Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 PM GMT

PDB ID	:	3W8Z
Title	:	The complex structure of EncM with hydroxytetraketide
Authors	:	Teufel, R.; Miyanaga, A.; Stull, F.; Michaudel, Q.; Louie, G.; Noel, J.P.; Baran, P.S.; Palfey, B.; Moore, B.S.
Deposited on	:	2013-03-22
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

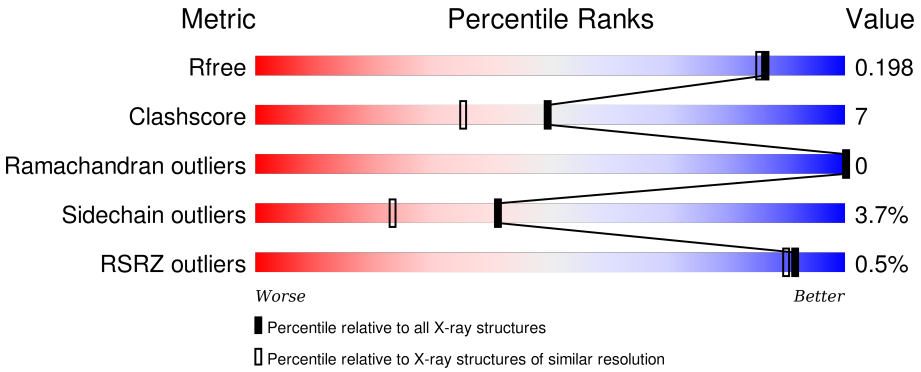
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 >=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 <=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	468	83% 13%
1	B	468	% 85% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HTK	A	601	-	-	-	X
3	HTK	B	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7874 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.

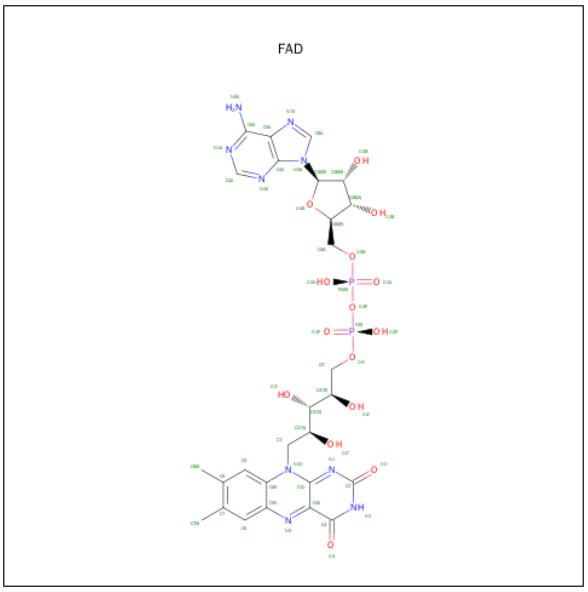
- Molecule 1 is a protein called Putative FAD-dependent oxygenase EncM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3501	2213	625	650	13			
1	B	461	Total	C	N	O	S	0	0	0
			3507	2216	626	652	13			

There are 8 discrepancies between the modelled and reference sequences:

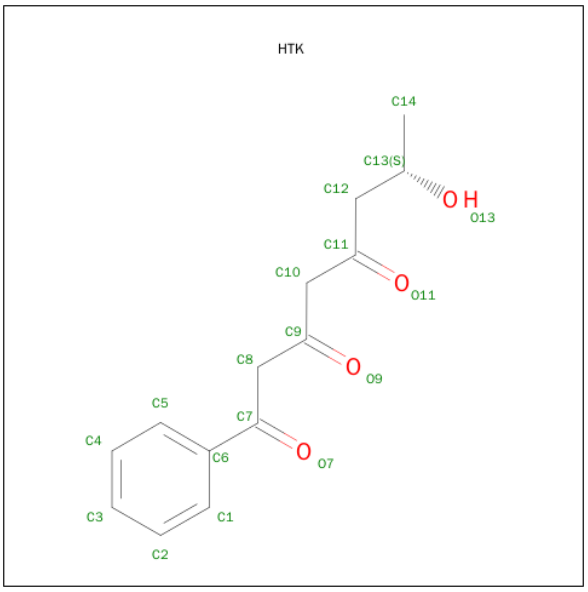
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q9KHK2
A	-2	SER	-	EXPRESSION TAG	UNP Q9KHK2
A	-1	HIS	-	EXPRESSION TAG	UNP Q9KHK2
A	0	GLY	-	EXPRESSION TAG	UNP Q9KHK2
B	-3	GLY	-	EXPRESSION TAG	UNP Q9KHK2
B	-2	SER	-	EXPRESSION TAG	UNP Q9KHK2
B	-1	HIS	-	EXPRESSION TAG	UNP Q9KHK2
B	0	GLY	-	EXPRESSION TAG	UNP Q9KHK2

- 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 (7S)-7-HYDROXY-1-PHENYLOCTANE-1,3,5-TRIONE (three-letter code: HTK) (formula: $C_{14}H_{16}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	14	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			18	14	4		

- Molecule 4 is water.

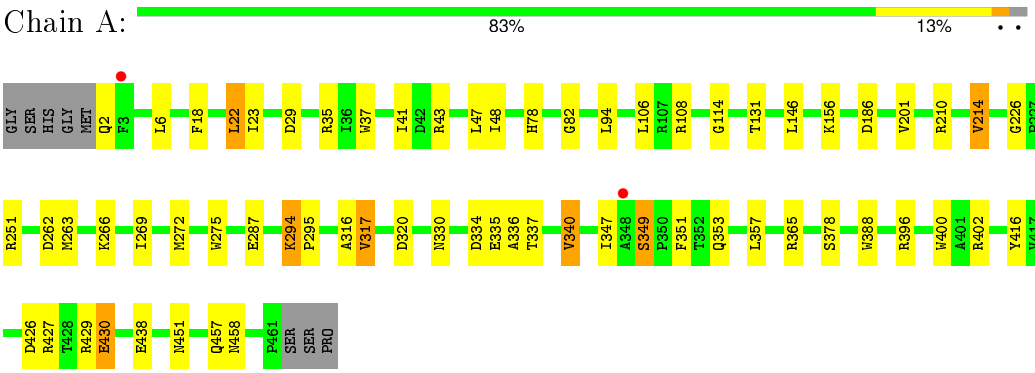
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	376	Total	O	0	0
			376	376		
4	B	348	Total	O	0	0
			348	348		

3 Residue-property plots (i)

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.

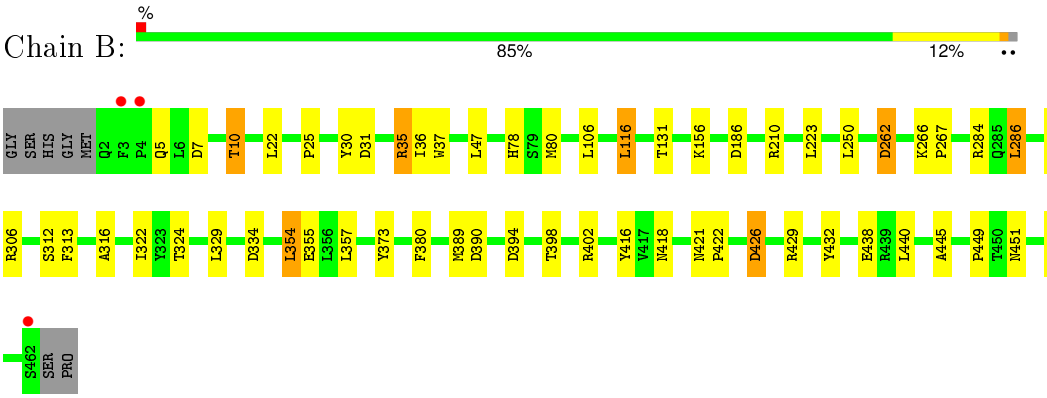
- Molecule 1: Putative FAD-dependent oxygenase EncM

Chain A:



- Molecule 1: Putative FAD-dependent oxygenase EncM

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.07Å 85.12Å 79.34Å 90.00° 99.58° 90.00°	Depositor
Resolution (Å)	42.60 – 1.80 42.56 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.60-1.80) 99.8 (42.56-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.158 , 0.196 0.158 , 0.198	Depositor DCC
R_{free} test set	4318 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 86188 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7874	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HTK, 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	1.13	3/3592 (0.1%)	1.09	11/4896 (0.2%)
1	B	1.09	3/3598 (0.1%)	1.08	12/4904 (0.2%)
All	All	1.11	6/7190 (0.1%)	1.08	23/9800 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	TRP	CG-CD1	6.66	1.46	1.36
1	A	388	TRP	CG-CD1	5.69	1.44	1.36
1	B	432	TYR	CE1-CZ	5.45	1.45	1.38
1	A	275	TRP	CE3-CZ3	5.36	1.47	1.38
1	B	373	TYR	CG-CD1	5.31	1.46	1.39
1	B	373	TYR	CE2-CZ	5.05	1.45	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	402	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	B	390	ASP	CB-CG-OD1	8.37	125.83	118.30
1	B	116	LEU	CB-CG-CD1	7.63	123.97	111.00
1	A	340	VAL	CG1-CB-CG2	6.84	121.84	110.90
1	A	29	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	334	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	306	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	186	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	390	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	B	286	LEU	CB-CG-CD1	5.75	120.77	111.00
1	B	31	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	402	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	214	VAL	CG1-CB-CG2	5.48	119.67	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	354	LEU	CB-CG-CD2	5.41	120.19	111.00
1	B	186	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	214	VAL	CA-CB-CG1	5.34	118.91	110.90
1	A	402	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	334	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	347	ILE	C-N-CA	-5.25	108.58	121.70
1	B	426	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	396	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	106	LEU	CB-CG-CD1	-5.04	102.43	111.00

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	3501	0	3413	52	0
1	B	3507	0	3418	46	0
2	A	53	0	31	8	0
2	B	53	0	31	7	0
3	A	18	0	16	3	0
3	B	18	0	16	5	0
4	A	376	0	0	10	1
4	B	348	0	0	4	0
All	All	7874	0	6925	100	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (100) 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:78:HIS:ND1	2:A:600:FAD:HM83	1.18	1.43
1:B:78:HIS:ND1	2:B:600:FAD:HM83	1.11	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:HIS:ND1	2:A:600:FAD:C8M	1.91	1.30
1:B:78:HIS:ND1	2:B:600:FAD:C8M	1.91	1.30
1:B:438:GLU:HB2	4:B:838:HOH:O	1.40	1.21
1:A:78:HIS:CE1	2:A:600:FAD:HM83	1.86	1.10
1:B:7:ASP:HB3	1:B:10:THR:CG2	1.84	1.06
1:B:35:ARG:HG2	1:B:35:ARG:HH21	1.17	1.05
1:B:7:ASP:HB3	1:B:10:THR:HG22	1.41	1.02
1:B:78:HIS:CE1	2:B:600:FAD:HM83	1.96	1.00
1:A:349:SER:HB2	4:A:965:HOH:O	1.60	0.99
1:A:231:ARG:HH11	1:A:231:ARG:HG3	1.30	0.92
1:B:35:ARG:NH2	1:B:36:ILE:O	2.06	0.87
1:A:228:GLN:H	1:A:228:GLN:HE21	1.27	0.83
1:B:35:ARG:CG	1:B:35:ARG:HH21	1.91	0.82
1:A:294:LYS:HD2	1:A:295:PRO:HD2	1.63	0.81
1:B:451:ASN:HD21	1:B:458:ASN:HD21	1.29	0.79
1:B:223:LEU:H	1:B:266:LYS:HZ1	1.31	0.75
1:B:7:ASP:CB	1:B:10:THR:HG22	2.15	0.75
1:B:223:LEU:H	1:B:266:LYS:NZ	1.89	0.71
1:A:231:ARG:NH1	1:A:231:ARG:HG3	2.04	0.70
1:B:357:LEU:HD11	3:B:601:HTK:H7	1.74	0.69
1:B:35:ARG:NH2	1:B:35:ARG:HG2	1.99	0.69
1:B:398:THR:HG21	4:B:1029:HOH:O	1.94	0.68
1:A:35:ARG:HD2	4:A:707:HOH:O	1.97	0.65
1:A:294:LYS:HD2	1:A:295:PRO:CD	2.27	0.65
1:A:317:VAL:CG2	1:A:351:PHE:CZ	2.80	0.65
1:B:357:LEU:CD1	3:B:601:HTK:H7	2.26	0.64
1:B:262:ASP:OD1	1:B:262:ASP:N	2.24	0.63
1:A:263:MET:HA	1:A:266:LYS:HE2	1.81	0.62
1:B:78:HIS:ND1	2:B:600:FAD:C8	2.61	0.62
1:B:7:ASP:OD2	1:B:10:THR:HG22	1.99	0.62
1:A:78:HIS:ND1	2:A:600:FAD:C8	2.62	0.61
1:A:18:PHE:CE2	1:A:22:LEU:HD13	2.36	0.60
3:B:601:HTK:O11	3:B:601:HTK:H15	2.02	0.59
1:B:156:LYS:HE2	4:B:895:HOH:O	2.00	0.59
2:B:600:FAD:O4	3:B:601:HTK:O7	2.20	0.58
1:A:78:HIS:ND1	2:A:600:FAD:HM81	2.10	0.57
1:A:228:GLN:HE21	1:A:228:GLN:N	1.99	0.57
1:B:37:TRP:CH2	2:B:600:FAD:HM82	2.41	0.56
1:A:317:VAL:HG22	1:A:351:PHE:CZ	2.41	0.56
1:A:317:VAL:HG21	1:A:351:PHE:CZ	2.40	0.55
1:A:451:ASN:HD21	1:A:458:ASN:HD21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HH12	1:A:337:THR:HG21	1.72	0.54
2:A:600:FAD:O4	3:A:601:HTK:O7	2.26	0.54
1:B:37:TRP:CZ3	2:B:600:FAD:HM82	2.42	0.54
1:A:365:ARG:NH2	4:A:1067:HOH:O	2.23	0.54
1:A:335:GLU:HG2	4:A:717:HOH:O	2.08	0.54
1:A:251:ARG:HD2	1:A:353:GLN:HE21	1.73	0.53
1:A:228:GLN:H	1:A:228:GLN:NE2	2.01	0.53
1:A:156:LYS:HE2	4:A:837:HOH:O	2.09	0.53
1:A:37:TRP:CZ3	2:A:600:FAD:HM82	2.44	0.52
3:A:601:HTK:H15	3:A:601:HTK:O11	2.09	0.52
1:A:317:VAL:HG22	1:A:351:PHE:CE1	2.45	0.52
1:A:316:ALA:O	1:B:210:ARG:NH2	2.42	0.51
1:B:7:ASP:HB3	1:B:10:THR:HG21	1.84	0.50
1:A:262:ASP:O	1:A:266:LYS:HE2	2.11	0.49
1:B:266:LYS:HG2	1:B:267:PRO:N	2.27	0.49
1:A:35:ARG:NH2	4:A:1021:HOH:O	2.45	0.49
1:B:421:ASN:HB2	1:B:422:PRO:CD	2.43	0.49
1:B:394:ASP:O	1:B:398:THR:HG23	2.13	0.48
1:A:37:TRP:CH2	2:A:600:FAD:HM82	2.49	0.47
1:A:231:ARG:NH1	1:A:337:THR:HG21	2.29	0.47
1:B:223:LEU:N	1:B:266:LYS:HZ1	2.07	0.47
1:A:320:ASP:OD1	4:A:766:HOH:O	2.20	0.47
1:B:35:ARG:NH2	1:B:35:ARG:CG	2.61	0.47
1:A:210:ARG:NH2	1:B:316:ALA:O	2.48	0.47
1:A:94:LEU:O	1:A:114:GLY:HA3	2.16	0.46
1:B:329:LEU:HB2	1:B:380:PHE:HB2	1.98	0.45
1:A:457:GLN:HG2	4:A:920:HOH:O	2.17	0.44
1:A:416:TYR:CZ	1:A:418:ASN:HB2	2.53	0.44
1:B:7:ASP:CG	1:B:10:THR:HG22	2.38	0.44
1:A:336:ALA:O	1:A:340:VAL:HG13	2.18	0.44
1:B:22:LEU:HB3	1:B:47:LEU:HD11	1.99	0.44
1:B:355:GLU:OE1	3:B:601:HTK:H12	2.19	0.43
1:A:421:ASN:HB2	1:A:422:PRO:CD	2.48	0.43
1:A:429:ARG:HD3	4:A:721:HOH:O	2.18	0.43
1:A:23:ILE:HB	1:A:48:ILE:HB	1.99	0.43
1:B:80:MET:SD	1:B:324:THR:HG21	2.57	0.43
1:B:440:LEU:HB3	1:B:459:ILE:HD13	2.00	0.43
1:A:330:ASN:ND2	1:A:378:SER:OG	2.52	0.43
1:B:416:TYR:CZ	1:B:418:ASN:HB2	2.53	0.42
1:A:272:MET:HE3	1:A:272:MET:HB2	1.98	0.42
1:A:41:ILE:HG13	1:A:82:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PRO:HA	1:B:30:TYR:CG	2.54	0.42
1:B:389:MET:HG3	4:B:956:HOH:O	2.19	0.42
1:A:226:GLY:HA2	1:A:269:ILE:HD11	2.02	0.42
1:A:146:LEU:HD21	1:A:201:VAL:HG21	2.01	0.42
1:A:108:ARG:NH1	4:A:1029:HOH:O	2.37	0.42
1:A:22:LEU:HG	1:A:47:LEU:HD11	2.02	0.42
1:B:312:SER:HA	1:B:313:PHE:HA	1.94	0.42
1:A:357:LEU:HD11	3:A:601:HTK:C8	2.50	0.42
1:A:427:ARG:O	1:A:430:GLU:HG3	2.21	0.41
1:B:294:LYS:HE3	1:B:296:HIS:CE1	2.55	0.41
1:A:231:ARG:NH1	1:A:231:ARG:CG	2.76	0.41
1:A:294:LYS:C	1:A:294:LYS:HD2	2.42	0.41
1:B:322:ILE:C	1:B:322:ILE:HD12	2.40	0.41
1:B:250:LEU:HD12	1:B:250:LEU:N	2.36	0.41
1:B:445:ALA:O	1:B:449:PRO:HB3	2.22	0.40
1:B:421:ASN:HB2	1:B:422:PRO:HD2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1033:HOH:O	4:A:1073:HOH:O[2_546]	1.99	0.21

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	458/468 (98%)	451 (98%)	7 (2%)	0	100	100
1	B	459/468 (98%)	451 (98%)	8 (2%)	0	100	100
All	All	917/936 (98%)	902 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	355/361 (98%)	342 (96%)	13 (4%)	41	23
1	B	356/361 (99%)	343 (96%)	13 (4%)	41	23
All	All	711/722 (98%)	685 (96%)	26 (4%)	41	23

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	6	LEU
1	A	22	LEU
1	A	131	THR
1	A	214	VAL
1	A	228	GLN
1	A	287	GLU
1	A	294	LYS
1	A	317	VAL
1	A	349	SER
1	A	426	ASP
1	A	430	GLU
1	A	438	GLU
1	B	5	GLN
1	B	10	THR
1	B	35	ARG
1	B	106	LEU
1	B	116	LEU
1	B	131	THR
1	B	262	ASP
1	B	284	ARG
1	B	286	LEU
1	B	354	LEU
1	B	426	ASP
1	B	429	ARG

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Mol	Chain	Res	Type
1	B	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	228	GLN
1	A	264	HIS
1	A	330	ASN
1	A	353	GLN
1	A	375	ASN
1	A	418	ASN
1	A	458	ASN
1	B	125	GLN
1	B	163	ASN
1	B	330	ASN
1	B	441	GLN
1	B	457	GLN
1	B	458	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

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	600	-	48,58,58	1.48	6 (12%)	54,89,89	2.35	11 (20%)
3	HTK	A	601	-	18,18,18	0.45	0	19,23,23	0.71	0
2	FAD	B	600	-	48,58,58	1.52	9 (18%)	54,89,89	2.86	12 (22%)
3	HTK	B	601	-	18,18,18	0.43	0	19,23,23	0.84	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	600	-	-	0/30/50/50	0/6/6/6
3	HTK	A	601	-	-	0/16/16/16	0/1/1/1
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	HTK	B	601	-	-	0/16/16/16	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	O4B-C4B	2.14	1.50	1.45
2	B	600	FAD	C4'-C3'	2.35	1.58	1.53
2	B	600	FAD	C7M-C7	2.41	1.55	1.51
2	A	600	FAD	C4X-N5	2.41	1.37	1.33
2	B	600	FAD	C2A-N1A	2.53	1.38	1.33
2	B	600	FAD	C8M-C8	2.74	1.56	1.51
2	B	600	FAD	C4X-C10	2.84	1.46	1.41
2	B	600	FAD	C8A-N7A	2.96	1.40	1.34
2	B	600	FAD	C2A-N3A	3.08	1.37	1.32
2	B	600	FAD	C10-N10	3.42	1.43	1.39
2	A	600	FAD	C5X-N5	3.49	1.40	1.35
2	A	600	FAD	C10-N10	3.60	1.43	1.39
2	B	600	FAD	C4X-N5	3.74	1.39	1.33
2	A	600	FAD	O4B-C1B	3.83	1.46	1.41
2	A	600	FAD	C4X-C10	4.28	1.49	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	C4X-C10-N10	-11.59	113.69	120.52
2	B	600	FAD	N3A-C2A-N1A	-8.42	122.45	128.89
2	B	600	FAD	C4-C4X-C10	-5.65	116.33	119.94
2	A	600	FAD	C4X-C4-N3	-5.24	116.43	123.59
2	A	600	FAD	C4X-C10-N10	-5.20	117.45	120.52
2	A	600	FAD	N3A-C2A-N1A	-4.41	125.52	128.89
2	A	600	FAD	C1B-N9A-C4A	-4.25	120.53	126.94
2	B	600	FAD	C4X-C4-N3	-3.82	118.36	123.59
2	B	600	FAD	C1B-N9A-C4A	-3.54	121.60	126.94
2	B	600	FAD	C9A-C5X-N5	-2.82	118.19	122.36
2	B	600	FAD	O4B-C1B-N9A	-2.71	102.43	108.10
2	A	600	FAD	O4B-C1B-N9A	-2.62	102.61	108.10
2	B	600	FAD	O2A-PA-O3P	2.01	114.22	105.09
2	B	600	FAD	C6-C5X-C9A	2.12	121.78	118.98
2	A	600	FAD	C4B-O4B-C1B	2.95	112.96	109.72
2	A	600	FAD	C2B-C1B-N9A	3.29	119.32	114.29
2	A	600	FAD	C4-C4X-N5	3.47	122.93	118.72
2	B	600	FAD	C4-C4X-N5	3.59	123.08	118.72
2	A	600	FAD	C1'-N10-C9A	4.09	123.45	118.86
2	A	600	FAD	C4X-N5-C5X	4.48	121.92	116.76
2	B	600	FAD	C4X-N5-C5X	5.69	123.30	116.76
2	B	600	FAD	C4-N3-C2	7.72	121.92	115.25
2	A	600	FAD	C4-N3-C2	9.73	123.66	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	8	0
3	A	601	HTK	3	0
2	B	600	FAD	7	0
3	B	601	HTK	5	0

5.7 Other polymers (i)

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

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, 95^{th} 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	460/468 (98%)	-0.44	2 (0%)	93	91	7, 14, 28, 43	0
1	B	461/468 (98%)	-0.38	3 (0%)	89	87	7, 16, 32, 49	0
All	All	921/936 (98%)	-0.41	5 (0%)	91	90	7, 15, 30, 49	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	ALA	2.7
1	B	4	PRO	2.6
1	A	3	PHE	2.4
1	B	3	PHE	2.2
1	B	462	SER	2.2

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

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
3	HTK	A	601	18/18	0.70	0.27	7.27	21,33,43,43	18
3	HTK	B	601	18/18	0.67	0.26	7.25	19,32,43,46	18
2	FAD	A	600	53/53	0.98	0.09	0.09	7,8,11,12	0
2	FAD	B	600	53/53	0.98	0.08	-0.18	8,10,12,14	0

6.5 Other polymers (i)

There are no such residues in this entry.