



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:32 pm GMT

PDB ID : 1S3E
Title : Crystal structure of MAOB in complex with 6-hydroxy-N-propargyl-1(R)-aminoindan
Authors : Binda, C.; Hubalek, F.; Li, M.; Herzig, Y.; Sterling, J.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2004-01-13
Resolution : 1.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

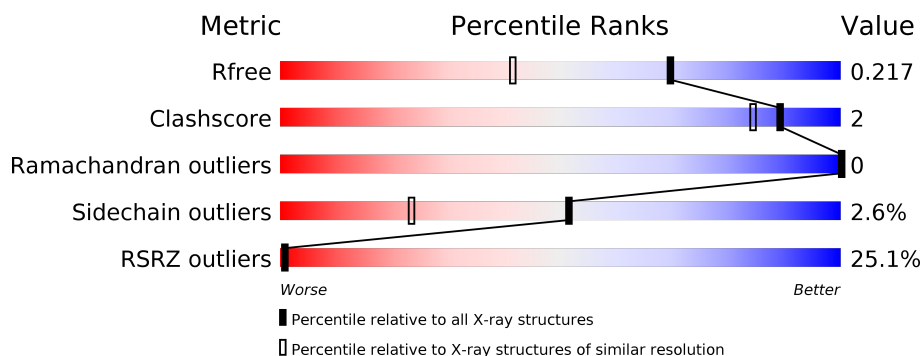
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

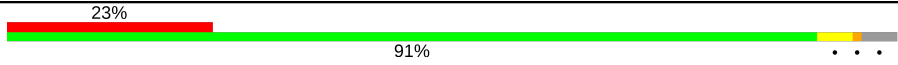

The reported resolution of this entry is 1.60 Å.

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}	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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	520	
1	B	520	

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
2	RHP	A	601	-	-	-	X
2	RHP	B	601	-	-	-	X

2 Entry composition [i](#)

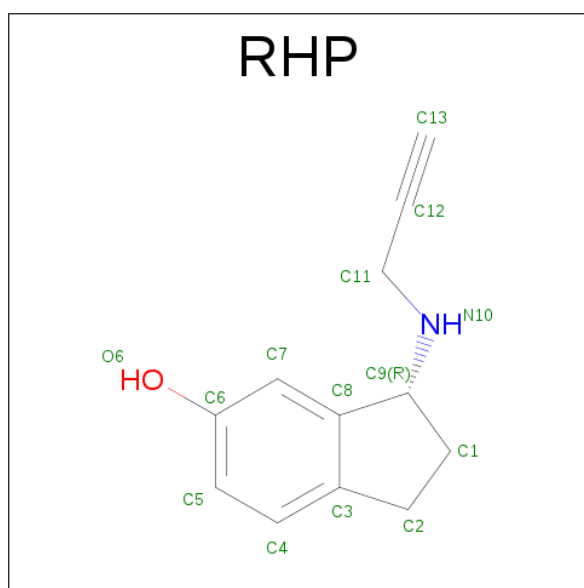
There are 3 unique types of molecules in this entry. The entry contains 8838 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Amine oxidase [flavin-containing] B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	1	0
			3972	2538	681	728	25			
1	B	494	Total	C	N	O	S	0	1	0
			3941	2519	676	721	25			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: RHP, FAD) (formula: $C_{12}H_{13}NO$, $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	N	O	P	0	0
			67	39	10	16	2		
2	B	2	Total	C	N	O	P	0	0
			67	39	10	16	2		

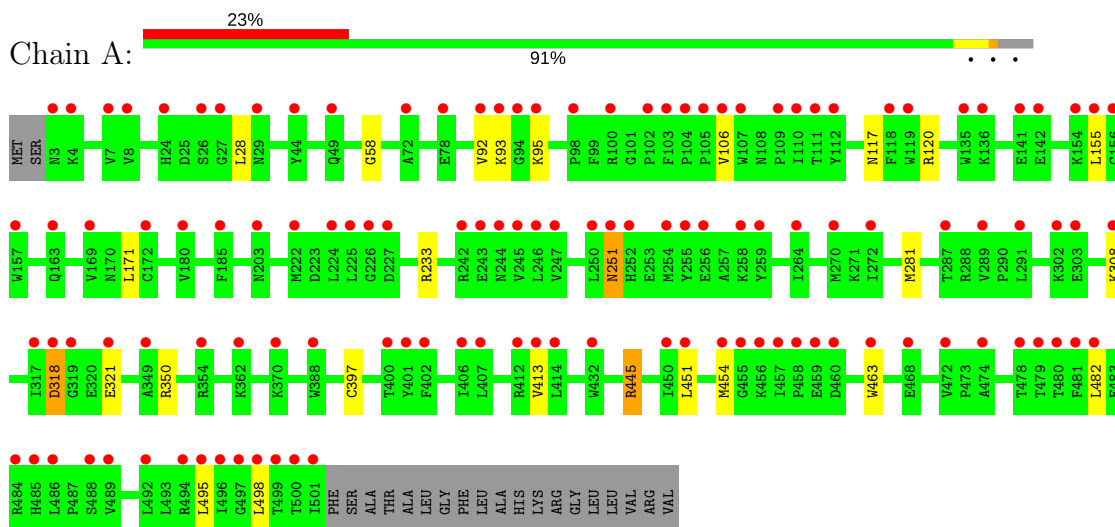
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	359	Total 359	O 359	0	0
3	B	432	Total 432	O 432	0	0

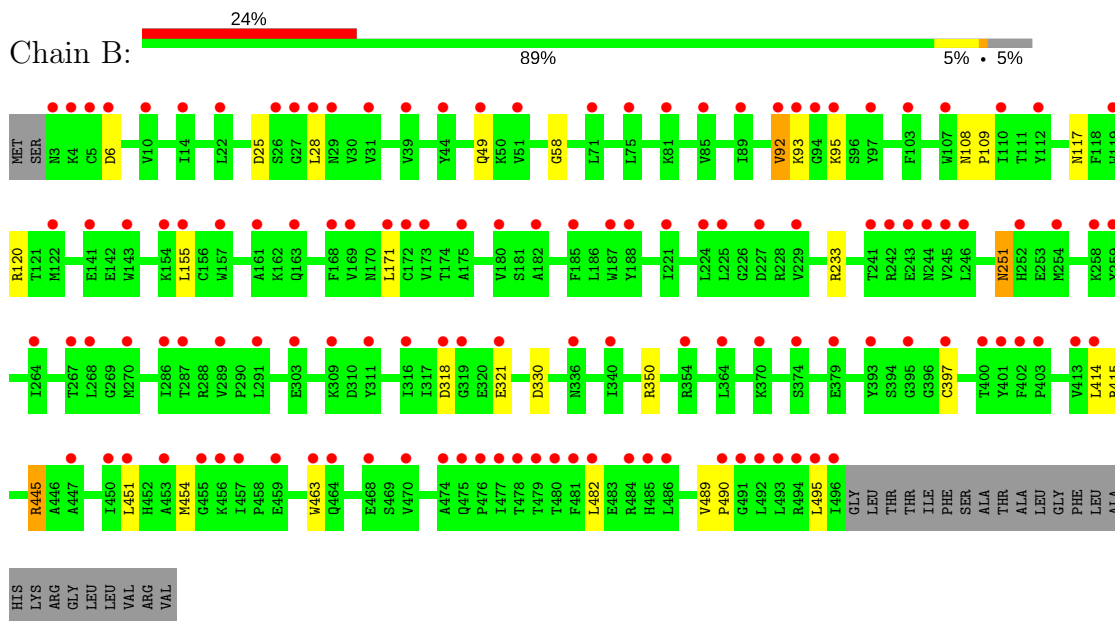
3 Residue-property plots [i](#)

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

• Molecule 1: Amine oxidase [flavin-containing] B



• Molecule 1: Amine oxidase [flavin-containing] B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.96Å 224.06Å 86.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 47.04 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.6 (15.00-1.60) 88.6 (47.04-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.216 0.199 , 0.217	Depositor DCC
R_{free} test set	3823 reflections (2.63%)	DCC
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 76.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8838	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RHP, 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	0.36	0/4074	0.64	3/5530 (0.1%)
1	B	0.36	0/4043	0.64	4/5487 (0.1%)
All	All	0.36	0/8117	0.64	7/11017 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	445	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	445	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	445	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	6	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	330	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	318	ASP	CB-CG-OD2	5.15	122.93	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	3972	0	3968	16	0
1	B	3941	0	3938	19	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	67	0	42	2	0
2	B	67	0	42	2	0
3	A	359	0	0	1	0
3	B	432	0	0	4	0
All	All	8838	0	7990	35	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 2.

All (35) 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:B:92:VAL:HB	3:B:1022:HOH:O	1.55	1.06
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.39	0.69
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.39	0.68
1:B:251:ASN:H	1:B:251:ASN:HD22	1.43	0.66
1:A:251:ASN:H	1:A:251:ASN:HD22	1.43	0.66
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.34	0.63
1:B:445:ARG:HD2	1:B:463:TRP:CH2	2.34	0.61
1:B:445:ARG:HD3	3:B:602:HOH:O	2.01	0.61
1:A:451:LEU:HD23	1:A:454:MET:HE1	1.83	0.58
1:B:451:LEU:HD23	1:B:454:MET:HE1	1.86	0.56
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.42	0.54
1:B:233:ARG:HG3	1:B:251:ASN:HD21	1.73	0.53
1:A:445:ARG:HD3	3:A:628:HOH:O	2.09	0.52
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.44	0.51
1:A:233:ARG:HG3	1:A:251:ASN:HD21	1.76	0.51
1:B:414:LEU:HD12	3:B:859:HOH:O	2.12	0.49
1:A:321:GLU:H	1:A:321:GLU:CD	2.20	0.46
1:B:321:GLU:CD	1:B:321:GLU:H	2.19	0.45
1:B:454:MET:HB2	1:B:454:MET:HE2	1.56	0.45
1:A:58:GLY:HA2	2:A:600:FAD:C4X	2.47	0.44
1:A:171:LEU:HD21	2:A:601:RHP:H21	1.99	0.44
1:B:108:ASN:HA	1:B:109:PRO:HD3	1.88	0.44
1:A:28:LEU:HD11	1:A:454:MET:HE1	2.00	0.43
1:A:308:LYS:HB2	1:A:308:LYS:HE2	1.78	0.43
1:A:251:ASN:H	1:A:251:ASN:ND2	2.15	0.43
1:B:171:LEU:HD21	2:B:601:RHP:H21	2.00	0.42
1:B:28:LEU:HD11	1:B:454:MET:HE1	2.02	0.42
1:A:117:ASN:HD22	1:A:120:ARG:NH2	2.11	0.42
1:B:58:GLY:HA2	2:B:600:FAD:C4X	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASN:HD22	1:B:120:ARG:NH2	2.13	0.41
1:B:415:ARG:NH1	3:B:897:HOH:O	2.52	0.41
1:B:251:ASN:H	1:B:251:ASN:ND2	2.15	0.41
1:A:454:MET:HB2	1:A:454:MET:HE2	1.57	0.41
1:B:489:VAL:N	1:B:490:PRO:HD2	2.36	0.41
1:A:281:MET:HB3	1:A:413:VAL:HG21	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)
1:B:25:ASP:O	1:B:49:GLN:NE2[4_565]	1.59	0.61

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	498/520 (96%)	487 (98%)	11 (2%)	0	100	100
1	B	493/520 (95%)	481 (98%)	12 (2%)	0	100	100
All	All	991/1040 (95%)	968 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	428/444 (96%)	416 (97%)	12 (3%)	49	21
1	B	425/444 (96%)	415 (98%)	10 (2%)	54	26
All	All	853/888 (96%)	831 (97%)	22 (3%)	51	23

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	93	LYS
1	A	95	LYS
1	A	106	VAL
1	A	155	LEU
1	A	251	ASN
1	A	318	ASP
1	A	350	ARG
1	A	397	CYS
1	A	482	LEU
1	A	495	LEU
1	A	498	LEU
1	B	92	VAL
1	B	93	LYS
1	B	95	LYS
1	B	155	LEU
1	B	251	ASN
1	B	318	ASP
1	B	350	ARG
1	B	397	CYS
1	B	482	LEU
1	B	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	251	ASN
1	B	117	ASN
1	B	251	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	1,2	51,58,58	1.31	7 (13%)	54,89,89	1.87	7 (12%)
2	RHP	A	601	2	14,15,15	4.84	3 (21%)	19,20,20	12.14	5 (26%)
2	FAD	B	600	1,2	51,58,58	1.34	7 (13%)	54,89,89	1.91	7 (12%)
2	RHP	B	601	2	14,15,15	4.78	3 (21%)	19,20,20	12.13	5 (26%)

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	1,2	-	0/28/50/50	0/6/6/6
2	RHP	A	601	2	-	0/3/13/13	0/2/2/2
2	FAD	B	600	1,2	-	0/28/50/50	0/6/6/6
2	RHP	B	601	2	-	0/3/13/13	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	RHP	C11-N10	-15.58	1.29	1.46
2	B	601	RHP	C11-N10	-15.34	1.29	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C5X-N5	2.01	1.38	1.35
2	A	600	FAD	C5X-N5	2.26	1.38	1.35
2	A	600	FAD	C2A-N1A	2.34	1.38	1.33
2	B	600	FAD	C2A-N1A	2.39	1.38	1.33
2	A	600	FAD	C1'-N10	2.50	1.51	1.48
2	B	600	FAD	C4-N3	2.66	1.37	1.33
2	A	600	FAD	C4-N3	2.73	1.38	1.33
2	B	600	FAD	C1'-N10	2.89	1.51	1.48
2	A	600	FAD	C2A-N3A	3.34	1.37	1.32
2	B	600	FAD	C2A-N3A	3.49	1.38	1.32
2	A	600	FAD	C10-N1	3.94	1.38	1.33
2	B	600	FAD	C10-N1	4.12	1.39	1.33
2	B	600	FAD	C4X-N5	4.33	1.39	1.33
2	A	600	FAD	C4X-N5	4.41	1.39	1.33
2	A	601	RHP	C12-C13	5.33	1.30	1.18
2	B	601	RHP	C12-C13	5.36	1.30	1.18
2	B	601	RHP	C11-C12	7.14	1.53	1.47
2	A	601	RHP	C11-C12	7.25	1.54	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	RHP	C11-C12-C13	-52.22	125.76	178.30
2	B	601	RHP	C11-C12-C13	-52.17	125.81	178.30
2	B	600	FAD	N3A-C2A-N1A	-9.91	120.23	128.86
2	A	600	FAD	N3A-C2A-N1A	-9.75	120.37	128.86
2	B	601	RHP	C5-C4-C3	-2.86	117.59	121.40
2	A	601	RHP	C5-C4-C3	-2.66	117.86	121.40
2	B	600	FAD	C4X-C4-N3	-2.49	119.93	123.48
2	B	600	FAD	C9A-C5X-N5	-2.46	118.58	122.24
2	A	600	FAD	C4X-C4-N3	-2.40	120.06	123.48
2	A	600	FAD	C9A-C5X-N5	-2.22	118.94	122.24
2	B	600	FAD	C4A-C5A-N7A	-2.21	107.28	109.41
2	A	600	FAD	C1B-N9A-C4A	-2.14	122.94	126.64
2	A	600	FAD	C1'-N10-C9A	2.09	120.26	118.35
2	A	600	FAD	C4-C4X-N5	2.24	121.14	118.68
2	B	601	RHP	C3-C8-C9	2.42	112.50	110.27
2	A	601	RHP	C3-C8-C9	2.49	112.57	110.27
2	B	600	FAD	C4X-N5-C5X	2.64	119.55	116.76
2	B	600	FAD	C4-C4X-N5	2.64	121.58	118.68
2	B	601	RHP	C11-N10-C9	2.66	119.00	113.90
2	A	601	RHP	C11-N10-C9	2.69	119.05	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	RHP	C12-C11-N10	6.12	120.18	112.26
2	A	600	FAD	C4-N3-C2	6.25	120.62	115.16
2	A	601	RHP	C12-C11-N10	6.36	120.50	112.26
2	B	600	FAD	C4-N3-C2	6.48	120.83	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	1	0
2	A	601	RHP	1	0
2	B	600	FAD	1	0
2	B	601	RHP	1	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 ⓘ

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	499/520 (95%)	1.54	122 (24%)	1 1	28, 34, 51, 77	1 (0%)
1	B	494/520 (95%)	1.57	127 (25%)	1 1	26, 34, 48, 69	1 (0%)
All	All	993/1040 (95%)	1.56	249 (25%)	1 1	26, 34, 49, 77	2 (0%)

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	LEU	10.0
1	A	500	THR	9.6
1	A	499	THR	9.6
1	B	496	ILE	8.6
1	A	107	TRP	7.6
1	A	252	HIS	7.5
1	A	501	ILE	7.5
1	B	494	ARG	7.1
1	B	107	TRP	6.3
1	A	103	PHE	6.2
1	B	481	PHE	5.9
1	B	244	ASN	5.9
1	A	498	LEU	5.8
1	B	492	LEU	5.7
1	A	496	ILE	5.7
1	A	354	ARG	5.7
1	A	246	LEU	5.5
1	B	243	GLU	5.5
1	A	478	THR	5.5
1	A	479	THR	5.4
1	B	482	LEU	5.4
1	B	252	HIS	5.4
1	B	242	ARG	5.4
1	A	482	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	93	LYS	4.9
1	A	480	THR	4.7
1	A	495	LEU	4.6
1	B	493	LEU	4.6
1	A	243	GLU	4.6
1	A	242	ARG	4.6
1	B	3	ASN	4.4
1	B	119	TRP	4.4
1	A	494	ARG	4.3
1	A	484	ARG	4.3
1	B	157	TRP	4.3
1	A	3	ASN	4.2
1	A	106	VAL	4.0
1	A	92	VAL	4.0
1	A	251	ASN	4.0
1	B	478	THR	3.9
1	A	49	GLN	3.9
1	B	459	GLU	3.8
1	B	95	LYS	3.8
1	B	303	GLU	3.8
1	A	105	PRO	3.8
1	B	491	GLY	3.7
1	A	451	LEU	3.7
1	B	457	ILE	3.7
1	A	110	ILE	3.6
1	A	93	LYS	3.6
1	B	490	PRO	3.6
1	B	103	PHE	3.6
1	B	354	ARG	3.6
1	A	4	LYS	3.6
1	A	226	GLY	3.6
1	B	414	LEU	3.6
1	A	112	TYR	3.5
1	B	5	CYS	3.5
1	A	227	ASP	3.5
1	B	453	ALA	3.4
1	B	49	GLN	3.4
1	A	459	GLU	3.4
1	B	254	MET	3.3
1	A	259	TYR	3.3
1	A	302	LYS	3.3
1	B	110	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	318	ASP	3.3
1	B	27	GLY	3.3
1	B	475	GLN	3.2
1	A	308	LYS	3.2
1	B	155	LEU	3.2
1	A	497	GLY	3.2
1	A	78	GLU	3.2
1	A	481	PHE	3.2
1	A	102	PRO	3.2
1	A	458	PRO	3.1
1	B	92	VAL	3.1
1	B	289	VAL	3.1
1	A	245	VAL	3.1
1	A	163	GLN	3.1
1	B	485	HIS	3.1
1	A	100	ARG	3.0
1	B	450	ILE	3.0
1	A	321	GLU	3.0
1	A	460	ASP	3.0
1	B	477	ILE	3.0
1	A	486	LEU	3.0
1	A	457	ILE	3.0
1	B	270	MET	3.0
1	A	119	TRP	3.0
1	B	112	TYR	3.0
1	B	267	THR	3.0
1	B	229	VAL	3.0
1	A	454	MET	2.9
1	B	479	THR	2.9
1	B	224	LEU	2.9
1	A	406	ILE	2.9
1	B	393	TYR	2.9
1	A	26	SER	2.9
1	A	224	LEU	2.9
1	B	4	LYS	2.9
1	A	169	VAL	2.8
1	B	245	VAL	2.8
1	B	318	ASP	2.8
1	A	142	GLU	2.8
1	A	468	GLU	2.8
1	A	256	GLU	2.8
1	B	28	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	264	ILE	2.8
1	B	246	LEU	2.8
1	A	157	TRP	2.8
1	A	104	PRO	2.7
1	B	319	GLY	2.7
1	B	468	GLU	2.7
1	B	241	THR	2.7
1	B	268	LEU	2.7
1	A	319	GLY	2.7
1	A	29	ASN	2.7
1	A	349	ALA	2.7
1	A	264	ILE	2.7
1	B	29	ASN	2.7
1	B	225	LEU	2.7
1	A	118	PHE	2.7
1	A	270	MET	2.6
1	A	456	LYS	2.6
1	B	97	TYR	2.6
1	B	476	PRO	2.6
1	A	244	ASN	2.6
1	B	480	THR	2.6
1	B	484	ARG	2.5
1	A	72	ALA	2.5
1	A	489	VAL	2.5
1	A	94	GLY	2.5
1	A	141	GLU	2.5
1	B	259	TYR	2.5
1	B	321	GLU	2.5
1	B	122	MET	2.5
1	B	175	ALA	2.5
1	A	463	TRP	2.5
1	A	272	ILE	2.5
1	B	221	ILE	2.5
1	B	85	VAL	2.5
1	B	168	PHE	2.5
1	A	413	VAL	2.5
1	B	31	VAL	2.5
1	B	340	ILE	2.5
1	B	470	VAL	2.5
1	B	397	CYS	2.5
1	A	136	LYS	2.5
1	B	89	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	414	LEU	2.5
1	B	370	LYS	2.5
1	B	44	TYR	2.4
1	B	474	ALA	2.4
1	A	154	LYS	2.4
1	A	250	LEU	2.4
1	A	407	LEU	2.4
1	B	75	LEU	2.4
1	A	24	HIS	2.4
1	A	155	LEU	2.4
1	A	402	PHE	2.4
1	A	474	ALA	2.4
1	B	163	GLN	2.4
1	B	182	ALA	2.4
1	B	188	TYR	2.4
1	B	463	TRP	2.4
1	A	109	PRO	2.4
1	B	464	GLN	2.4
1	B	141	GLU	2.4
1	A	258	LYS	2.4
1	B	39	VAL	2.4
1	B	169	VAL	2.4
1	B	291	LEU	2.4
1	B	402	PHE	2.4
1	B	171	LEU	2.3
1	B	486	LEU	2.3
1	A	254	MET	2.3
1	A	370	LYS	2.3
1	B	403	PRO	2.3
1	A	472	VAL	2.3
1	A	488	SER	2.3
1	A	492	LEU	2.3
1	B	364	LEU	2.3
1	B	185	PHE	2.3
1	B	447	ALA	2.3
1	B	173	VAL	2.3
1	A	27	GLY	2.3
1	A	317	ILE	2.3
1	B	227	ASP	2.3
1	B	311	TYR	2.3
1	A	95	LYS	2.3
1	B	286	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	455	GLY	2.3
1	A	135	TRP	2.2
1	A	450	ILE	2.2
1	A	8	VAL	2.2
1	B	374	SER	2.2
1	A	412	ARG	2.2
1	B	51	VAL	2.2
1	B	180	VAL	2.2
1	B	451	LEU	2.2
1	B	258	LYS	2.2
1	A	98	PRO	2.2
1	A	485	HIS	2.2
1	B	143	TRP	2.2
1	A	111	THR	2.2
1	B	81	LYS	2.2
1	A	247	VAL	2.2
1	A	225	LEU	2.2
1	B	14	ILE	2.2
1	B	287	THR	2.2
1	A	185	PHE	2.1
1	A	255	TYR	2.1
1	A	401	TYR	2.1
1	B	413	VAL	2.1
1	A	388	TRP	2.1
1	A	432	TRP	2.1
1	A	303	GLU	2.1
1	A	289	VAL	2.1
1	B	10	VAL	2.1
1	A	400	THR	2.1
1	B	71	LEU	2.1
1	A	362	LYS	2.1
1	B	309	LYS	2.1
1	B	455	GLY	2.1
1	A	44	TYR	2.1
1	A	287	THR	2.1
1	A	180	VAL	2.1
1	B	400	THR	2.1
1	A	7	VAL	2.1
1	B	395	GLY	2.1
1	A	203	ASN	2.1
1	B	172[A]	CYS	2.1
1	A	291	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	26	SER	2.0
1	B	187	TRP	2.0
1	B	456	LYS	2.0
1	A	156	CYS	2.0
1	A	172[A]	CYS	2.0
1	B	316	ILE	2.0
1	A	222	MET	2.0
1	B	161	ALA	2.0
1	B	154	LYS	2.0
1	B	379	GLU	2.0
1	B	401	TYR	2.0
1	B	22	LEU	2.0
1	B	6	ASP	2.0
1	B	94	GLY	2.0
1	B	336	ASN	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
2	RHP	B	601	14/14	0.68	0.24	4.89	38,44,45,46	0
2	RHP	A	601	14/14	0.78	0.20	3.66	38,44,45,46	0
2	FAD	A	600	53/53	0.91	0.14	-0.37	27,29,31,31	0
2	FAD	B	600	53/53	0.94	0.14	-0.96	27,29,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.