



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:30 PM GMT

PDB ID : 4TM0
Title : Kutzneria sp. 744 ornithine N-hydroxylase, KtzI-FADred-ox-NADP+-L-orn
Authors : Setser, J.W.; Drennan, C.L.
Deposited on : 2014-05-30
Resolution : 2.74 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

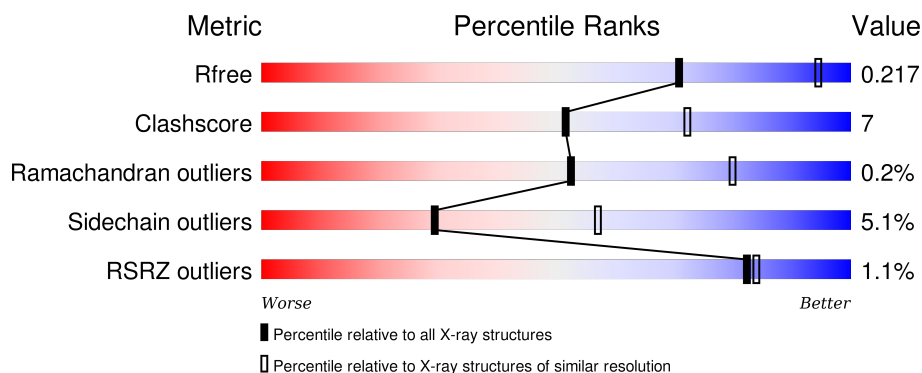
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 $\leq 5\%$. 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	443	
1	B	443	
1	C	443	
1	D	443	

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
4	ORN	A	503	-	-	-	X
4	ORN	C	503	-	-	-	X
4	ORN	D	503	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13461 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 KtzI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3202	2013	573	606	10			
1	B	414	Total	C	N	O	S	0	0	0
			3214	2020	579	605	10			
1	C	414	Total	C	N	O	S	0	0	0
			3164	1994	563	597	10			
1	D	415	Total	C	N	O	S	0	0	0
			3194	2009	565	610	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A8CF85
A	-17	GLY	-	expression tag	UNP A8CF85
A	-16	SER	-	expression tag	UNP A8CF85
A	-15	SER	-	expression tag	UNP A8CF85
A	-14	HIS	-	expression tag	UNP A8CF85
A	-13	HIS	-	expression tag	UNP A8CF85
A	-12	HIS	-	expression tag	UNP A8CF85
A	-11	HIS	-	expression tag	UNP A8CF85
A	-10	HIS	-	expression tag	UNP A8CF85
A	-9	HIS	-	expression tag	UNP A8CF85
A	-8	SER	-	expression tag	UNP A8CF85
A	-7	SER	-	expression tag	UNP A8CF85
A	-6	GLY	-	expression tag	UNP A8CF85
A	-5	LEU	-	expression tag	UNP A8CF85
A	-4	VAL	-	expression tag	UNP A8CF85
A	-3	PRO	-	expression tag	UNP A8CF85
A	-2	ARG	-	expression tag	UNP A8CF85
A	-1	GLY	-	expression tag	UNP A8CF85
A	0	SER	-	expression tag	UNP A8CF85
A	1	HIS	-	expression tag	UNP A8CF85
A	2	MET	-	expression tag	UNP A8CF85

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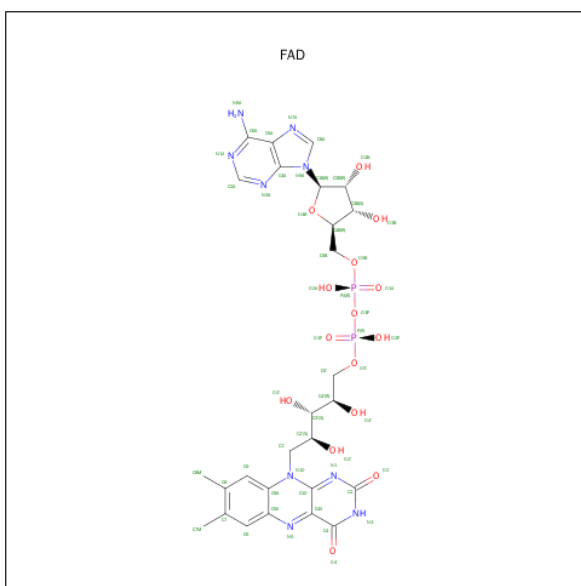
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP A8CF85
B	-17	GLY	-	expression tag	UNP A8CF85
B	-16	SER	-	expression tag	UNP A8CF85
B	-15	SER	-	expression tag	UNP A8CF85
B	-14	HIS	-	expression tag	UNP A8CF85
B	-13	HIS	-	expression tag	UNP A8CF85
B	-12	HIS	-	expression tag	UNP A8CF85
B	-11	HIS	-	expression tag	UNP A8CF85
B	-10	HIS	-	expression tag	UNP A8CF85
B	-9	HIS	-	expression tag	UNP A8CF85
B	-8	SER	-	expression tag	UNP A8CF85
B	-7	SER	-	expression tag	UNP A8CF85
B	-6	GLY	-	expression tag	UNP A8CF85
B	-5	LEU	-	expression tag	UNP A8CF85
B	-4	VAL	-	expression tag	UNP A8CF85
B	-3	PRO	-	expression tag	UNP A8CF85
B	-2	ARG	-	expression tag	UNP A8CF85
B	-1	GLY	-	expression tag	UNP A8CF85
B	0	SER	-	expression tag	UNP A8CF85
B	1	HIS	-	expression tag	UNP A8CF85
B	2	MET	-	expression tag	UNP A8CF85
C	-18	MET	-	initiating methionine	UNP A8CF85
C	-17	GLY	-	expression tag	UNP A8CF85
C	-16	SER	-	expression tag	UNP A8CF85
C	-15	SER	-	expression tag	UNP A8CF85
C	-14	HIS	-	expression tag	UNP A8CF85
C	-13	HIS	-	expression tag	UNP A8CF85
C	-12	HIS	-	expression tag	UNP A8CF85
C	-11	HIS	-	expression tag	UNP A8CF85
C	-10	HIS	-	expression tag	UNP A8CF85
C	-9	HIS	-	expression tag	UNP A8CF85
C	-8	SER	-	expression tag	UNP A8CF85
C	-7	SER	-	expression tag	UNP A8CF85
C	-6	GLY	-	expression tag	UNP A8CF85
C	-5	LEU	-	expression tag	UNP A8CF85
C	-4	VAL	-	expression tag	UNP A8CF85
C	-3	PRO	-	expression tag	UNP A8CF85
C	-2	ARG	-	expression tag	UNP A8CF85
C	-1	GLY	-	expression tag	UNP A8CF85
C	0	SER	-	expression tag	UNP A8CF85
C	1	HIS	-	expression tag	UNP A8CF85
C	2	MET	-	expression tag	UNP A8CF85

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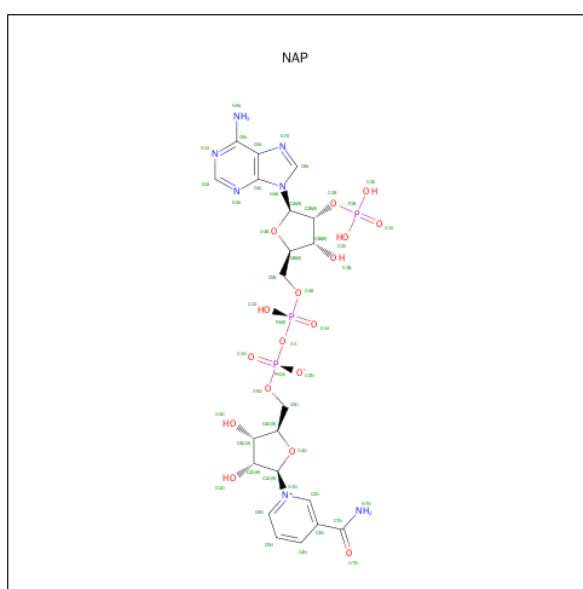
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP A8CF85
D	-17	GLY	-	expression tag	UNP A8CF85
D	-16	SER	-	expression tag	UNP A8CF85
D	-15	SER	-	expression tag	UNP A8CF85
D	-14	HIS	-	expression tag	UNP A8CF85
D	-13	HIS	-	expression tag	UNP A8CF85
D	-12	HIS	-	expression tag	UNP A8CF85
D	-11	HIS	-	expression tag	UNP A8CF85
D	-10	HIS	-	expression tag	UNP A8CF85
D	-9	HIS	-	expression tag	UNP A8CF85
D	-8	SER	-	expression tag	UNP A8CF85
D	-7	SER	-	expression tag	UNP A8CF85
D	-6	GLY	-	expression tag	UNP A8CF85
D	-5	LEU	-	expression tag	UNP A8CF85
D	-4	VAL	-	expression tag	UNP A8CF85
D	-3	PRO	-	expression tag	UNP A8CF85
D	-2	ARG	-	expression tag	UNP A8CF85
D	-1	GLY	-	expression tag	UNP A8CF85
D	0	SER	-	expression tag	UNP A8CF85
D	1	HIS	-	expression tag	UNP A8CF85
D	2	MET	-	expression tag	UNP A8CF85

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



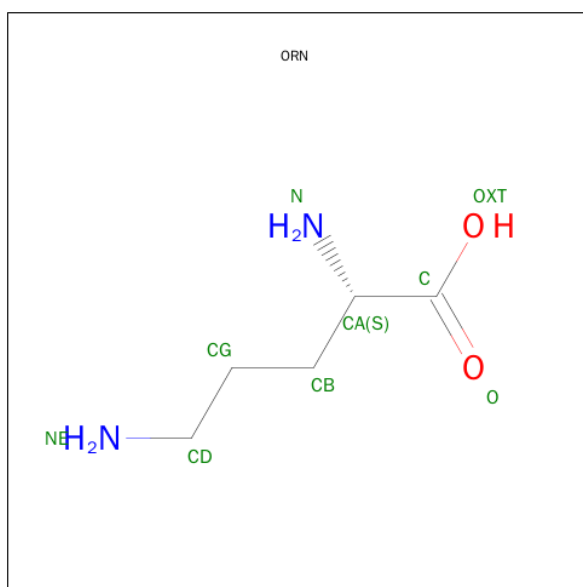
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	2	2		
4	B	1	Total	C	N	O	0	0
			9	5	2	2		
4	C	1	Total	C	N	O	0	0
			9	5	2	2		
4	D	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	K	0	0
			2	2		
5	A	2	Total	K	0	0
			2	2		
5	D	2	Total	K	0	0
			2	2		
5	C	2	Total	K	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total	O	0	0
			78	78		

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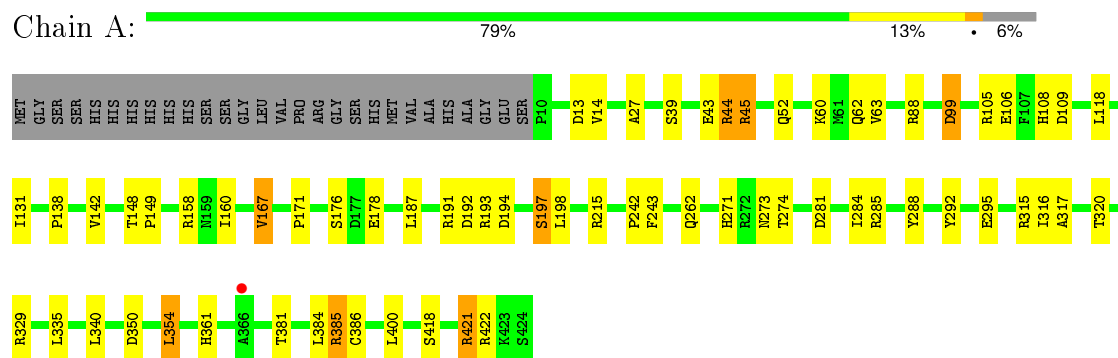
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	70	Total	O	0	0
			70	70		
6	C	47	Total	O	0	0
			47	47		
6	D	44	Total	O	0	0
			44	44		

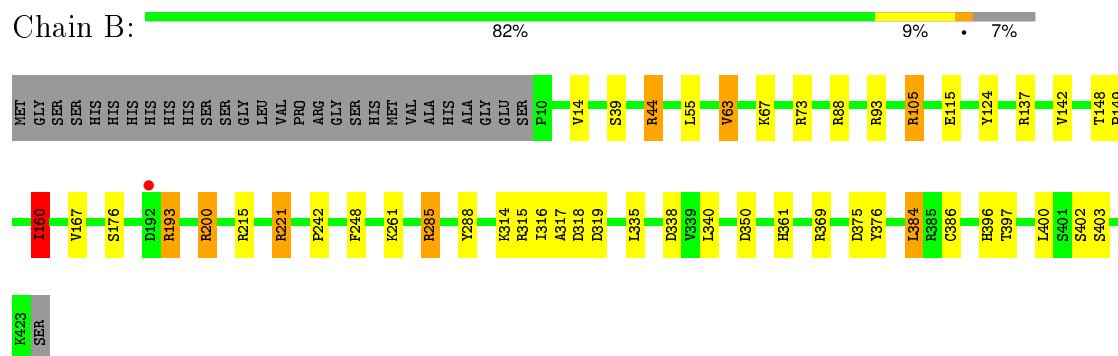
3 Residue-property plots [i](#)

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.

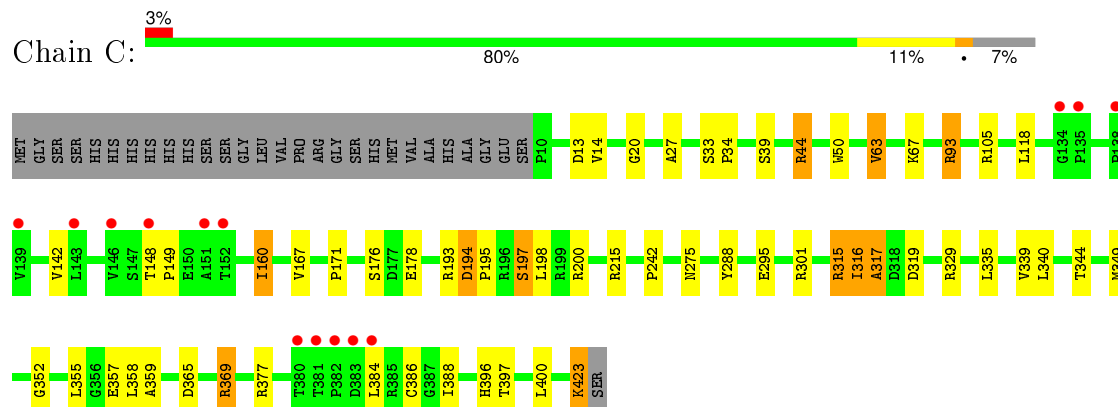
• Molecule 1: KtzI



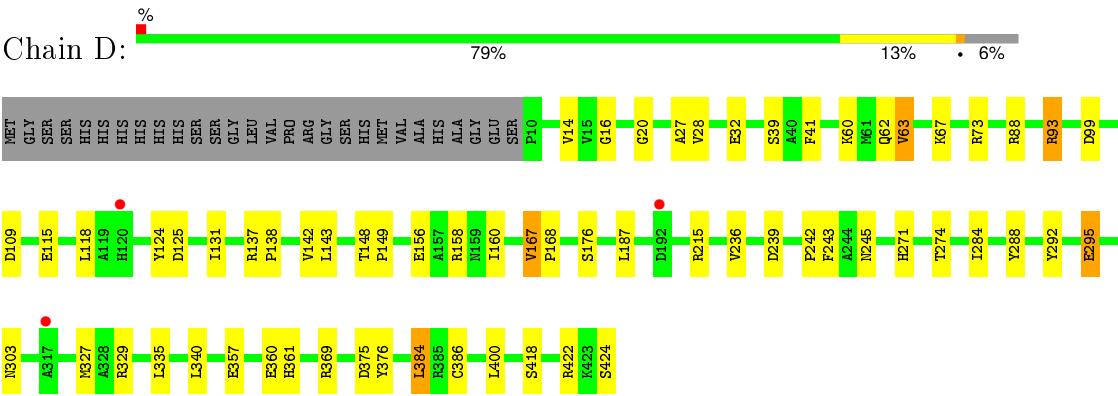
• Molecule 1: KtzI



• Molecule 1: KtzI



● Molecule 1: KtzI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.03Å 156.40Å 164.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.16 – 2.74 49.70 – 2.73	Depositor EDS
% Data completeness (in resolution range)	91.3 (47.16-2.74) 91.3 (49.70-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.186 , 0.216 0.191 , 0.217	Depositor DCC
R_{free} test set	2738 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.1	EDS
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 54056 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13461	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, 0.375 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: ORN, K, 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	0.72	0/3282	0.65	3/4474 (0.1%)
1	B	0.73	0/3294	0.68	4/4486 (0.1%)
1	C	0.70	1/3243 (0.0%)	0.65	0/4425
1	D	0.65	0/3274	0.63	1/4465 (0.0%)
All	All	0.70	1/13093 (0.0%)	0.66	8/17850 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	194	ASP	CB-CG	-5.72	1.39	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	ASP	C-N-CD	5.83	140.65	128.40
1	A	350	ASP	C-N-CD	5.77	140.51	128.40
1	A	381	THR	C-N-CD	5.73	140.43	128.40
1	D	329	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	319	ASP	N-CA-C	-5.67	95.69	111.00
1	B	200	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	160	ILE	CB-CA-C	-5.30	101.00	111.60
1	A	99	ASP	CB-CG-OD1	5.05	122.85	118.30

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	3202	0	3025	53	0
1	B	3214	0	3058	40	0
1	C	3164	0	2977	43	0
1	D	3194	0	3007	43	0
2	A	53	0	30	7	0
2	B	53	0	30	3	0
2	C	53	0	30	7	0
2	D	53	0	30	3	0
3	A	48	0	24	7	0
3	B	48	0	25	0	0
3	C	48	0	25	2	0
3	D	48	0	25	3	0
4	A	9	0	11	1	0
4	B	9	0	11	2	0
4	C	9	0	11	1	0
4	D	9	0	11	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	78	0	0	3	0
6	B	70	0	0	2	0
6	C	47	0	0	1	0
6	D	44	0	0	0	0
All	All	13461	0	12330	173	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 7.

All (173) 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:262:GLN:NE2	1:D:327:MET:HG2	1.52	1.21
1:C:194:ASP:OD2	1:C:195:PRO:HD2	1.42	1.16
1:A:262:GLN:HE22	1:D:327:MET:HG2	1.19	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLN:NE2	1:D:327:MET:CG	2.31	0.94
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.36	0.91
2:A:501:FAD:O4	3:A:502:NAP:H51N	1.74	0.88
1:B:317:ALA:O	1:B:318:ASP:HB2	1.71	0.88
3:D:502:NAP:H51N	3:D:502:NAP:H6N	1.53	0.87
1:C:194:ASP:O	1:C:197:SER:HB3	1.77	0.84
1:C:194:ASP:OD2	1:C:195:PRO:CD	2.24	0.84
1:A:43:GLU:OE2	1:A:45:ARG:HG2	1.84	0.77
1:A:138:PRO:HG2	1:A:385:ARG:NH2	2.02	0.74
1:A:138:PRO:HB2	1:A:385:ARG:NH2	2.02	0.74
1:B:315:ARG:NH2	1:B:318:ASP:HA	2.05	0.72
1:B:55:LEU:O	1:B:105:ARG:NH1	2.23	0.71
1:B:73:ARG:NH2	6:B:612:HOH:O	2.23	0.71
1:A:262:GLN:HE21	1:D:327:MET:CG	2.03	0.69
1:C:63:VAL:HG22	1:C:67:LYS:HD2	1.74	0.69
2:A:501:FAD:C4	3:A:502:NAP:H51N	2.23	0.69
1:C:384:LEU:CD2	1:C:386:CYS:SG	2.81	0.68
1:B:193:ARG:HG2	1:B:193:ARG:NH1	2.08	0.68
1:A:44:ARG:HG2	2:A:501:FAD:C4A	2.25	0.67
1:D:143:LEU:HD23	1:D:156:GLU:HG3	1.75	0.67
1:C:50:TRP:HE1	2:C:501:FAD:H4'	1.59	0.66
1:B:384:LEU:CD2	1:B:386:CYS:SG	2.84	0.66
1:C:194:ASP:CG	1:C:195:PRO:HD2	2.17	0.65
1:A:191:ARG:NH2	6:A:628:HOH:O	2.24	0.64
1:B:142:VAL:HG21	1:B:160:ILE:HG12	1.78	0.64
1:A:60:LYS:NZ	1:A:99:ASP:OD2	2.29	0.64
1:A:138:PRO:CG	1:A:385:ARG:NH2	2.59	0.64
1:B:384:LEU:HD21	1:B:386:CYS:SG	2.38	0.64
1:B:44:ARG:HG2	2:B:501:FAD:C4A	2.27	0.64
1:C:365:ASP:OD2	1:C:369:ARG:HD2	1.99	0.62
1:C:148:THR:HB	1:C:149:PRO:CD	2.30	0.62
1:C:384:LEU:HD21	1:C:386:CYS:SG	2.40	0.62
1:A:138:PRO:HB2	1:A:385:ARG:HH21	1.63	0.61
1:C:200:ARG:NH2	1:C:319:ASP:OD1	2.27	0.60
1:A:148:THR:HB	1:A:149:PRO:CD	2.32	0.60
1:A:138:PRO:CB	1:A:385:ARG:NH2	2.65	0.60
1:C:44:ARG:HG2	2:C:501:FAD:N3A	2.18	0.59
1:C:198:LEU:HD22	1:C:339:VAL:CG2	2.34	0.57
1:B:248:PHE:CD2	4:B:503:ORN:HA	2.40	0.57
1:C:44:ARG:HG2	2:C:501:FAD:C4A	2.35	0.57
1:A:178:GLU:O	1:A:193:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ASN:OD1	4:C:503:ORN:NE	2.39	0.56
2:A:501:FAD:C4	3:A:502:NAP:H4D	2.35	0.56
1:A:315:ARG:NH1	1:A:320:THR:OG1	2.39	0.55
1:C:355:LEU:O	1:C:358:LEU:HD12	2.06	0.55
1:B:400:LEU:N	1:B:400:LEU:HD12	2.22	0.55
1:C:301:ARG:NH1	6:C:645:HOH:O	2.27	0.54
1:D:131:ILE:HD13	1:D:160:ILE:HD13	1.89	0.54
1:D:20:GLY:HA3	2:D:501:FAD:H52A	1.89	0.54
1:C:316:ILE:O	1:C:317:ALA:HB3	2.07	0.54
2:D:501:FAD:C4	3:D:502:NAP:H4D	2.38	0.54
1:A:138:PRO:CB	1:A:385:ARG:HH21	2.18	0.54
1:B:221:ARG:CG	1:B:221:ARG:HH11	2.20	0.54
1:D:271:HIS:O	1:D:274:THR:OG1	2.24	0.54
1:B:288:TYR:OH	1:D:93:ARG:HG3	2.09	0.53
1:A:131:ILE:HD13	1:A:160:ILE:HD13	1.91	0.53
1:C:400:LEU:HD12	1:C:400:LEU:N	2.24	0.53
1:A:418:SER:O	1:A:422:ARG:HG3	2.09	0.53
1:C:20:GLY:HA3	2:C:501:FAD:H52A	1.91	0.52
1:D:124:TYR:O	1:D:125:ASP:HB2	2.08	0.52
1:A:421:ARG:NH2	6:A:637:HOH:O	2.42	0.52
1:B:248:PHE:CE2	4:B:503:ORN:HA	2.44	0.52
1:A:292:TYR:HD2	1:C:93:ARG:HG2	1.74	0.52
1:D:28:VAL:O	1:D:32:GLU:HG3	2.09	0.52
1:C:195:PRO:C	1:C:197:SER:H	2.11	0.52
1:B:242:PRO:HB2	1:C:288:TYR:CD1	2.44	0.52
1:B:193:ARG:CG	1:B:193:ARG:NH1	2.73	0.51
1:A:271:HIS:O	1:A:274:THR:OG1	2.21	0.51
1:A:13:ASP:OD1	1:A:158:ARG:NH2	2.43	0.51
2:C:501:FAD:C4	3:C:502:NAP:H4D	2.40	0.51
1:A:62:GLN:O	4:A:503:ORN:HB3	2.10	0.51
1:B:314:LYS:HD2	1:B:316:ILE:HD11	1.92	0.51
1:B:142:VAL:HG13	1:B:386:CYS:SG	2.51	0.51
1:C:148:THR:HB	1:C:149:PRO:HD2	1.92	0.51
2:A:501:FAD:C4X	3:A:502:NAP:H4D	2.41	0.50
1:C:198:LEU:HD22	1:C:339:VAL:HG23	1.92	0.50
1:C:14:VAL:O	1:C:39:SER:HA	2.11	0.50
1:A:284:ILE:HG23	1:D:243:PHE:HD2	1.76	0.50
1:D:400:LEU:N	1:D:400:LEU:HD12	2.27	0.50
1:B:221:ARG:HG3	1:B:221:ARG:HH11	1.77	0.50
1:D:60:LYS:NZ	1:D:99:ASP:OD2	2.45	0.50
1:D:67:LYS:NZ	4:D:503:ORN:O	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HD2	2:B:501:FAD:O2B	2.12	0.49
1:D:14:VAL:O	1:D:39:SER:HA	2.12	0.49
1:A:243:PHE:HD2	1:D:284:ILE:HG23	1.77	0.49
1:A:138:PRO:HB2	1:A:385:ARG:HG3	1.95	0.49
1:A:148:THR:HB	1:A:149:PRO:HD2	1.93	0.49
1:C:142:VAL:HG21	1:C:160:ILE:HG12	1.95	0.48
1:A:171:PRO:HB3	3:A:502:NAP:N6A	2.29	0.48
2:C:501:FAD:HM72	3:C:502:NAP:C5N	2.44	0.48
1:D:245:ASN:OD1	4:D:503:ORN:N	2.42	0.48
1:A:400:LEU:HD12	1:A:400:LEU:N	2.29	0.48
1:B:288:TYR:CD1	1:C:242:PRO:HB2	2.49	0.48
1:B:315:ARG:C	1:B:316:ILE:HG13	2.34	0.47
1:C:178:GLU:O	1:C:193:ARG:NH1	2.47	0.47
1:A:106:GLU:O	1:A:109:ASP:HB3	2.15	0.47
1:A:361:HIS:HB2	1:A:384:LEU:HD12	1.96	0.46
1:D:239:ASP:O	1:D:274:THR:HG22	2.15	0.46
1:A:14:VAL:O	1:A:39:SER:HA	2.14	0.46
1:B:44:ARG:HG2	2:B:501:FAD:N3A	2.31	0.46
1:C:365:ASP:OD2	1:C:369:ARG:CD	2.64	0.46
1:B:221:ARG:CG	1:B:221:ARG:NH1	2.77	0.46
1:B:93:ARG:NH1	1:D:295:GLU:OE2	2.48	0.46
1:C:27:ALA:HB1	1:C:118:LEU:HD21	1.98	0.46
1:B:361:HIS:HB2	1:B:384:LEU:HD12	1.97	0.45
1:C:198:LEU:HD22	1:C:339:VAL:HG21	1.98	0.45
1:B:93:ARG:HG2	1:D:292:TYR:HD2	1.80	0.45
1:A:242:PRO:HB2	1:D:288:TYR:CD1	2.52	0.45
1:B:148:THR:HB	1:B:149:PRO:HD2	1.98	0.45
1:A:167:VAL:HG22	6:A:619:HOH:O	2.17	0.45
1:A:138:PRO:CG	1:A:385:ARG:HH21	2.31	0.44
1:B:63:VAL:HG22	1:B:67:LYS:HD2	1.99	0.44
1:D:143:LEU:CD2	1:D:156:GLU:HG3	2.44	0.44
1:B:315:ARG:HH21	1:B:318:ASP:HA	1.79	0.44
1:C:357:GLU:C	1:C:359:ALA:N	2.69	0.44
1:A:138:PRO:CG	1:A:385:ARG:HH22	2.28	0.44
1:D:62:GLN:HG2	3:D:502:NAP:N7N	2.33	0.44
1:B:14:VAL:O	1:B:39:SER:HA	2.18	0.44
1:C:20:GLY:CA	2:C:501:FAD:H52A	2.47	0.44
1:D:142:VAL:HG13	1:D:386:CYS:SG	2.58	0.44
1:C:13:ASP:OD1	1:C:423:LYS:HE3	2.18	0.44
1:C:316:ILE:O	1:C:316:ILE:HG22	2.18	0.43
1:D:32:GLU:OE1	1:D:73:ARG:NH2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:THR:HB	1:D:149:PRO:CD	2.48	0.43
1:D:167:VAL:HA	1:D:168:PRO:HD3	1.89	0.43
1:A:385:ARG:HG3	1:A:385:ARG:NH2	2.32	0.43
1:A:316:ILE:O	1:A:317:ALA:HB3	2.19	0.43
1:D:137:ARG:HA	1:D:138:PRO:C	2.38	0.43
1:A:142:VAL:HG13	1:A:386:CYS:SG	2.58	0.43
1:D:375:ASP:O	1:D:376:TYR:HB2	2.19	0.43
1:D:418:SER:O	1:D:422:ARG:HG3	2.17	0.43
1:D:361:HIS:HB2	1:D:384:LEU:HD12	2.00	0.43
1:D:27:ALA:HB1	1:D:118:LEU:HD21	2.01	0.43
1:B:314:LYS:HG2	6:B:644:HOH:O	2.18	0.43
1:A:197:SER:O	1:A:198:LEU:HD23	2.18	0.43
1:A:45:ARG:HG2	1:A:45:ARG:H	1.61	0.43
1:D:357:GLU:O	1:D:360:GLU:HG2	2.19	0.43
1:C:195:PRO:C	1:C:197:SER:N	2.73	0.42
2:A:501:FAD:C4X	3:A:502:NAP:C4D	2.96	0.42
1:C:396:HIS:CD2	1:C:397:THR:HG23	2.54	0.42
1:C:33:SER:HA	1:C:34:PRO:HD3	1.92	0.42
1:B:285:ARG:CG	1:B:285:ARG:HH11	2.32	0.42
1:B:200:ARG:NH1	1:B:338:ASP:OD1	2.53	0.42
1:A:273:ASN:HD21	1:D:236:VAL:HG13	1.84	0.42
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.80	0.42
1:D:20:GLY:CA	2:D:501:FAD:H52A	2.49	0.42
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.86	0.42
1:D:115:GLU:OE2	1:D:124:TYR:OH	2.32	0.42
1:B:137:ARG:HD3	1:B:137:ARG:HH11	1.71	0.42
1:A:138:PRO:HG2	1:A:385:ARG:HH21	1.77	0.41
1:B:400:LEU:H	1:B:400:LEU:HD12	1.84	0.41
1:C:400:LEU:HD12	1:C:400:LEU:H	1.85	0.41
1:A:194:ASP:O	1:A:197:SER:HB3	2.19	0.41
1:A:288:TYR:CD1	1:D:242:PRO:HB2	2.56	0.41
1:C:315:ARG:O	1:C:316:ILE:HG13	2.20	0.41
2:A:501:FAD:C4	3:A:502:NAP:C5D	2.97	0.41
1:A:292:TYR:CD2	1:C:93:ARG:HG2	2.54	0.41
1:D:158:ARG:O	1:D:386:CYS:HB2	2.21	0.41
1:A:52:GLN:HE21	1:A:108:HIS:CE1	2.39	0.41
1:C:171:PRO:HG3	1:C:344:THR:HG21	2.03	0.41
1:B:375:ASP:O	1:B:376:TYR:HB2	2.21	0.41
1:D:148:THR:HB	1:D:149:PRO:HD2	2.03	0.41
1:A:281:ASP:O	1:A:285:ARG:HG3	2.20	0.41
1:B:396:HIS:CD2	1:B:397:THR:HG23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:HB1	1:A:118:LEU:HD21	2.03	0.40
1:A:385:ARG:HG3	1:A:385:ARG:HH21	1.87	0.40
1:A:187:LEU:HD13	1:A:191:ARG:NH2	2.36	0.40
1:B:115:GLU:OE2	1:B:124:TYR:OH	2.29	0.40
1:D:16:GLY:HA3	1:D:41:PHE:CD1	2.57	0.40
1:D:63:VAL:HG23	4:D:503:ORN:HB2	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	413/443 (93%)	397 (96%)	16 (4%)	0	100	100
1	B	412/443 (93%)	397 (96%)	15 (4%)	0	100	100
1	C	412/443 (93%)	392 (95%)	17 (4%)	3 (1%)	26	54
1	D	413/443 (93%)	402 (97%)	11 (3%)	0	100	100
All	All	1650/1772 (93%)	1588 (96%)	59 (4%)	3 (0%)	52	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	317	ALA
1	C	316	ILE
1	C	352	GLY

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	334/372 (90%)	317 (95%)	17 (5%)	29	57
1	B	337/372 (91%)	319 (95%)	18 (5%)	28	55
1	C	326/372 (88%)	307 (94%)	19 (6%)	25	50
1	D	334/372 (90%)	320 (96%)	14 (4%)	36	66
All	All	1331/1488 (89%)	1263 (95%)	68 (5%)	29	57

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	45	ARG
1	A	63	VAL
1	A	88	ARG
1	A	105	ARG
1	A	167	VAL
1	A	176	SER
1	A	192	ASP
1	A	197	SER
1	A	215	ARG
1	A	295	GLU
1	A	329	ARG
1	A	335	LEU
1	A	340	LEU
1	A	354	LEU
1	A	385	ARG
1	A	421	ARG
1	B	44	ARG
1	B	63	VAL
1	B	88	ARG
1	B	105	ARG
1	B	160	ILE
1	B	167	VAL
1	B	176	SER
1	B	193	ARG
1	B	215	ARG
1	B	221	ARG
1	B	261	LYS
1	B	285	ARG
1	B	335	LEU

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Mol	Chain	Res	Type
1	B	340	LEU
1	B	369	ARG
1	B	384	LEU
1	B	402	SER
1	B	403	SER
1	C	44	ARG
1	C	63	VAL
1	C	93	ARG
1	C	105	ARG
1	C	160	ILE
1	C	167	VAL
1	C	176	SER
1	C	197	SER
1	C	215	ARG
1	C	295	GLU
1	C	315	ARG
1	C	329	ARG
1	C	335	LEU
1	C	340	LEU
1	C	349	MET
1	C	369	ARG
1	C	377	ARG
1	C	388	ILE
1	C	423	LYS
1	D	63	VAL
1	D	88	ARG
1	D	93	ARG
1	D	109	ASP
1	D	167	VAL
1	D	176	SER
1	D	215	ARG
1	D	295	GLU
1	D	303	ASN
1	D	335	LEU
1	D	340	LEU
1	D	369	ARG
1	D	384	LEU
1	D	424	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	189	HIS
1	A	262	GLN
1	B	189	HIS
1	C	189	HIS
1	D	120	HIS
1	D	189	HIS
1	D	275	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 ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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	501	-	48,58,58	2.49	14 (29%)	54,89,89	3.53	22 (40%)
3	NAP	A	502	-	42,52,52	1.56	6 (14%)	54,80,80	2.35	12 (22%)
4	ORN	A	503	-	5,8,8	0.49	0	3,9,9	0.70	0
2	FAD	B	501	-	48,58,58	2.42	16 (33%)	54,89,89	2.81	16 (29%)
3	NAP	B	502	-	42,52,52	1.51	6 (14%)	54,80,80	2.02	10 (18%)
4	ORN	B	503	-	5,8,8	0.54	0	3,9,9	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	C	501	-	48,58,58	2.66	13 (27%)	54,89,89	3.57	20 (37%)
3	NAP	C	502	-	42,52,52	1.54	6 (14%)	54,80,80	1.74	6 (11%)
4	ORN	C	503	-	5,8,8	0.68	0	3,9,9	0.22	0
2	FAD	D	501	-	48,58,58	2.27	14 (29%)	54,89,89	2.95	20 (37%)
3	NAP	D	502	-	42,52,52	1.59	6 (14%)	54,80,80	1.95	12 (22%)
4	ORN	D	503	-	5,8,8	0.69	0	3,9,9	0.58	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	501	-	-	0/30/50/50	0/6/6/6
3	NAP	A	502	-	-	0/27/67/67	0/5/5/5
4	ORN	A	503	-	-	0/4/8/8	0/0/0/0
2	FAD	B	501	-	-	0/30/50/50	0/6/6/6
3	NAP	B	502	-	-	0/27/67/67	0/5/5/5
4	ORN	B	503	-	-	0/4/8/8	0/0/0/0
2	FAD	C	501	-	-	0/30/50/50	0/6/6/6
3	NAP	C	502	-	-	0/27/67/67	0/5/5/5
4	ORN	C	503	-	-	0/4/8/8	0/0/0/0
2	FAD	D	501	-	-	0/30/50/50	0/6/6/6
3	NAP	D	502	-	-	0/27/67/67	0/5/5/5
4	ORN	D	503	-	-	0/4/8/8	0/0/0/0

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C2'-C3'	-9.85	1.33	1.53
2	B	501	FAD	O3'-C3'	-7.48	1.25	1.43
2	A	501	FAD	O3'-C3'	-7.38	1.25	1.43
2	C	501	FAD	C4'-C3'	-5.94	1.41	1.53
3	B	502	NAP	C2D-C3D	-4.23	1.41	1.53
3	C	502	NAP	C2D-C3D	-4.17	1.42	1.53
3	D	502	NAP	C2D-C3D	-4.06	1.42	1.53
3	D	502	NAP	C3B-C2B	-3.75	1.44	1.53
3	B	502	NAP	C3B-C2B	-3.63	1.44	1.53
3	A	502	NAP	C3B-C2B	-3.54	1.45	1.53
2	D	501	FAD	O3'-C3'	-3.30	1.35	1.43
3	C	502	NAP	C3B-C2B	-3.20	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C2'-C3'	-3.19	1.47	1.53
2	B	501	FAD	C1'-N10	-3.17	1.45	1.48
3	A	502	NAP	C2D-C3D	-3.04	1.45	1.53
3	A	502	NAP	PA-O5B	-2.87	1.45	1.59
2	B	501	FAD	O2'-C2'	-2.87	1.36	1.43
3	D	502	NAP	O4D-C4D	-2.65	1.38	1.45
3	A	502	NAP	O4D-C1D	-2.36	1.38	1.41
2	B	501	FAD	C8M-C8	-2.29	1.46	1.51
2	D	501	FAD	O2'-C2'	-2.28	1.38	1.43
2	D	501	FAD	O4'-C4'	-2.22	1.38	1.43
3	C	502	NAP	O4D-C4D	-2.21	1.39	1.45
2	D	501	FAD	C1'-N10	-2.18	1.46	1.48
2	B	501	FAD	O4B-C4B	-2.12	1.40	1.45
3	B	502	NAP	O4D-C4D	-2.12	1.40	1.45
2	C	501	FAD	PA-O1A	2.10	1.58	1.51
3	B	502	NAP	C2A-N3A	2.13	1.36	1.32
2	B	501	FAD	C2A-N3A	2.17	1.36	1.32
3	D	502	NAP	C2A-N3A	2.19	1.36	1.32
3	C	502	NAP	C2A-N3A	2.24	1.36	1.32
2	B	501	FAD	PA-O5B	2.27	1.69	1.59
2	C	501	FAD	PA-O5B	2.27	1.69	1.59
2	B	501	FAD	PA-O1A	2.35	1.59	1.51
2	B	501	FAD	PA-O2A	2.37	1.65	1.54
2	A	501	FAD	C10-N10	2.39	1.41	1.39
2	A	501	FAD	PA-O5B	2.46	1.70	1.59
2	B	501	FAD	C9A-N10	2.49	1.42	1.38
2	D	501	FAD	C4'-C3'	2.56	1.58	1.53
2	C	501	FAD	PA-O2A	2.56	1.65	1.54
2	A	501	FAD	PA-O2A	2.57	1.65	1.54
2	D	501	FAD	PA-O5B	2.61	1.71	1.59
2	A	501	FAD	C2A-N3A	2.65	1.36	1.32
2	A	501	FAD	C2'-C3'	2.69	1.59	1.53
2	D	501	FAD	PA-O2A	2.73	1.66	1.54
2	C	501	FAD	C6A-N6A	2.74	1.43	1.34
2	D	501	FAD	C6A-N6A	2.86	1.43	1.34
2	C	501	FAD	C9A-N10	2.94	1.42	1.38
2	B	501	FAD	C6A-N6A	2.99	1.44	1.34
2	B	501	FAD	C4-C4X	3.00	1.47	1.41
2	A	501	FAD	C6A-N6A	3.03	1.44	1.34
2	C	501	FAD	O3'-C3'	3.08	1.50	1.43
2	C	501	FAD	C4-C4X	3.25	1.47	1.41
2	D	501	FAD	C4-C4X	3.37	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C5'-C4'	3.42	1.56	1.51
2	D	501	FAD	C9A-N10	3.48	1.43	1.38
2	A	501	FAD	C4-C4X	3.56	1.48	1.41
2	A	501	FAD	C9A-N10	3.75	1.44	1.38
2	A	501	FAD	C4'-C3'	3.85	1.61	1.53
2	A	501	FAD	C4-N3	3.86	1.40	1.33
3	A	502	NAP	C6A-N6A	3.92	1.47	1.34
3	B	502	NAP	C6A-N6A	3.92	1.47	1.34
3	D	502	NAP	C6A-N6A	3.94	1.47	1.34
2	B	501	FAD	C4'-C3'	3.96	1.61	1.53
2	A	501	FAD	C5'-C4'	3.98	1.57	1.51
3	C	502	NAP	C7N-N7N	4.02	1.41	1.33
2	B	501	FAD	C4-N3	4.09	1.40	1.33
3	C	502	NAP	C6A-N6A	4.16	1.47	1.34
2	C	501	FAD	C4X-C10	4.21	1.48	1.41
2	C	501	FAD	C4-N3	4.28	1.41	1.33
2	D	501	FAD	C4-N3	4.31	1.41	1.33
2	B	501	FAD	C4X-C10	4.35	1.49	1.41
3	A	502	NAP	C7N-N7N	4.61	1.42	1.33
3	B	502	NAP	C7N-N7N	4.62	1.42	1.33
2	D	501	FAD	C4X-C10	4.79	1.50	1.41
3	D	502	NAP	C7N-N7N	5.30	1.43	1.33
2	A	501	FAD	C4X-C10	5.48	1.51	1.41
2	A	501	FAD	C5X-N5	7.59	1.47	1.35
2	C	501	FAD	C5X-N5	7.82	1.47	1.35
2	B	501	FAD	C5X-N5	8.10	1.48	1.35
2	D	501	FAD	C5X-N5	8.65	1.49	1.35

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C2A-N1A	-14.70	117.64	128.89
2	C	501	FAD	N3A-C2A-N1A	-12.10	119.63	128.89
2	D	501	FAD	N3A-C2A-N1A	-11.47	120.11	128.89
3	A	502	NAP	N3A-C2A-N1A	-10.59	120.78	128.89
2	B	501	FAD	N3A-C2A-N1A	-10.26	121.04	128.89
2	C	501	FAD	C4B-O4B-C1B	-9.78	98.98	109.72
3	B	502	NAP	N3A-C2A-N1A	-9.53	121.59	128.89
3	C	502	NAP	N3A-C2A-N1A	-9.48	121.64	128.89
3	D	502	NAP	N3A-C2A-N1A	-9.24	121.82	128.89
2	C	501	FAD	O2'-C2'-C3'	-8.69	87.16	109.02
2	C	501	FAD	O5B-PA-O1A	-8.64	76.08	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O5B-PA-O1A	-7.60	80.11	109.62
2	D	501	FAD	C4B-O4B-C1B	-7.26	101.74	109.72
2	B	501	FAD	O5B-PA-O1A	-7.24	81.50	109.62
2	B	501	FAD	O2A-PA-O1A	-6.86	75.35	112.53
2	A	501	FAD	O3P-P-O5'	-6.42	85.91	102.94
3	A	502	NAP	O3-PA-O5B	-6.13	86.67	102.94
2	A	501	FAD	O2A-PA-O1A	-5.92	80.45	112.53
2	C	501	FAD	C4X-C10-N10	-5.86	117.07	120.52
2	C	501	FAD	O2A-PA-O1A	-5.75	81.38	112.53
2	D	501	FAD	C4X-C10-N10	-5.61	117.21	120.52
2	A	501	FAD	O2P-P-O5'	-5.16	82.46	108.46
2	A	501	FAD	C4X-C10-N10	-4.95	117.61	120.52
2	A	501	FAD	O5'-P-O1P	-4.84	90.82	109.62
2	C	501	FAD	O3'-C3'-C2'	-4.82	96.61	108.75
2	C	501	FAD	P-O3P-PA	-4.72	119.49	132.73
2	A	501	FAD	P-O3P-PA	-4.63	119.72	132.73
2	D	501	FAD	O2'-C2'-C3'	-4.26	98.31	109.02
3	A	502	NAP	O3D-C3D-C2D	-4.00	98.82	111.83
2	B	501	FAD	C4-C4X-C10	-3.82	117.50	119.94
2	B	501	FAD	C1'-C2'-C3'	-3.74	99.13	109.82
2	B	501	FAD	C4X-C10-N10	-3.68	118.35	120.52
2	D	501	FAD	O5B-PA-O1A	-3.54	95.86	109.62
3	A	502	NAP	O2A-PA-O3	-3.47	89.35	105.09
2	B	501	FAD	P-O3P-PA	-3.41	123.15	132.73
2	A	501	FAD	C4X-C4-N3	-3.32	119.05	123.59
3	D	502	NAP	C3N-C7N-N7N	-3.30	114.21	117.82
3	B	502	NAP	O7N-C7N-C3N	-3.23	116.06	119.59
2	D	501	FAD	P-O3P-PA	-2.91	124.55	132.73
2	C	501	FAD	C4A-C5A-N7A	-2.91	106.80	109.48
2	A	501	FAD	C1'-C2'-C3'	-2.91	101.50	109.82
3	B	502	NAP	C4A-C5A-N7A	-2.86	106.84	109.48
2	C	501	FAD	C4X-C4-N3	-2.85	119.69	123.59
3	B	502	NAP	C3N-C2N-N1N	-2.85	117.08	120.36
2	B	501	FAD	C4X-C4-N3	-2.78	119.79	123.59
2	D	501	FAD	C4X-C4-N3	-2.73	119.85	123.59
2	D	501	FAD	C4-C4X-C10	-2.63	118.26	119.94
3	B	502	NAP	O4B-C1B-C2B	-2.60	101.90	106.60
3	B	502	NAP	C4B-O4B-C1B	-2.58	106.88	109.72
3	C	502	NAP	O4B-C1B-C2B	-2.51	102.06	106.60
3	B	502	NAP	C6N-C5N-C4N	-2.41	115.80	119.44
3	D	502	NAP	PN-O3-PA	-2.35	126.13	132.73
3	D	502	NAP	C6N-C5N-C4N	-2.29	115.98	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAP	O5D-PN-O1N	-2.23	100.95	109.62
3	A	502	NAP	O2N-PN-O1N	-2.20	100.61	112.53
2	A	501	FAD	C1B-N9A-C4A	-2.18	123.65	126.94
2	D	501	FAD	C1'-C2'-C3'	-2.18	103.59	109.82
3	C	502	NAP	PN-O3-PA	-2.16	126.67	132.73
2	D	501	FAD	O2A-PA-O1A	-2.11	101.10	112.53
2	A	501	FAD	C4B-O4B-C1B	-2.07	107.44	109.72
2	C	501	FAD	C1B-N9A-C4A	-2.06	123.84	126.94
3	D	502	NAP	C3N-C2N-N1N	-2.01	118.05	120.36
2	B	501	FAD	O4B-C4B-C3B	2.08	109.33	105.15
2	B	501	FAD	C4X-N5-C5X	2.09	119.16	116.76
2	A	501	FAD	O4'-C4'-C5'	2.09	114.74	110.19
3	C	502	NAP	O4B-C4B-C5B	2.10	116.82	109.32
3	D	502	NAP	O5B-C5B-C4B	2.10	116.88	109.12
2	A	501	FAD	C2B-C1B-N9A	2.12	117.54	114.29
3	A	502	NAP	C2N-C3N-C4N	2.14	120.67	118.29
3	D	502	NAP	C5N-C6N-N1N	2.14	124.18	120.47
2	D	501	FAD	O2A-PA-O5B	2.19	119.50	108.46
3	B	502	NAP	O3-PN-O5D	2.24	108.87	102.94
2	A	501	FAD	C2A-N1A-C6A	2.27	122.83	118.77
2	A	501	FAD	C4X-N5-C5X	2.32	119.43	116.76
2	B	501	FAD	O3P-PA-O5B	2.35	109.16	102.94
2	B	501	FAD	O3'-C3'-C2'	2.35	114.67	108.75
2	A	501	FAD	O2P-P-O1P	2.36	125.34	112.53
3	C	502	NAP	O2N-PN-O3	2.41	116.05	105.09
3	D	502	NAP	O5D-C5D-C4D	2.42	118.03	109.12
2	D	501	FAD	O2P-P-O3P	2.42	116.08	105.09
2	A	501	FAD	O4B-C4B-C3B	2.60	110.39	105.15
2	C	501	FAD	C4-C4X-N5	2.69	121.98	118.72
3	D	502	NAP	O3-PA-O5B	2.74	110.19	102.94
3	C	502	NAP	O4D-C1D-N1N	2.75	111.16	108.13
2	C	501	FAD	C4X-N5-C5X	2.87	120.07	116.76
2	C	501	FAD	O2A-PA-O3P	3.09	119.10	105.09
2	D	501	FAD	O2A-PA-O3P	3.11	119.18	105.09
2	D	501	FAD	C4X-N5-C5X	3.11	120.34	116.76
3	D	502	NAP	O7N-C7N-N7N	3.15	127.03	122.59
3	A	502	NAP	O2A-PA-O5B	3.27	124.94	108.46
2	C	501	FAD	O3P-P-O5'	3.28	111.64	102.94
2	D	501	FAD	C4-C4X-N5	3.33	122.76	118.72
2	D	501	FAD	O3P-P-O5'	3.40	111.95	102.94
3	A	502	NAP	O2N-PN-O3	3.47	120.82	105.09
3	A	502	NAP	O5B-C5B-C4B	3.50	122.03	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O2P-P-O3P	3.59	121.39	105.09
2	C	501	FAD	O4'-C4'-C5'	3.65	118.13	110.19
3	D	502	NAP	C2N-C3N-C4N	3.83	122.55	118.29
3	A	502	NAP	O4D-C1D-N1N	3.83	112.34	108.13
3	A	502	NAP	C5B-C4B-C3B	3.93	130.79	115.21
3	B	502	NAP	C2N-C3N-C4N	3.93	122.66	118.29
2	B	501	FAD	C4-C4X-N5	3.99	123.57	118.72
2	B	501	FAD	O2A-PA-O3P	4.02	123.34	105.09
2	D	501	FAD	C2B-C1B-N9A	4.20	120.71	114.29
2	C	501	FAD	O3P-PA-O5B	4.24	114.18	102.94
2	C	501	FAD	C2B-C1B-N9A	4.49	121.15	114.29
3	D	502	NAP	O4D-C1D-N1N	4.57	113.16	108.13
2	D	501	FAD	O3P-PA-O5B	4.63	115.22	102.94
2	C	501	FAD	C1'-C2'-C3'	4.72	123.31	109.82
3	B	502	NAP	O4D-C1D-N1N	5.25	113.90	108.13
2	C	501	FAD	C4-N3-C2	5.45	119.96	115.25
2	D	501	FAD	O4'-C4'-C3'	5.59	123.07	109.02
2	B	501	FAD	O4'-C4'-C3'	5.81	123.62	109.02
2	D	501	FAD	C4-N3-C2	6.01	120.44	115.25
2	A	501	FAD	O4'-C4'-C3'	6.16	124.50	109.02
2	A	501	FAD	O3P-PA-O5B	6.30	119.65	102.94
2	B	501	FAD	C4-N3-C2	6.33	120.72	115.25
2	A	501	FAD	C4-N3-C2	6.71	121.05	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	7	0
3	A	502	NAP	7	0
4	A	503	ORN	1	0
2	B	501	FAD	3	0
4	B	503	ORN	2	0
2	C	501	FAD	7	0
3	C	502	NAP	2	0
4	C	503	ORN	1	0
2	D	501	FAD	3	0
3	D	502	NAP	3	0
4	D	503	ORN	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

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	415/443 (93%)	-0.25	1 (0%) 95 96	11, 23, 49, 61	0
1	B	414/443 (93%)	-0.18	1 (0%) 95 96	10, 22, 47, 61	0
1	C	414/443 (93%)	-0.02	14 (3%) 49 51	10, 27, 62, 78	0
1	D	415/443 (93%)	-0.22	3 (0%) 89 90	14, 27, 52, 75	0
All	All	1658/1772 (93%)	-0.17	19 (1%) 82 84	10, 25, 53, 78	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	384	LEU	4.7
1	C	135	PRO	4.6
1	C	138	PRO	4.0
1	C	143	LEU	2.8
1	C	383	ASP	2.7
1	C	380	THR	2.6
1	C	146	VAL	2.6
1	C	152	THR	2.6
1	C	139	VAL	2.5
1	C	148	THR	2.4
1	C	151	ALA	2.4
1	D	317	ALA	2.4
1	C	134	GLY	2.3
1	D	192	ASP	2.3
1	C	382	PRO	2.3
1	A	366	ALA	2.2
1	B	192	ASP	2.0
1	D	120	HIS	2.0
1	C	381	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	ORN	D	503	9/9	0.89	0.22	2.26	28,31,35,43	0
4	ORN	C	503	9/9	0.91	0.21	2.25	33,35,40,46	0
4	ORN	A	503	9/9	0.91	0.22	2.05	29,33,39,46	0
3	NAP	D	502	48/48	0.94	0.22	1.73	24,37,48,54	0
3	NAP	A	502	48/48	0.94	0.18	1.03	24,35,44,56	0
2	FAD	B	501	53/53	0.97	0.15	0.19	12,18,30,39	0
4	ORN	B	503	9/9	0.95	0.17	-0.09	16,22,25,33	0
2	FAD	D	501	53/53	0.97	0.14	-0.23	14,25,32,39	0
2	FAD	C	501	53/53	0.96	0.14	-0.40	15,26,36,40	0
3	NAP	C	502	48/48	0.97	0.13	-0.63	17,24,32,36	0
5	K	C	504	1/1	0.83	0.15	-0.63	63,63,63,63	0
5	K	D	504	1/1	0.91	0.11	-0.69	48,48,48,48	0
3	NAP	B	502	48/48	0.97	0.13	-0.85	15,23,28,33	0
5	K	A	504	1/1	0.94	0.09	-0.87	37,37,37,37	0
2	FAD	A	501	53/53	0.97	0.12	-0.90	12,22,36,40	0
5	K	B	504	1/1	0.92	0.11	-1.19	43,43,43,43	0
5	K	D	505	1/1	0.97	0.07	-2.34	47,47,47,47	0
5	K	B	505	1/1	0.95	0.08	-2.37	42,42,42,42	0
5	K	A	505	1/1	0.94	0.08	-3.28	44,44,44,44	0
5	K	C	505	1/1	0.82	0.08	-3.35	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.