



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

PDB ID : 3VTE  
Title : Crystal structure of tetrahydrocannabinolic acid synthase from Cannabis sativa  
Authors : Shoyama, Y.; Tamada, T.; Kurihara, K.; Takeuchi, A.; Taura, F.; Arai, S.; Blaber, M.; Shoyama, Y.; Morimoto, S.; Kuroki, R.  
Deposited on : 2012-05-28  
Resolution : 2.75 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

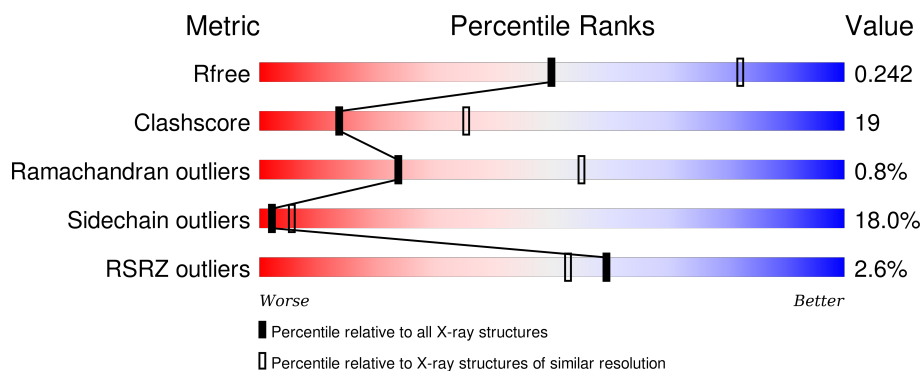
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	518	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4211 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 Tetrahydrocannabinolic acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			4023	2594	683	730	16			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



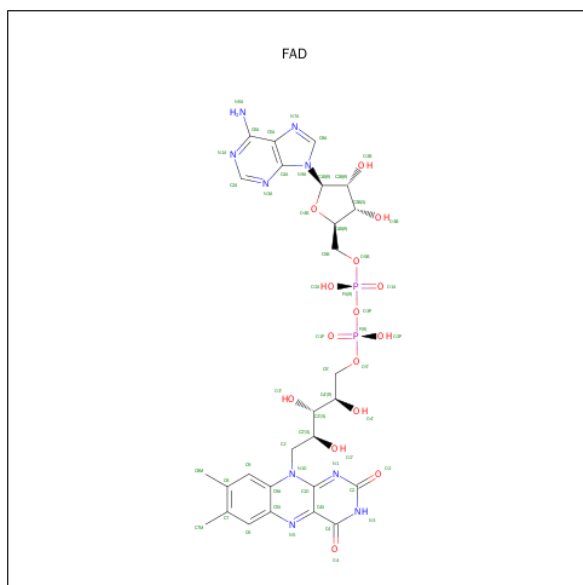
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

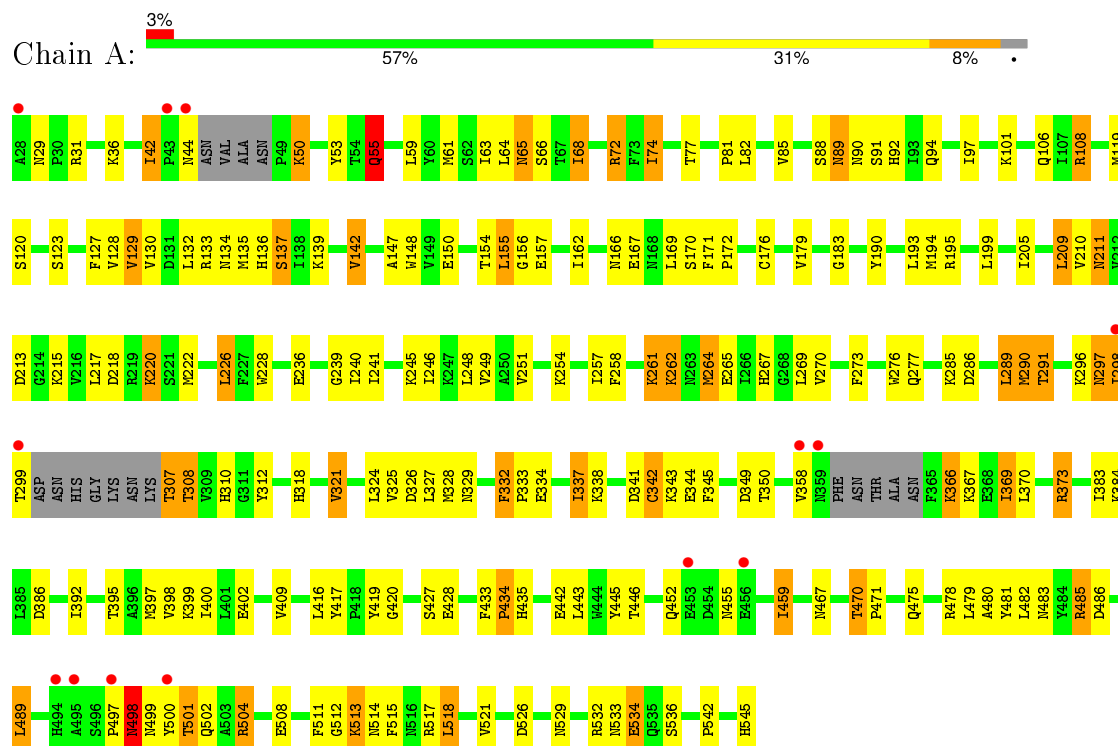
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		

### 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: Tetrahydrocannabinolic acid synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.95Å 177.95Å 177.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.49 – 2.75 44.49 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.49-2.75) 98.9 (44.49-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.198 , 0.250 0.194 , 0.242	Depositor DCC
$R_{free}$ test set	1309 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 25393 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: NAG, 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	0.88	1/4130 (0.0%)	0.90	4/5591 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	GLU	CG-CD	5.17	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	511	PHE	C-N-CA	-5.70	110.33	122.30
1	A	142	VAL	CB-CA-C	-5.33	101.28	111.40
1	A	526	ASP	CB-CG-OD2	5.03	122.82	118.30

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	4023	0	3976	148	0
2	A	84	0	78	2	0
3	A	53	0	29	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	51	0	0	5	0
All	All	4211	0	4083	153	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 19.

All (153) 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:467:ASN:O	1:A:470:THR:HG22	1.23	1.27
1:A:467:ASN:O	1:A:470:THR:CG2	2.05	1.04
1:A:119:MET:CE	1:A:485:ARG:HD3	1.90	1.00
1:A:119:MET:HE3	1:A:485:ARG:HD3	1.43	0.99
1:A:209:LEU:HD12	1:A:241:ILE:HD13	1.47	0.95
1:A:211:ASN:ND2	1:A:213:ASP:H	1.66	0.94
1:A:383:ILE:HG13	1:A:446:THR:HG22	1.48	0.94
1:A:211:ASN:HD22	1:A:211:ASN:C	1.73	0.92
1:A:513:LYS:H	1:A:513:LYS:HZ3	1.15	0.91
1:A:512:GLY:HA3	1:A:513:LYS:HZ1	1.34	0.91
1:A:373:ARG:HH11	1:A:373:ARG:HG2	1.44	0.83
1:A:504:ARG:HG2	1:A:504:ARG:HH21	1.45	0.81
1:A:470:THR:HB	1:A:478:ARG:NH2	1.96	0.80
3:A:607:FAD:H8A	3:A:607:FAD:H51A	1.61	0.80
1:A:183:GLY:HA3	3:A:607:FAD:H52A	1.65	0.78
1:A:222:MET:HG2	1:A:226:LEU:HB3	1.67	0.76
1:A:88:SER:H	1:A:92:HIS:HD2	1.31	0.75
1:A:262:LYS:HD3	1:A:264:MET:HE1	1.67	0.75
1:A:209:LEU:CD1	1:A:241:ILE:HD13	2.16	0.74
1:A:512:GLY:HA3	1:A:513:LYS:NZ	2.02	0.74
1:A:119:MET:HE1	1:A:485:ARG:HD3	1.69	0.74
1:A:497:PRO:O	1:A:498:ASN:HB2	1.88	0.73
1:A:265:GLU:OE1	1:A:267:HIS:HB2	1.89	0.73
1:A:297:ASN:HB2	1:A:307:THR:HA	1.71	0.72
1:A:397:MET:HA	1:A:400:ILE:HD12	1.71	0.72
1:A:513:LYS:NZ	1:A:513:LYS:H	1.88	0.71
1:A:542:PRO:HA	1:A:545:HIS:CD2	2.26	0.70
1:A:119:MET:HE3	1:A:485:ARG:CD	2.21	0.68
1:A:297:ASN:O	1:A:307:THR:HB	1.94	0.67
1:A:504:ARG:HD2	1:A:508:GLU:OE1	1.95	0.67
1:A:337:ILE:HD12	1:A:337:ILE:O	1.95	0.66
1:A:338:LYS:O	1:A:341:ASP:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG13	1:A:68:ILE:O	1.96	0.65
1:A:481:TYR:CZ	1:A:483:ASN:HB2	2.32	0.64
1:A:504:ARG:HH21	1:A:504:ARG:CG	2.11	0.64
1:A:211:ASN:ND2	1:A:213:ASP:N	2.43	0.63
1:A:91:SER:HA	1:A:94:GLN:HE21	1.63	0.63
1:A:205:ILE:HB	1:A:245:LYS:HG2	1.80	0.63
1:A:211:ASN:HD22	1:A:213:ASP:H	1.44	0.62
1:A:321:VAL:O	1:A:325:VAL:HG23	2.00	0.61
1:A:258:PHE:HB3	1:A:342:CYS:HB3	1.82	0.61
1:A:512:GLY:H	1:A:514:ASN:HB2	1.66	0.61
1:A:209:LEU:HG	1:A:210:VAL:N	2.16	0.61
1:A:74:ILE:O	1:A:74:ILE:HG22	2.01	0.61
1:A:50:LYS:HD3	1:A:53:TYR:CE2	2.37	0.60
1:A:171:PHE:CZ	1:A:246:ILE:HG13	2.37	0.59
1:A:533:ASN:OD1	1:A:536:SER:HB3	2.03	0.59
1:A:176:CYS:HB2	1:A:179:VAL:HG23	1.85	0.59
1:A:211:ASN:ND2	1:A:211:ASN:C	2.46	0.58
1:A:486:ASP:HB3	1:A:489:LEU:HD22	1.84	0.58
1:A:176:CYS:HB3	4:A:848:HOH:O	2.04	0.58
1:A:499:ASN:OD1	1:A:501:THR:N	2.37	0.57
1:A:532:ARG:HD3	4:A:814:HOH:O	2.04	0.57
1:A:395:THR:O	1:A:398:VAL:HG22	2.05	0.57
1:A:504:ARG:HG2	1:A:504:ARG:NH2	2.19	0.56
1:A:183:GLY:CA	3:A:607:FAD:H52A	2.34	0.56
3:A:607:FAD:H8A	3:A:607:FAD:C5B	2.34	0.55
1:A:88:SER:HA	1:A:135:MET:HG3	1.88	0.55
1:A:383:ILE:HG12	1:A:384:LYS:N	2.21	0.54
1:A:119:MET:SD	1:A:534:GLU:HG2	2.47	0.54
1:A:106:GLN:OE1	1:A:108:ARG:NH1	2.40	0.54
1:A:276:TRP:CD1	1:A:289:LEU:HD13	2.43	0.54
1:A:90:ASN:O	1:A:94:GLN:HG3	2.08	0.54
1:A:228:TRP:CZ3	1:A:518:LEU:HD13	2.42	0.54
1:A:435:HIS:HE1	1:A:480:ALA:O	1.91	0.54
3:A:607:FAD:C8A	3:A:607:FAD:H51A	2.33	0.54
1:A:334:GLU:H	1:A:334:GLU:CD	2.11	0.53
1:A:89:ASN:OD1	2:A:602:NAG:H2	2.08	0.53
1:A:470:THR:HB	1:A:478:ARG:HH22	1.74	0.53
1:A:137:SER:HB3	1:A:150:GLU:OE1	2.08	0.53
1:A:308:THR:O	1:A:310:HIS:HD2	1.93	0.52
1:A:483:ASN:ND2	4:A:801:HOH:O	2.42	0.51
1:A:329:ASN:O	1:A:333:PRO:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG21	1:A:398:VAL:HG12	1.91	0.51
1:A:81:PRO:HG3	1:A:129:VAL:HG13	1.92	0.50
1:A:42:ILE:HG22	1:A:42:ILE:O	2.12	0.50
1:A:171:PHE:CE2	1:A:246:ILE:HG13	2.47	0.49
1:A:257:ILE:HD11	1:A:350:THR:HG23	1.95	0.49
1:A:169:LEU:HD13	1:A:248:LEU:HD12	1.94	0.48
1:A:291:THR:HG23	1:A:416:LEU:HD22	1.95	0.48
1:A:61:MET:O	1:A:65:ASN:HB2	2.14	0.48
1:A:500:TYR:OH	1:A:504:ARG:NH1	2.47	0.47
1:A:195:ARG:HE	1:A:420:GLY:H	1.62	0.47
1:A:108:ARG:NH1	1:A:123:SER:HB2	2.29	0.47
1:A:435:HIS:CD2	1:A:479:LEU:HD13	2.49	0.47
1:A:210:VAL:HA	1:A:215:LYS:O	2.14	0.47
1:A:81:PRO:HB3	1:A:127:PHE:CE1	2.50	0.47
1:A:517:ARG:O	1:A:521:VAL:HG23	2.14	0.47
1:A:296:LYS:O	1:A:297:ASN:HB2	2.14	0.47
1:A:373:ARG:HH11	1:A:373:ARG:CG	2.19	0.47
1:A:328:MET:CB	1:A:337:ILE:HD11	2.44	0.47
1:A:366:LYS:O	1:A:369:ILE:HG13	2.14	0.47
1:A:515:PHE:HB3	4:A:845:HOH:O	2.15	0.46
1:A:74:ILE:CG2	1:A:74:ILE:O	2.64	0.46
1:A:72:ARG:HA	1:A:452:GLN:HE22	1.81	0.46
1:A:273:PHE:CD1	1:A:397:MET:HG2	2.50	0.46
1:A:470:THR:N	1:A:471:PRO:CD	2.79	0.46
1:A:130:VAL:HG12	1:A:130:VAL:O	2.15	0.45
1:A:218:ASP:O	1:A:222:MET:HB2	2.17	0.45
1:A:97:ILE:HD11	1:A:240:ILE:HD12	1.99	0.45
1:A:89:ASN:OD1	2:A:602:NAG:H83	2.17	0.45
3:A:607:FAD:H1'2	3:A:607:FAD:H9	1.45	0.44
1:A:290:MET:HE1	1:A:417:TYR:HE2	1.82	0.44
1:A:276:TRP:HD1	1:A:289:LEU:HD13	1.82	0.44
1:A:308:THR:O	1:A:310:HIS:CD2	2.69	0.44
1:A:55:GLN:HE21	1:A:55:GLN:HB2	1.62	0.44
1:A:498:ASN:O	1:A:499:ASN:C	2.55	0.44
1:A:123:SER:HB3	1:A:127:PHE:CD2	2.53	0.44
1:A:290:MET:CE	1:A:417:TYR:HE2	2.31	0.44
1:A:499:ASN:OD1	1:A:502:GLN:N	2.50	0.44
1:A:328:MET:HG3	1:A:337:ILE:HG12	1.99	0.44
1:A:277:GLN:OE1	1:A:392:ILE:N	2.45	0.43
1:A:239:GLY:O	3:A:607:FAD:H2A	2.18	0.43
1:A:166:ASN:C	1:A:166:ASN:OD1	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:O	1:A:136:HIS:HD2	2.01	0.43
1:A:261:LYS:O	1:A:262:LYS:HG2	2.18	0.43
1:A:499:ASN:C	1:A:499:ASN:OD1	2.57	0.43
1:A:261:LYS:HG2	1:A:312:TYR:CE1	2.53	0.43
1:A:398:VAL:CG2	1:A:399:LYS:N	2.81	0.43
1:A:162:ILE:HG21	1:A:170:SER:HA	2.00	0.43
1:A:236:GLU:HB3	3:A:607:FAD:H1B	2.00	0.43
1:A:199:LEU:HD21	1:A:433:PHE:CD1	2.54	0.43
1:A:120:SER:HB3	3:A:607:FAD:H3B	2.01	0.43
1:A:42:ILE:HD13	1:A:42:ILE:HA	1.79	0.42
1:A:66:SER:OG	1:A:133:ARG:NH1	2.39	0.42
1:A:273:PHE:HE2	1:A:416:LEU:HD21	1.85	0.42
1:A:513:LYS:N	1:A:513:LYS:HZ3	1.99	0.42
1:A:81:PRO:HG3	1:A:129:VAL:CG1	2.49	0.42
1:A:504:ARG:HD2	1:A:508:GLU:CD	2.40	0.42
1:A:172:PRO:HD3	1:A:249:VAL:CG2	2.49	0.42
1:A:190:TYR:OH	1:A:442:GLU:OE1	2.28	0.42
1:A:59:LEU:O	1:A:63:ILE:HG13	2.19	0.42
1:A:154:THR:OG1	1:A:157:GLU:HG3	2.20	0.42
1:A:211:ASN:HD22	1:A:213:ASP:N	2.11	0.41
1:A:286:ASP:HB2	1:A:318:HIS:HB2	2.02	0.41
1:A:148:TRP:NE1	1:A:245:LYS:HD3	2.35	0.41
1:A:133:ARG:HG3	1:A:134:ASN:ND2	2.35	0.41
1:A:373:ARG:NH1	1:A:373:ARG:HG2	2.21	0.41
1:A:220:LYS:HB3	1:A:220:LYS:HE2	1.89	0.41
1:A:337:ILE:C	1:A:337:ILE:CD1	2.89	0.41
1:A:108:ARG:HD2	1:A:108:ARG:HA	1.97	0.41
3:A:607:FAD:O2B	4:A:824:HOH:O	2.22	0.41
1:A:332:PHE:N	1:A:333:PRO:HD3	2.36	0.41
1:A:369:ILE:H	1:A:369:ILE:HG13	1.51	0.41
1:A:36:LYS:HE2	1:A:36:LYS:HB3	1.74	0.41
1:A:155:LEU:O	1:A:156:GLY:C	2.60	0.40
1:A:345:PHE:HD1	1:A:349:ASP:HB3	1.86	0.40
1:A:147:ALA:HB3	1:A:246:ILE:HG22	2.01	0.40
1:A:328:MET:HB2	1:A:337:ILE:HD11	2.02	0.40
1:A:455:ASN:O	1:A:459:ILE:HG23	2.21	0.40
1:A:452:GLN:HE21	1:A:455:ASN:HD21	1.69	0.40
1:A:298:ILE:HA	1:A:409:VAL:HG21	2.02	0.40
1:A:428:GLU:HB3	1:A:513:LYS:HE3	2.04	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	494/518 (95%)	453 (92%)	37 (8%)	4 (1%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	55	GLN
1	A	498	ASN
1	A	434	PRO

### 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	439/452 (97%)	360 (82%)	79 (18%)	2	5

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	31	ARG
1	A	42	ILE
1	A	44	ASN
1	A	50	LYS
1	A	55	GLN
1	A	64	LEU

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Mol	Chain	Res	Type
1	A	65	ASN
1	A	68	ILE
1	A	72	ARG
1	A	74	ILE
1	A	77	THR
1	A	82	LEU
1	A	85	VAL
1	A	89	ASN
1	A	101	LYS
1	A	108	ARG
1	A	128	VAL
1	A	129	VAL
1	A	132	LEU
1	A	137	SER
1	A	139	LYS
1	A	142	VAL
1	A	155	LEU
1	A	193	LEU
1	A	194	MET
1	A	209	LEU
1	A	211	ASN
1	A	217	LEU
1	A	220	LYS
1	A	226	LEU
1	A	251	VAL
1	A	254	LYS
1	A	261	LYS
1	A	262	LYS
1	A	264	MET
1	A	269	LEU
1	A	285	LYS
1	A	289	LEU
1	A	290	MET
1	A	291	THR
1	A	298	ILE
1	A	299	THR
1	A	307	THR
1	A	308	THR
1	A	321	VAL
1	A	324	LEU
1	A	326	ASP
1	A	327	LEU

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Mol	Chain	Res	Type
1	A	332	PHE
1	A	337	ILE
1	A	342	CYS
1	A	343	LYS
1	A	344	GLU
1	A	358	VAL
1	A	366	LYS
1	A	367	LYS
1	A	369	ILE
1	A	370	LEU
1	A	373	ARG
1	A	386	ASP
1	A	402	GLU
1	A	419	TYR
1	A	427	SER
1	A	434	PRO
1	A	443	LEU
1	A	445	TYR
1	A	459	ILE
1	A	470	THR
1	A	475	GLN
1	A	482	LEU
1	A	489	LEU
1	A	498	ASN
1	A	501	THR
1	A	504	ARG
1	A	513	LYS
1	A	518	LEU
1	A	529	ASN
1	A	534	GLU

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	56	HIS
1	A	90	ASN
1	A	92	HIS
1	A	94	GLN
1	A	134	ASN
1	A	136	HIS
1	A	211	ASN

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Mol	Chain	Res	Type
1	A	310	HIS
1	A	435	HIS
1	A	452	GLN
1	A	475	GLN
1	A	483	ASN
1	A	498	ASN
1	A	529	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

7 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	NAG	A	601	1	14,14,15	0.72	0	15,19,21	2.06	4 (26%)
2	NAG	A	602	1	14,14,15	1.04	1 (7%)	15,19,21	3.17	9 (60%)
2	NAG	A	603	1	14,14,15	1.30	2 (14%)	15,19,21	2.83	6 (40%)
2	NAG	A	604	1	14,14,15	0.43	0	15,19,21	1.92	4 (26%)
2	NAG	A	605	1	14,14,15	1.00	0	15,19,21	1.82	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	606	1	14,14,15	0.84	1 (7%)	15,19,21	2.11	6 (40%)
3	FAD	A	607	1	48,58,58	1.37	7 (14%)	54,89,89	2.34	15 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
2	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	NAG	A	605	1	-	0/6/23/26	0/1/1/1
2	NAG	A	606	1	-	0/6/23/26	0/1/1/1
3	FAD	A	607	1	-	0/30/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	FAD	O5B-C5B	-2.34	1.35	1.44
3	A	607	FAD	O4B-C4B	-2.05	1.40	1.45
2	A	603	NAG	C3-C2	2.13	1.57	1.52
2	A	602	NAG	C1-C2	2.16	1.55	1.52
2	A	606	NAG	C1-C2	2.20	1.55	1.52
3	A	607	FAD	C2A-N1A	2.41	1.38	1.33
3	A	607	FAD	C2A-N3A	2.58	1.36	1.32
3	A	607	FAD	C5X-N5	2.71	1.39	1.35
3	A	607	FAD	C4-N3	3.24	1.39	1.33
2	A	603	NAG	C1-C2	3.46	1.57	1.52
3	A	607	FAD	C4X-N5	3.76	1.39	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	FAD	N3A-C2A-N1A	-11.62	119.99	128.89
2	A	602	NAG	O7-C7-C8	-3.62	115.42	122.06
3	A	607	FAD	C1'-N10-C9A	-2.95	115.55	118.86
2	A	606	NAG	C3-C4-C5	-2.87	105.19	110.20
2	A	605	NAG	O7-C7-C8	-2.86	116.82	122.06
3	A	607	FAD	C2B-C1B-N9A	-2.83	109.96	114.29
2	A	603	NAG	O7-C7-C8	-2.81	116.90	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	NAG	C6-C5-C4	-2.81	106.09	113.02
3	A	607	FAD	C1B-N9A-C4A	-2.74	122.81	126.94
3	A	607	FAD	O4B-C4B-C3B	-2.68	99.75	105.15
3	A	607	FAD	C9A-C5X-N5	-2.52	118.63	122.36
2	A	604	NAG	C4-C3-C2	-2.39	107.51	111.23
2	A	602	NAG	C4-C3-C2	-2.23	107.75	111.23
2	A	606	NAG	O7-C7-C8	-2.13	118.15	122.06
3	A	607	FAD	P-O3P-PA	-2.06	126.93	132.73
2	A	602	NAG	O3-C3-C4	2.01	114.86	110.34
2	A	606	NAG	C6-C5-C4	2.02	118.01	113.02
3	A	607	FAD	O3P-P-O5'	2.06	108.39	102.94
2	A	605	NAG	C2-N2-C7	2.06	125.69	123.04
3	A	607	FAD	O2A-PA-O5B	2.13	119.18	108.46
2	A	605	NAG	C3-C2-N2	2.14	115.69	110.56
2	A	603	NAG	O4-C4-C5	2.16	114.96	109.24
2	A	602	NAG	O6-C6-C5	2.17	118.50	111.33
3	A	607	FAD	C4B-O4B-C1B	2.23	112.17	109.72
2	A	602	NAG	C6-C5-C4	2.24	118.54	113.02
2	A	603	NAG	O7-C7-N2	2.28	126.50	121.86
2	A	606	NAG	O4-C4-C5	2.33	115.41	109.24
2	A	601	NAG	C8-C7-N2	2.35	120.61	116.11
3	A	607	FAD	O2A-PA-O3P	2.37	115.82	105.09
2	A	605	NAG	C8-C7-N2	2.39	120.69	116.11
3	A	607	FAD	C6-C5X-N5	2.80	122.57	118.96
3	A	607	FAD	C4X-N5-C5X	2.84	120.03	116.76
2	A	603	NAG	C2-N2-C7	2.98	126.86	123.04
2	A	601	NAG	C1-O5-C5	2.99	116.05	112.25
2	A	604	NAG	C1-O5-C5	3.08	116.16	112.25
2	A	602	NAG	O5-C5-C6	3.12	114.11	107.35
2	A	601	NAG	C3-C4-C5	3.27	115.90	110.20
2	A	606	NAG	C2-N2-C7	3.29	127.27	123.04
2	A	604	NAG	C3-C2-N2	4.13	120.44	110.56
3	A	607	FAD	C4-N3-C2	4.33	118.99	115.25
2	A	603	NAG	O3-C3-C2	4.38	117.79	109.11
2	A	605	NAG	C1-O5-C5	4.40	117.83	112.25
2	A	602	NAG	C8-C7-N2	4.47	124.66	116.11
2	A	606	NAG	O5-C5-C6	4.58	117.25	107.35
2	A	602	NAG	C2-N2-C7	4.78	129.18	123.04
3	A	607	FAD	C5X-C9A-N10	4.83	121.29	117.62
2	A	601	NAG	C2-N2-C7	4.85	129.27	123.04
2	A	602	NAG	C1-O5-C5	7.88	122.25	112.25
2	A	603	NAG	C1-O5-C5	7.98	122.37	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	NAG	2	0
3	A	607	FAD	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	502/518 (96%)	-0.39	13 (2%) 59 53	26, 42, 71, 99	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	ALA	5.4
1	A	44	ASN	4.4
1	A	495	ALA	3.5
1	A	494	HIS	3.5
1	A	298	ILE	3.5
1	A	43	PRO	3.1
1	A	358	VAL	3.1
1	A	497	PRO	2.8
1	A	299	THR	2.6
1	A	500	TYR	2.5
1	A	456	GLU	2.3
1	A	359	ASN	2.2
1	A	453	GLU	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
3	FAD	A	607	53/53	0.98	0.16	0.95	21,30,36,39	0
2	NAG	A	602	14/15	0.76	0.35	-	89,93,98,102	0
2	NAG	A	606	14/15	0.78	0.36	-	118,121,127,128	0
2	NAG	A	601	14/15	0.82	0.21	-	75,81,85,87	0
2	NAG	A	603	14/15	0.89	0.11	-	69,73,75,78	0
2	NAG	A	604	14/15	0.90	0.42	-	97,103,108,109	0
2	NAG	A	605	14/15	0.75	0.32	-	82,89,91,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.