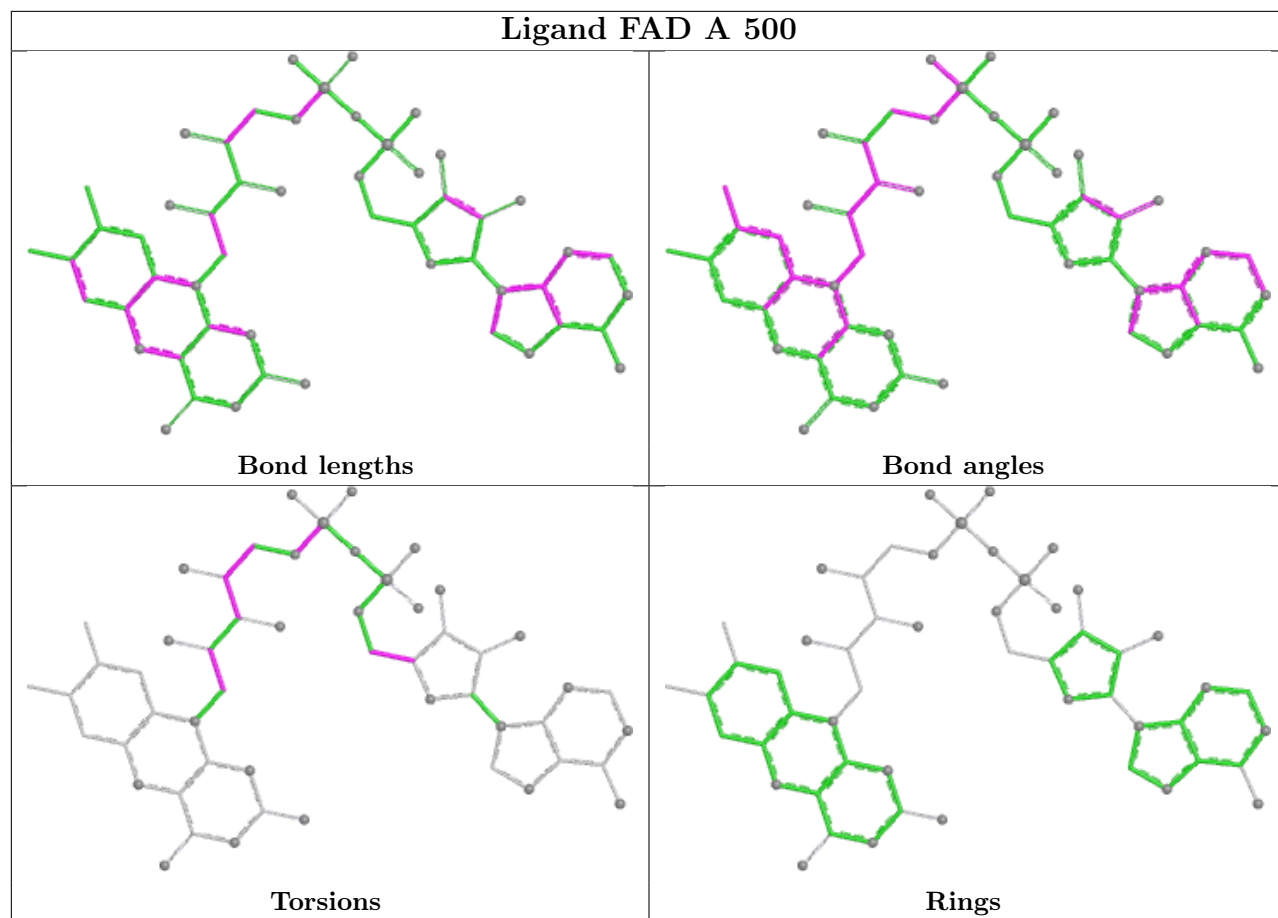
Mol	Chain	Res	Type	Atoms
3	B	501	NDP	C3B-C2B-O2B-P2B
4	A	502	GOL	C1-C2-C3-O3
4	B	502	GOL	C1-C2-C3-O3
2	A	500	FAD	C3'-C4'-C5'-O5'
2	B	500	FAD	C3'-C4'-C5'-O5'
4	A	502	GOL	O2-C2-C3-O3
4	B	502	GOL	O2-C2-C3-O3
3	A	501	NDP	C2N-C3N-C7N-N7N
3	B	501	NDP	C2N-C3N-C7N-N7N
3	A	501	NDP	PA-O3-PN-O1N
3	B	501	NDP	PA-O3-PN-O1N
3	A	501	NDP	C2N-C3N-C7N-O7N
3	B	501	NDP	C2N-C3N-C7N-O7N
2	A	500	FAD	C5'-O5'-P-O2P
3	B	501	NDP	PA-O3-PN-O2N
2	B	500	FAD	O4B-C4B-C5B-O5B
3	A	501	NDP	PA-O3-PN-O2N
2	A	500	FAD	O4B-C4B-C5B-O5B

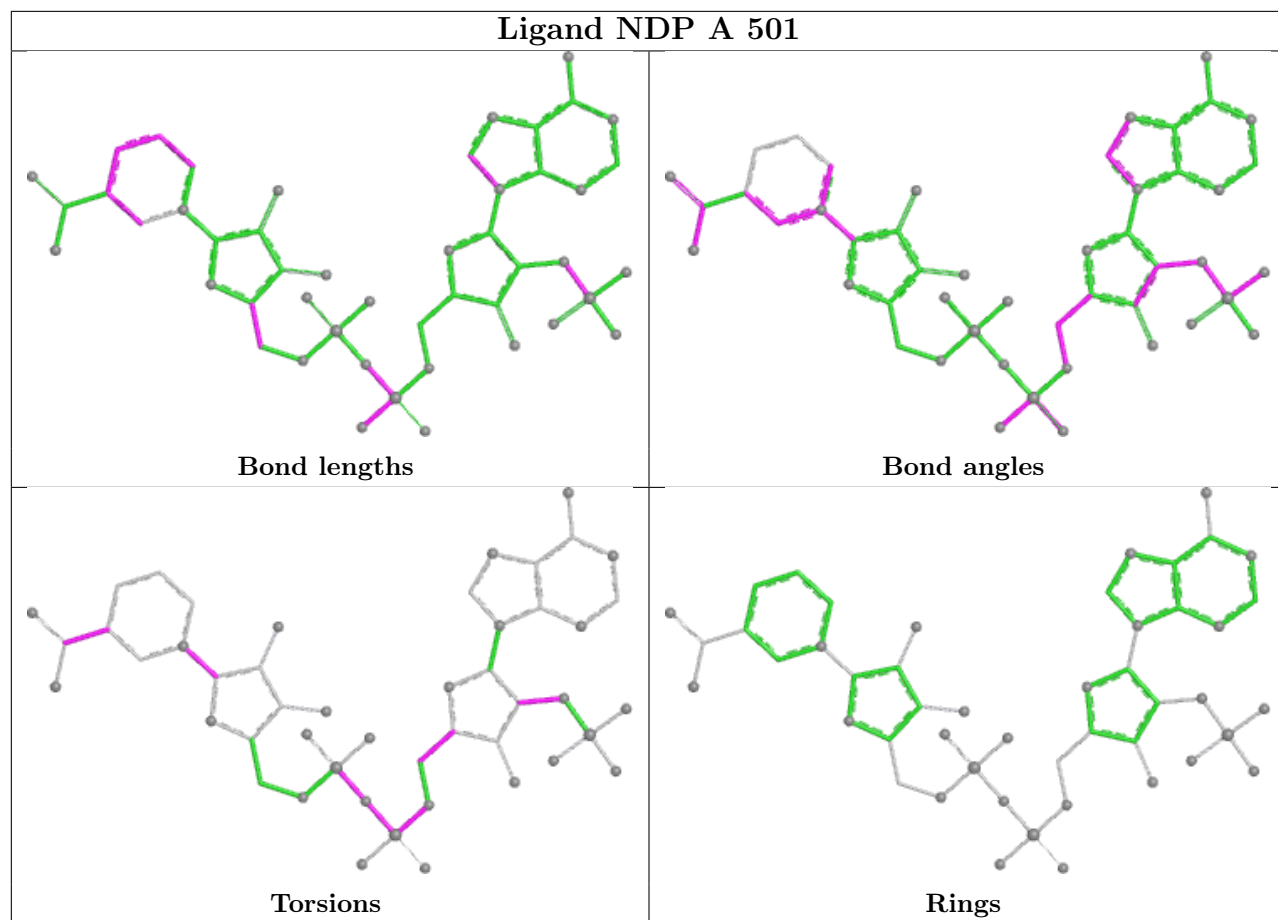
There are no ring outliers.

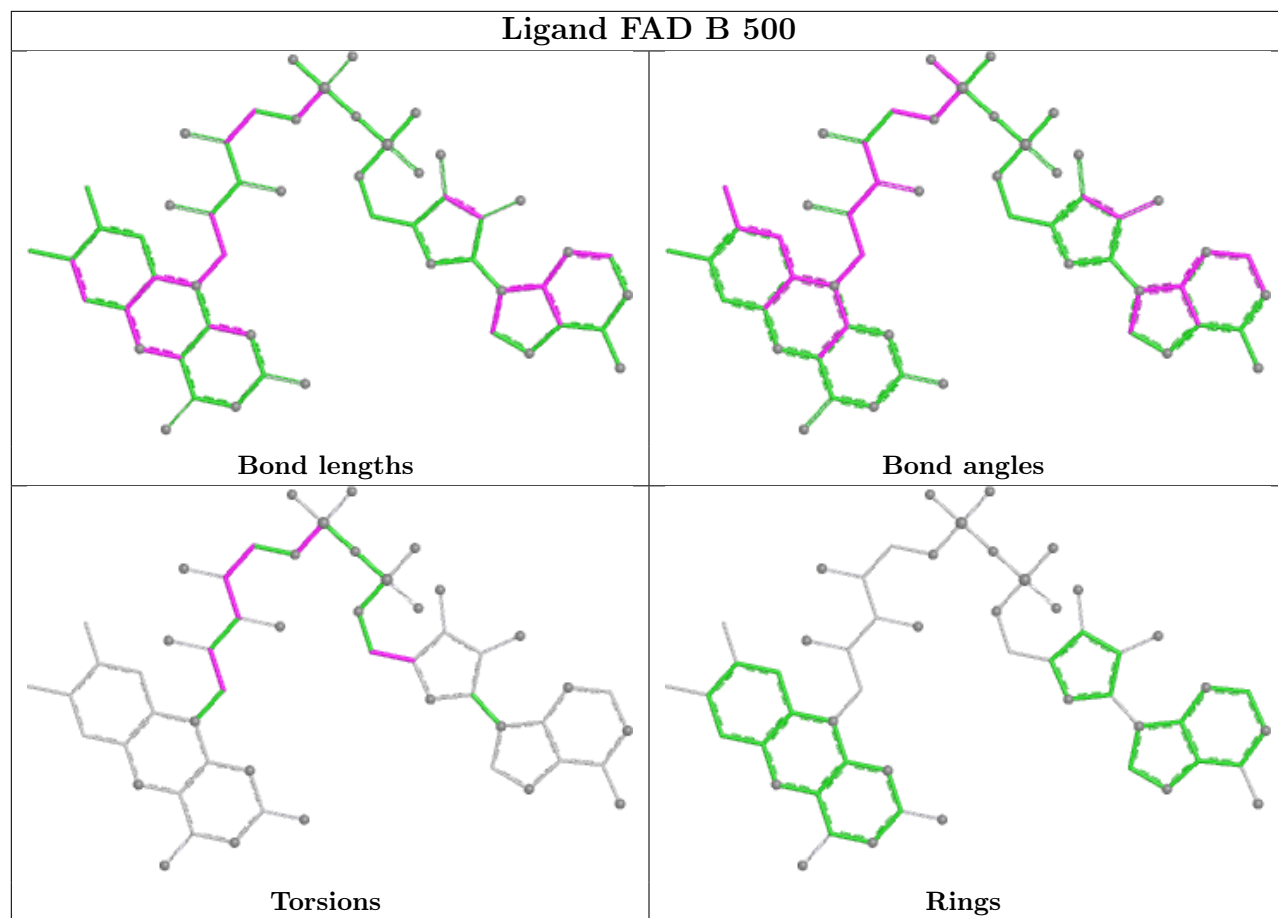
4 monomers are involved in 14 short contacts:

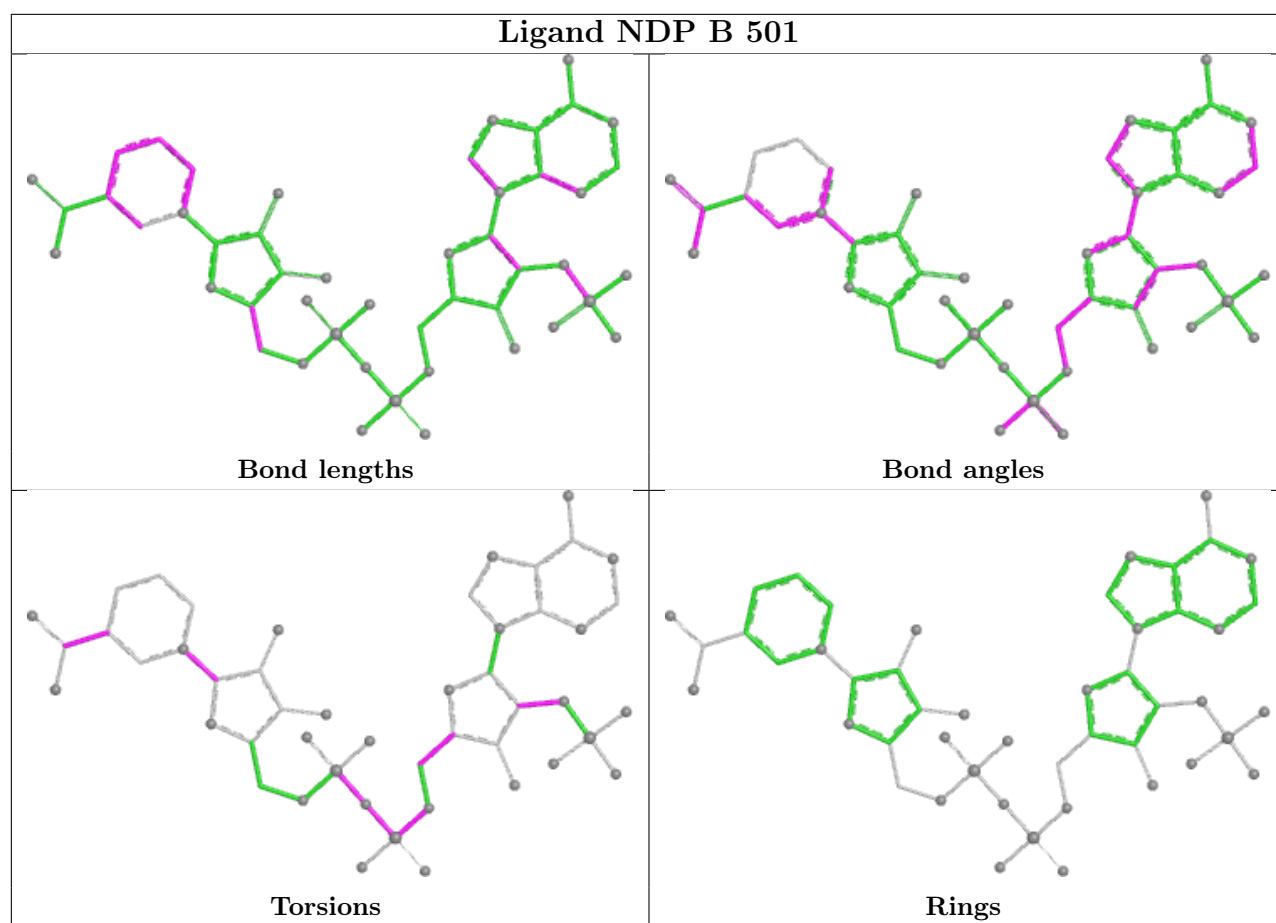
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	3	0
3	A	501	NDP	4	0
2	B	500	FAD	3	0
3	B	501	NDP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/447 (97%)	0.64	34 (7%) 19 20	11, 28, 42, 51	0
1	B	438/447 (97%)	0.89	70 (15%) 5 5	11, 30, 44, 52	0
All	All	876/894 (97%)	0.77	104 (11%) 9 9	11, 29, 43, 52	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	6.7
1	B	266	THR	6.6
1	A	3	LEU	5.7
1	B	271	TYR	5.5
1	A	4	PRO	5.4
1	B	4	PRO	5.4
1	B	444	GLU	4.6
1	B	263	PHE	4.6
1	B	267	THR	4.5
1	B	277	VAL	4.3
1	B	240	TYR	4.2
1	B	251	ASN	4.2
1	B	272	LEU	3.8
1	B	262	LYS	3.8
1	A	444	GLU	3.8
1	B	279	SER	3.7
1	B	189	GLU	3.6
1	B	264	ASP	3.4
1	B	244	LEU	3.4
1	B	5	THR	3.4
1	A	244	LEU	3.3
1	B	261	THR	3.3
1	B	238	PRO	3.2
1	B	280	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	278	LEU	3.2
1	B	281	ILE	3.2
1	A	251	ASN	3.1
1	A	146	GLY	3.1
1	B	239	ILE	3.1
1	A	157	ALA	3.1
1	A	275	GLY	3.0
1	B	249	ILE	3.0
1	A	271	TYR	3.0
1	B	270	ILE	2.9
1	A	266	THR	2.9
1	A	165	ILE	2.9
1	A	425	LYS	2.9
1	A	55	ASN	2.9
1	B	273	LYS	2.8
1	A	145	ASP	2.8
1	B	265	PRO	2.8
1	A	158	GLY	2.8
1	A	272	LEU	2.8
1	A	277	VAL	2.8
1	B	165	ILE	2.8
1	A	5	THR	2.7
1	B	146	GLY	2.7
1	B	218	VAL	2.7
1	B	252	GLU	2.7
1	A	162	SER	2.7
1	A	54	SER	2.7
1	B	237	HIS	2.6
1	B	245	GLY	2.6
1	B	155	THR	2.6
1	B	156	LYS	2.6
1	B	220	GLY	2.6
1	B	405	TRP	2.6
1	A	185	LYS	2.6
1	B	186	GLY	2.5
1	B	253	SER	2.5
1	B	269	GLU	2.5
1	B	424	GLU	2.5
1	B	187	LEU	2.5
1	B	246	GLY	2.5
1	B	275	GLY	2.5
1	A	156	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	255	GLN	2.4
1	A	194	VAL	2.4
1	B	162	SER	2.4
1	A	250	GLN	2.4
1	A	161	ILE	2.4
1	B	399	ILE	2.4
1	B	184	ILE	2.4
1	B	274	GLY	2.3
1	A	399	ILE	2.3
1	B	60	PRO	2.3
1	B	229	ARG	2.3
1	A	276	LYS	2.3
1	B	161	ILE	2.3
1	A	408	GLN	2.3
1	B	276	LYS	2.3
1	B	194	VAL	2.3
1	B	55	ASN	2.2
1	B	157	ALA	2.2
1	B	434	TRP	2.2
1	B	65	ILE	2.2
1	A	249	ILE	2.1
1	B	257	VAL	2.1
1	B	191	ALA	2.1
1	B	227	LEU	2.1
1	B	214	SER	2.1
1	B	367	GLU	2.1
1	A	155	THR	2.1
1	A	184	ILE	2.1
1	A	441	PHE	2.1
1	B	254	LEU	2.1
1	B	435	SER	2.1
1	B	158	GLY	2.1
1	A	367	GLU	2.0
1	B	54	SER	2.1
1	B	442	GLY	2.0
1	B	368	GLU	2.0
1	B	383	ALA	2.0
1	A	258	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

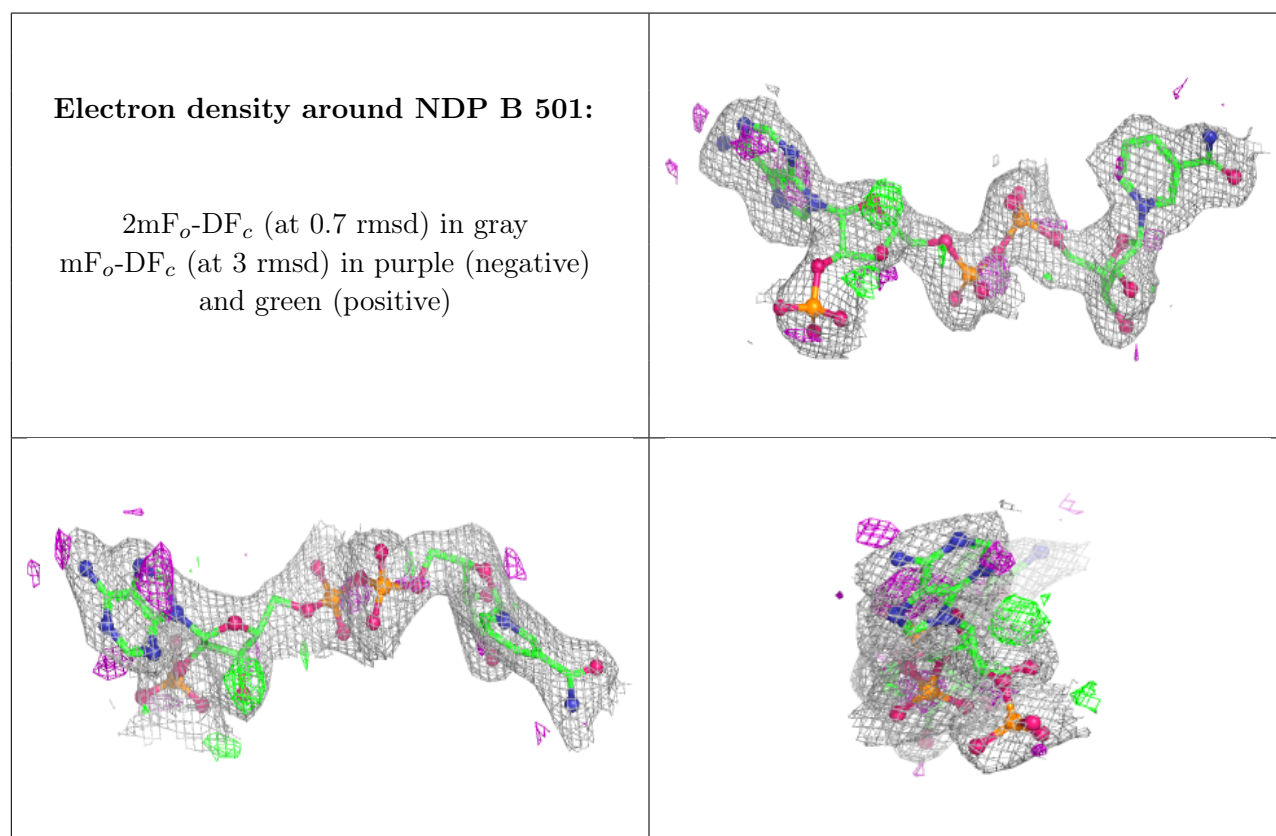
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

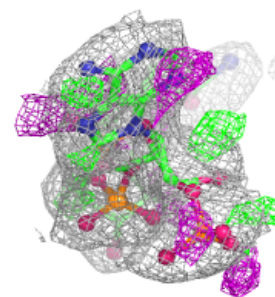
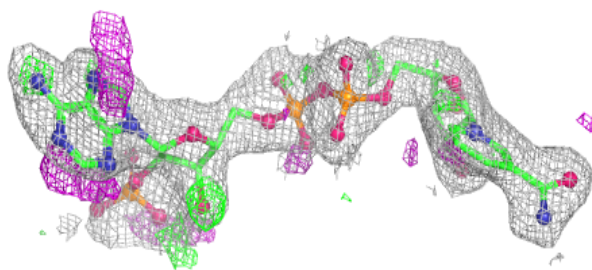
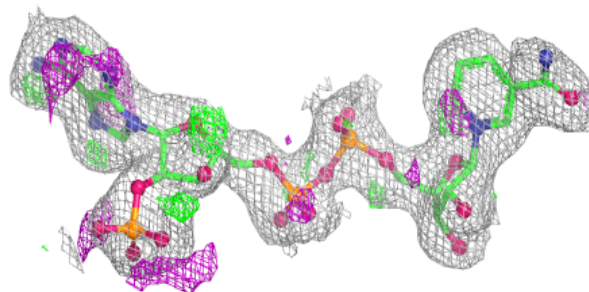
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NDP	B	501	48/48	0.88	0.12	27,32,47,48	0
3	NDP	A	501	48/48	0.89	0.13	24,27,43,45	0
2	FAD	A	500	53/53	0.94	0.09	15,18,24,24	0
2	FAD	B	500	53/53	0.94	0.10	14,20,23,25	0
4	GOL	B	502	6/6	0.94	0.07	16,18,20,21	0
4	GOL	A	502	6/6	0.95	0.07	15,18,19,20	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.

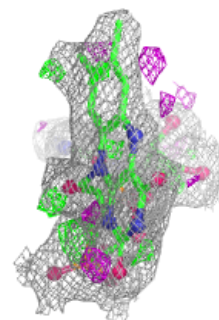
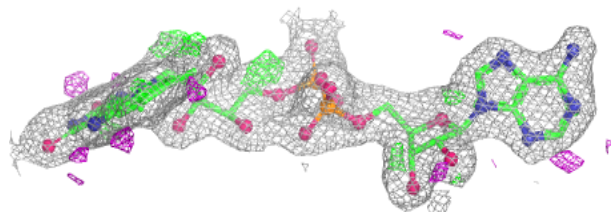
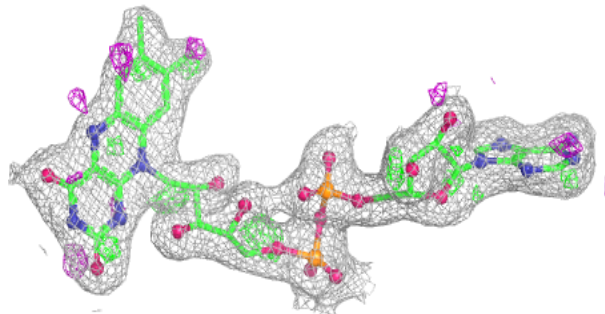


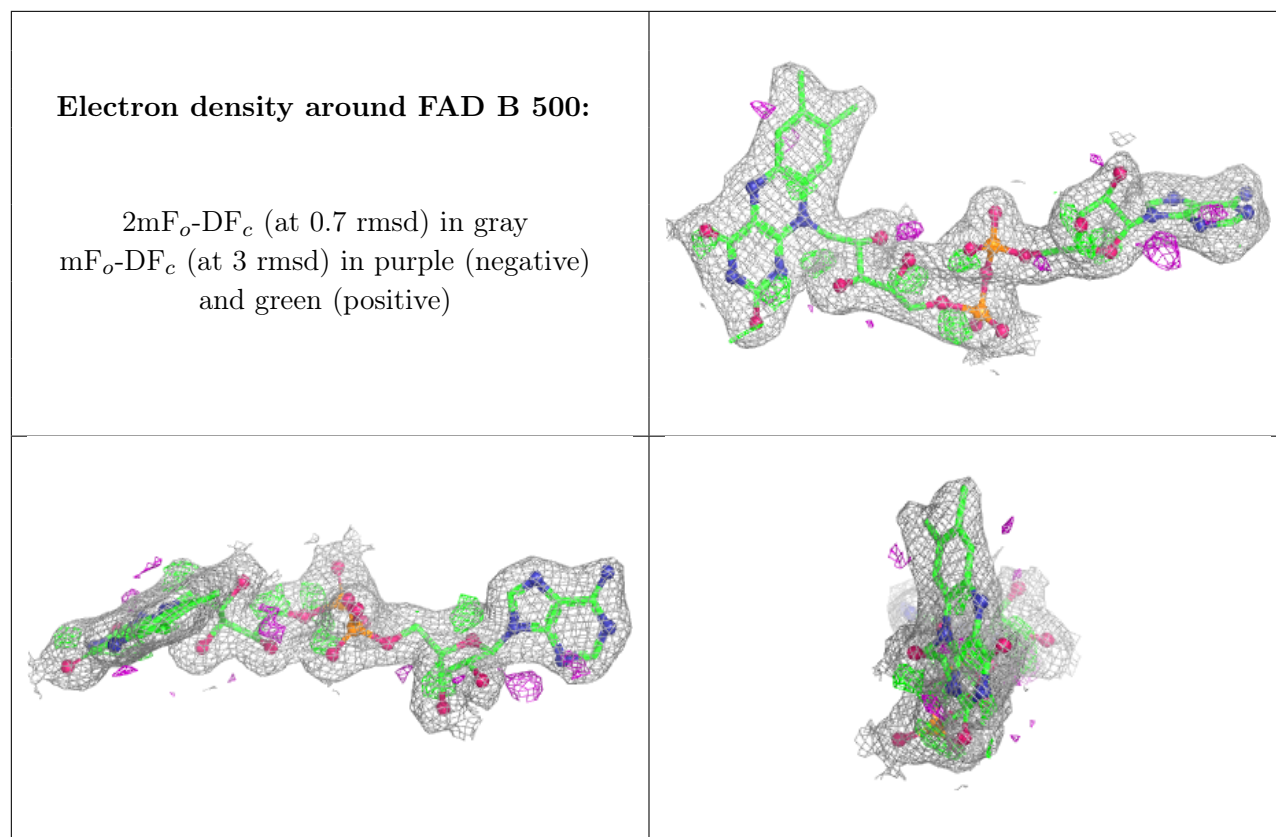
Electron density around NDP A 501:

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

**Electron density around FAD A 500:**

$2mF_o-DF_c$ (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.