



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 PM GMT

PDB ID : 3UP4  
Title : Crystal Structure of OTEMO complex with FAD and NADP (form 3)  
Authors : Shi, R.; Matte, A.; Cygler, M.; Lau, P.  
Deposited on : 2011-11-17  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

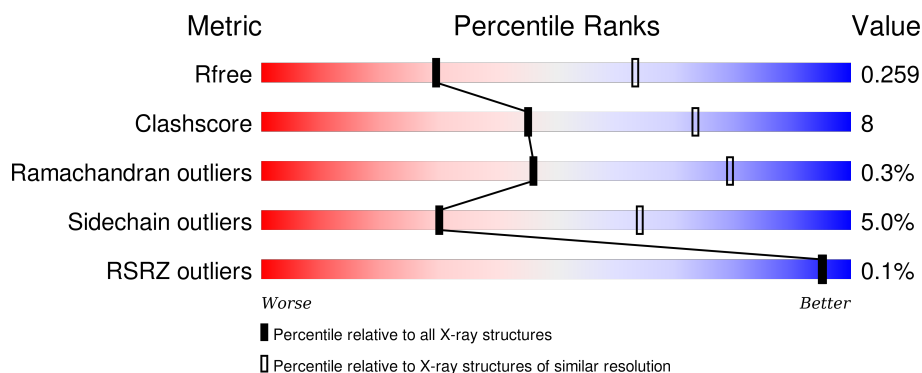
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	545	 76% 19% . .
1	B	545	 81% 15% . .

## 2 Entry composition [i](#)

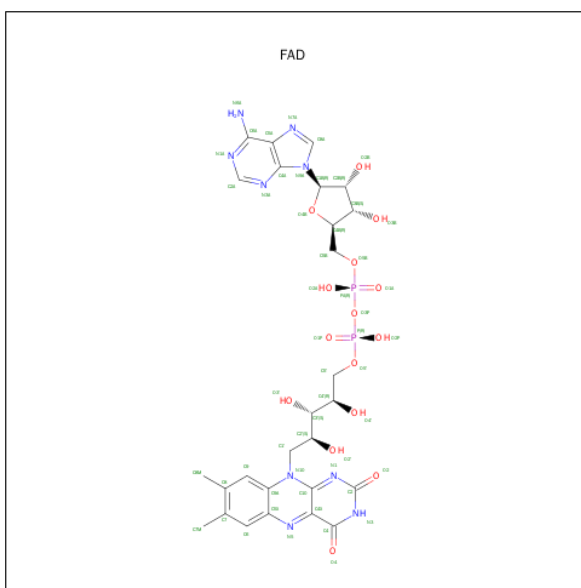
There are 4 unique types of molecules in this entry. The entry contains 8689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OTEMO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			4198	2671	725	787	15			
1	B	533	Total	C	N	O	S	0	0	0
			4240	2696	733	796	15			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

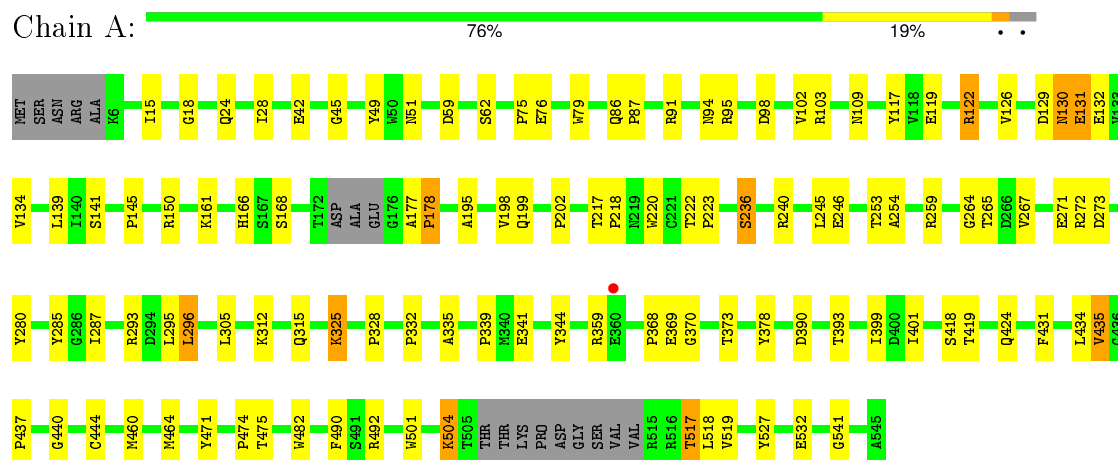
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	32	Total	O	0	0
			32	32		

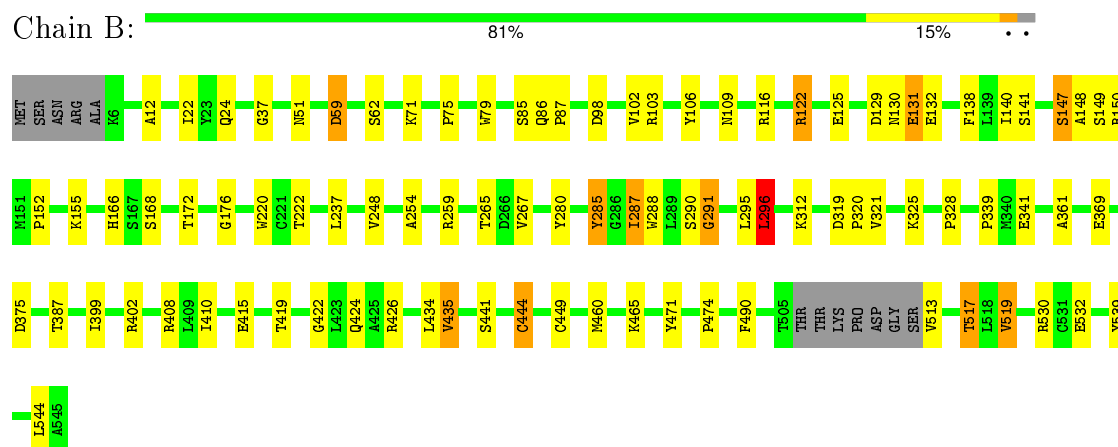
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: OTEMO



#### • Molecule 1: OTEMO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.31 Å 66.20 Å 282.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.80 48.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.5 (48.31-2.80) 87.5 (48.31-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.200 , 0.265 0.196 , 0.259	Depositor DCC
$R_{free}$ test set	1298 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 21.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 25667 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8689	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, FAD

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	0.64	0/4306	0.71	0/5847
1	B	0.70	0/4349	0.78	3/5907 (0.1%)
All	All	0.67	0/8655	0.75	3/11754 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASP	CB-CA-C	-5.53	99.35	110.40
1	B	296	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	237	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4198	0	4051	70	0
1	B	4240	0	4096	58	0
2	A	53	0	31	3	0
2	B	53	0	31	3	0
3	A	48	0	25	4	0
3	B	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	0	0	3	0
4	B	32	0	0	6	0
All	All	8689	0	8259	131	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 8.

All (131) 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:131:GLU:HG2	1:A:132:GLU:H	1.28	0.97
1:B:116:ARG:NH2	1:B:125:GLU:OE1	1.99	0.95
1:A:94:ASN:HD22	1:A:103:ARG:HH21	1.11	0.95
1:A:370:GLY:HA3	1:A:378:TYR:O	1.67	0.95
1:A:24:GLN:HE21	1:A:434:LEU:HD11	1.29	0.94
1:B:147:SER:O	1:B:148:ALA:HB3	1.87	0.75
1:A:131:GLU:HG2	1:A:132:GLU:N	2.00	0.75
1:A:94:ASN:HD22	1:A:103:ARG:NH2	1.84	0.71
1:A:435:VAL:HG22	1:A:435:VAL:O	1.90	0.71
1:A:51:ASN:O	1:A:86:GLN:HG3	1.93	0.68
1:A:435:VAL:CG2	1:A:435:VAL:O	2.44	0.66
1:A:129:ASP:C	1:A:130:ASN:OD1	2.34	0.66
1:B:222:THR:O	1:B:341:GLU:HG3	1.96	0.66
1:B:166:HIS:CD2	1:B:168:SER:H	2.13	0.66
1:B:402:ARG:HD3	1:B:408:ARG:HG2	1.78	0.65
1:A:424:GLN:HE21	1:A:474:PRO:HD3	1.59	0.65
1:A:94:ASN:ND2	1:A:103:ARG:HH21	1.91	0.63
1:B:280:TYR:CE2	1:B:312:LYS:HE3	2.34	0.63
1:A:280:TYR:CD2	1:A:312:LYS:HE2	2.33	0.63
2:B:551:FAD:HM73	3:B:552:NAP:C5N	2.29	0.63
3:B:552:NAP:H2N	4:B:554:HOH:O	1.97	0.62
1:B:166:HIS:HD2	1:B:168:SER:H	1.45	0.62
1:A:15:ILE:HD11	1:A:139:LEU:HD11	1.82	0.61
1:B:517:THR:HG21	1:B:519:VAL:O	2.00	0.61
1:B:220:TRP:O	1:B:339:PRO:HD2	2.00	0.61
1:A:199:GLN:OE1	3:A:552:NAP:H4N	2.01	0.60
1:A:131:GLU:CG	1:A:132:GLU:N	2.64	0.59
1:B:399:ILE:HD11	2:B:551:FAD:H61A	1.67	0.59
1:B:460:MET:HG3	1:B:539:TYR:CE2	2.38	0.59
1:B:24:GLN:HE21	1:B:434:LEU:HD11	1.68	0.58
1:B:152:PRO:HG3	1:B:387:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PRO:HG3	4:B:576:HOH:O	2.04	0.57
2:A:551:FAD:HM73	3:A:552:NAP:C5N	2.34	0.57
1:B:399:ILE:HD11	2:B:551:FAD:N6A	2.20	0.57
1:B:424:GLN:HE21	1:B:474:PRO:HD3	1.70	0.57
1:B:321:VAL:HG13	4:B:559:HOH:O	2.05	0.56
1:B:290:SER:O	1:B:291:GLY:O	2.22	0.56
1:A:195:ALA:HA	1:A:339:PRO:HB3	1.86	0.56
1:A:280:TYR:CE2	1:A:312:LYS:HE2	2.41	0.55
1:A:267:VAL:HG13	1:A:271:GLU:HB3	1.88	0.55
1:B:131:GLU:HG2	1:B:132:GLU:N	2.21	0.55
1:B:490:PHE:CE1	1:B:517:THR:HG23	2.42	0.55
1:A:460:MET:O	1:A:464:MET:HG3	2.07	0.55
1:A:75:PRO:HD2	1:A:76:GLU:OE1	2.07	0.54
1:A:532:GLU:HA	1:A:532:GLU:OE2	2.07	0.54
1:B:513:VAL:HG12	1:B:513:VAL:O	2.07	0.54
1:B:280:TYR:CD2	1:B:312:LYS:HE3	2.42	0.54
1:A:501:TRP:HE1	3:A:552:NAP:HO3N	1.55	0.54
1:A:122:ARG:HD2	1:A:471:TYR:HB2	1.89	0.54
1:A:492:ARG:CD	4:A:564:HOH:O	2.56	0.54
1:A:166:HIS:CD2	1:A:168:SER:H	2.26	0.53
1:A:126:VAL:HB	1:A:134:VAL:HG23	1.90	0.53
1:A:220:TRP:O	1:A:339:PRO:HD2	2.07	0.53
1:A:475:THR:HG23	1:A:541:GLY:O	2.08	0.53
1:A:424:GLN:HG2	1:A:431:PHE:O	2.08	0.53
1:A:492:ARG:HD2	4:A:564:HOH:O	2.07	0.52
1:B:410:ILE:HG13	4:B:565:HOH:O	2.09	0.52
1:B:122:ARG:NH1	4:B:578:HOH:O	2.41	0.52
1:A:236:SER:O	1:A:240:ARG:HG3	2.10	0.52
1:B:259:ARG:HH12	1:B:296:LEU:HD22	1.76	0.51
1:A:198:VAL:HG22	1:A:344:TYR:CE1	2.45	0.51
1:A:145:PRO:HD3	1:A:435:VAL:HG22	1.92	0.51
1:A:166:HIS:HD2	1:A:168:SER:H	1.59	0.50
1:B:419:THR:OG1	1:B:422:GLY:HA2	2.12	0.50
1:B:147:SER:O	1:B:148:ALA:CB	2.53	0.49
1:B:98:ASP:OD1	1:B:103:ARG:NH1	2.46	0.49
1:A:218:PRO:HG2	1:A:328:PRO:HA	1.94	0.49
1:B:441:SER:O	1:B:444:CYS:HB2	2.13	0.48
1:B:285:TYR:CE1	1:B:288:TRP:HE3	2.30	0.48
1:A:295:LEU:HD11	1:A:305:LEU:HD23	1.95	0.48
1:B:248:VAL:O	1:B:254:ALA:HA	2.14	0.48
1:A:62:SER:HB3	1:A:79:TRP:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:O	1:A:91:ARG:HG3	2.14	0.47
1:B:220:TRP:CE2	1:B:328:PRO:HG2	2.49	0.47
1:B:539:TYR:HB2	1:B:544:LEU:HD11	1.97	0.47
1:B:222:THR:HG21	1:B:287:ILE:HG21	1.96	0.46
1:A:24:GLN:O	1:A:28:ILE:HG13	2.14	0.46
1:A:198:VAL:CG1	1:A:341:GLU:HB3	2.45	0.46
1:A:246:GLU:HB3	1:B:532:GLU:HG3	1.97	0.46
1:B:172:THR:HB	1:B:176:GLY:HA2	1.96	0.46
1:A:259:ARG:HH22	1:A:296:LEU:HD22	1.81	0.46
1:A:264:GLY:O	1:A:272:ARG:HD3	2.16	0.46
1:B:37:GLY:O	1:B:106:TYR:HA	2.16	0.45
1:B:51:ASN:O	1:B:86:GLN:HG3	2.17	0.45
1:A:419:THR:O	1:A:482:TRP:HD1	1.99	0.45
1:A:393:THR:HG22	1:A:437:PRO:HG3	1.98	0.45
1:A:325:LYS:HE3	4:A:548:HOH:O	2.17	0.45
1:B:441:SER:HB2	1:B:449:CYS:HB3	1.98	0.45
1:B:75:PRO:HB3	4:B:564:HOH:O	2.17	0.44
1:A:24:GLN:HE21	1:A:434:LEU:CD1	2.16	0.44
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.68	0.44
1:A:253:THR:O	1:A:254:ALA:HB3	2.19	0.43
1:B:220:TRP:CD2	1:B:328:PRO:HG2	2.53	0.43
1:A:42:GLU:CG	1:A:109:ASN:HD21	2.31	0.43
1:B:59:ASP:OD2	3:B:552:NAP:O7N	2.36	0.43
1:B:424:GLN:NE2	1:B:474:PRO:HD3	2.34	0.43
1:A:222:THR:HB	1:A:223:PRO:CD	2.49	0.42
2:A:551:FAD:HM73	3:A:552:NAP:C6N	2.49	0.42
1:A:166:HIS:HD2	1:A:168:SER:OG	2.02	0.42
1:A:399:ILE:HG22	1:A:401:ILE:HG13	2.02	0.42
1:B:62:SER:HB3	1:B:79:TRP:CD2	2.55	0.42
1:A:130:ASN:N	1:A:130:ASN:OD1	2.53	0.42
1:B:295:LEU:HG	1:B:296:LEU:HD13	2.01	0.42
1:B:265:THR:C	1:B:267:VAL:H	2.23	0.42
1:A:202:PRO:HG3	1:A:344:TYR:HA	2.01	0.42
1:B:513:VAL:CG1	1:B:513:VAL:O	2.68	0.41
1:A:332:PRO:HG2	1:A:335:ALA:HB2	2.02	0.41
1:B:24:GLN:HG2	1:B:140:ILE:HG21	2.02	0.41
1:B:12:ALA:HA	1:B:138:PHE:O	2.20	0.41
1:A:217:THR:HG23	1:A:359:ARG:HH22	1.85	0.41
1:A:217:THR:HG23	1:A:359:ARG:NH2	2.34	0.41
1:B:22:ILE:HB	1:B:102:VAL:HG11	2.03	0.41
1:A:117:TYR:CE2	1:A:119:GLU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:TRP:O	1:B:288:TRP:CD1	2.74	0.41
1:B:435:VAL:O	1:B:435:VAL:HG22	2.20	0.41
1:A:45:GLY:HA3	1:A:49:TYR:HB2	2.02	0.41
1:A:18:GLY:HA3	2:A:551:FAD:O1P	2.21	0.41
1:A:267:VAL:CG1	1:A:271:GLU:HB3	2.51	0.41
1:A:440:GLY:HA3	1:A:527:TYR:CG	2.56	0.41
1:A:95:ARG:O	1:A:98:ASP:HB2	2.21	0.41
1:B:361:ALA:HB2	1:B:375:ASP:OD2	2.21	0.41
1:A:161:LYS:HG3	1:A:368:PRO:HB3	2.02	0.40
1:A:312:LYS:O	1:A:315:GLN:HB2	2.21	0.40
1:B:319:ASP:HA	1:B:320:PRO:HD2	1.96	0.40
1:B:129:ASP:O	1:B:130:ASN:HB2	2.20	0.40
1:A:177:ALA:HA	1:A:178:PRO:HD2	1.93	0.40
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.91	0.40
1:A:245:LEU:HD12	1:A:245:LEU:HA	1.79	0.40
1:B:85:SER:OG	1:B:87:PRO:HD2	2.22	0.40
1:A:504:LYS:HB2	1:A:518:LEU:HD21	2.02	0.40
1:A:490:PHE:CZ	1:A:517:THR:HG23	2.56	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	522/545 (96%)	493 (94%)	28 (5%)	1 (0%)	52	84
1	B	529/545 (97%)	502 (95%)	25 (5%)	2 (0%)	39	74
All	All	1051/1090 (96%)	995 (95%)	53 (5%)	3 (0%)	46	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	291	GLY
1	A	178	PRO
1	B	109	ASN

### 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	437/454 (96%)	413 (94%)	24 (6%)	27	59
1	B	442/454 (97%)	422 (96%)	20 (4%)	34	68
All	All	879/908 (97%)	835 (95%)	44 (5%)	30	64

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	102	VAL
1	A	122	ARG
1	A	130	ASN
1	A	131	GLU
1	A	141	SER
1	A	150	ARG
1	A	236	SER
1	A	265	THR
1	A	273	ASP
1	A	285	TYR
1	A	287	ILE
1	A	293	ARG
1	A	296	LEU
1	A	325	LYS
1	A	369	GLU
1	A	373	THR
1	A	390	ASP
1	A	418	SER
1	A	435	VAL
1	A	444	CYS

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Mol	Chain	Res	Type
1	A	504	LYS
1	A	517	THR
1	A	519	VAL
1	B	122	ARG
1	B	131	GLU
1	B	141	SER
1	B	147	SER
1	B	149	SER
1	B	150	ARG
1	B	285	TYR
1	B	287	ILE
1	B	296	LEU
1	B	325	LYS
1	B	369	GLU
1	B	415	GLU
1	B	426	ARG
1	B	435	VAL
1	B	444	CYS
1	B	465	LYS
1	B	471	TYR
1	B	517	THR
1	B	519	VAL
1	B	530	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	94	ASN
1	A	109	ASN
1	A	166	HIS
1	A	215	GLN
1	A	406	ASN
1	A	424	GLN
1	A	438	HIS
1	A	467	ASN
1	B	24	GLN
1	B	51	ASN
1	B	82	ASN
1	B	94	ASN
1	B	105	HIS
1	B	109	ASN

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Mol	Chain	Res	Type
1	B	166	HIS
1	B	315	GLN
1	B	424	GLN
1	B	467	ASN
1	B	537	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 carbohydrates 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$
2	FAD	A	551	-	48,58,58	1.24	5 (10%)	54,89,89	2.45	8 (14%)
3	NAP	A	552	-	42,52,52	1.70	3 (7%)	54,80,80	1.83	7 (12%)
2	FAD	B	551	-	48,58,58	1.29	6 (12%)	54,89,89	2.37	11 (20%)
3	NAP	B	552	-	42,52,52	1.76	3 (7%)	54,80,80	1.90	5 (9%)

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	551	-	-	0/30/50/50	0/6/6/6
3	NAP	A	552	-	-	0/27/67/67	0/5/5/5
2	FAD	B	551	-	-	0/30/50/50	0/6/6/6
3	NAP	B	552	-	-	0/27/67/67	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	551	FAD	C10-N1	2.01	1.39	1.35
2	B	551	FAD	C1'-N10	2.11	1.50	1.48
2	B	551	FAD	C5X-N5	2.15	1.38	1.35
3	B	552	NAP	C2A-N1A	2.36	1.38	1.33
2	A	551	FAD	C2A-N1A	2.38	1.38	1.33
2	A	551	FAD	C4-N3	2.72	1.38	1.33
2	B	551	FAD	C2A-N1A	2.73	1.39	1.33
3	A	552	NAP	C2A-N1A	2.79	1.39	1.33
2	A	551	FAD	C1'-N10	3.26	1.51	1.48
2	A	551	FAD	C4X-N5	3.28	1.38	1.33
2	A	551	FAD	C2A-N3A	3.49	1.38	1.32
2	B	551	FAD	C4X-N5	3.67	1.39	1.33
3	A	552	NAP	C2A-N3A	3.78	1.38	1.32
3	B	552	NAP	C2A-N3A	3.87	1.39	1.32
2	B	551	FAD	C2A-N3A	3.98	1.39	1.32
3	A	552	NAP	O7N-C7N	8.50	1.42	1.24
3	B	552	NAP	O7N-C7N	8.70	1.42	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	551	FAD	N3A-C2A-N1A	-13.67	118.43	128.89
2	B	551	FAD	N3A-C2A-N1A	-12.40	119.40	128.89
3	B	552	NAP	N3A-C2A-N1A	-11.56	120.05	128.89
3	A	552	NAP	N3A-C2A-N1A	-10.60	120.78	128.89
2	B	551	FAD	C2B-C1B-N9A	-4.50	107.41	114.29
2	A	551	FAD	P-O3P-PA	-4.34	120.54	132.73
3	A	552	NAP	O3-PN-O5D	-4.29	91.55	102.94
2	B	551	FAD	P-O3P-PA	-4.21	120.92	132.73
2	A	551	FAD	C4X-C4-N3	-2.99	119.49	123.59
3	B	552	NAP	O3B-C3B-C4B	-2.73	102.85	111.05
3	B	552	NAP	O3-PN-O5D	-2.65	95.90	102.94
3	A	552	NAP	C4A-C5A-N7A	-2.61	107.08	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	551	FAD	C4A-C5A-N7A	-2.45	107.22	109.48
2	A	551	FAD	C2B-C1B-N9A	-2.39	110.63	114.29
2	B	551	FAD	O2'-C2'-C1'	-2.16	104.63	109.94
2	B	551	FAD	O3B-C3B-C4B	-2.11	104.72	111.05
3	B	552	NAP	O5D-C5D-C4D	-2.08	101.47	109.12
2	B	551	FAD	N6A-C6A-N1A	-2.02	114.87	119.20
3	A	552	NAP	O2N-PN-O3	2.01	114.21	105.09
3	A	552	NAP	O4D-C1D-N1N	2.14	110.48	108.13
2	B	551	FAD	O4B-C1B-N9A	2.19	112.67	108.10
3	B	552	NAP	O3D-C3D-C4D	2.19	117.63	111.05
3	A	552	NAP	O2A-PA-O3	2.29	115.47	105.09
2	A	551	FAD	C5X-C9A-N10	2.46	119.49	117.62
3	A	552	NAP	O4B-C1B-N9A	2.50	113.33	108.10
2	A	551	FAD	C4-C4X-N5	2.76	122.07	118.72
2	B	551	FAD	C4-C4X-N5	3.28	122.69	118.72
2	A	551	FAD	C4X-N5-C5X	3.41	120.69	116.76
2	B	551	FAD	C4X-N5-C5X	3.73	121.06	116.76
2	B	551	FAD	C4-N3-C2	4.75	119.35	115.25
2	A	551	FAD	C4-N3-C2	5.63	120.12	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	551	FAD	3	0
3	A	552	NAP	4	0
2	B	551	FAD	3	0
3	B	552	NAP	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	528/545 (96%)	-0.43	1 (0%) 95   94	12, 33, 53, 79	0
1	B	533/545 (97%)	-0.57	0 100   100	8, 24, 41, 60	0
All	All	1061/1090 (97%)	-0.50	1 (0%) 95   95	8, 27, 51, 79	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	GLU	2.2

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAP	B	552	48/48	0.95	0.18	1.19	13,21,50,53	0
3	NAP	A	552	48/48	0.95	0.19	0.50	26,37,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	551	53/53	0.98	0.12	-0.56	5,11,15,18	0
2	FAD	A	551	53/53	0.98	0.12	-1.01	12,19,22,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.