Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:06 PM GMT

PDB ID	:	1S3B
Title	:	Crystal structure of MAOB in complex with N-methyl-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	:	1.65 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

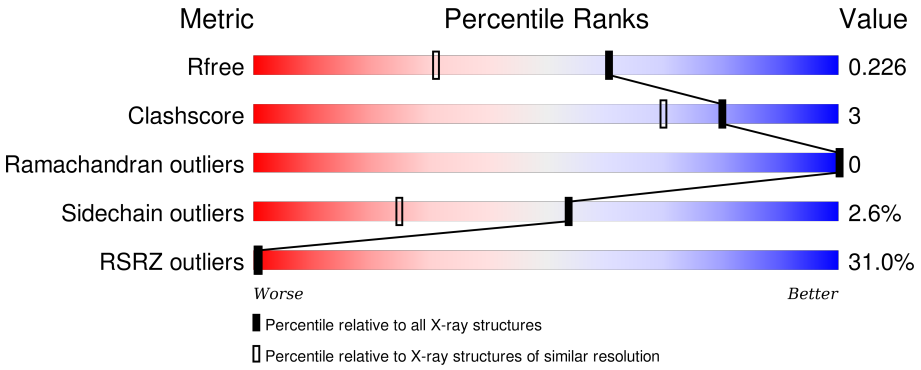
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.65 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	520	29% 88% 7% •
1	B	520	30% 85% 9% • 5%

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	RMA	A	601	-	-	-	X
2	RMA	B	601	-	-	-	X

2 Entry composition

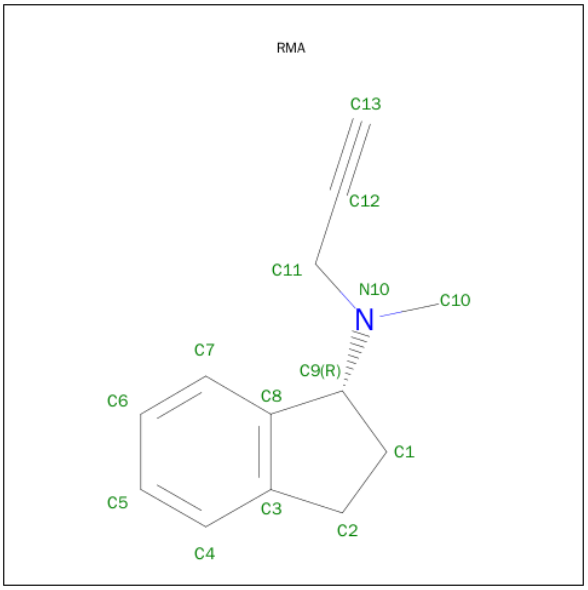
There are 3 unique types of molecules in this entry. The entry contains 8864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0
			3971	2538	681	728	24			
1	B	494	Total	C	N	O	S	0	0	0
			3940	2519	676	721	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: RMA, FAD) (formula: $C_{13}H_{15}N$, $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	N	O	P	0	0
			67	40	10	15	2		
2	B	2	Total	C	N	O	P	0	0
			67	40	10	15	2		

- Molecule 3 is water.

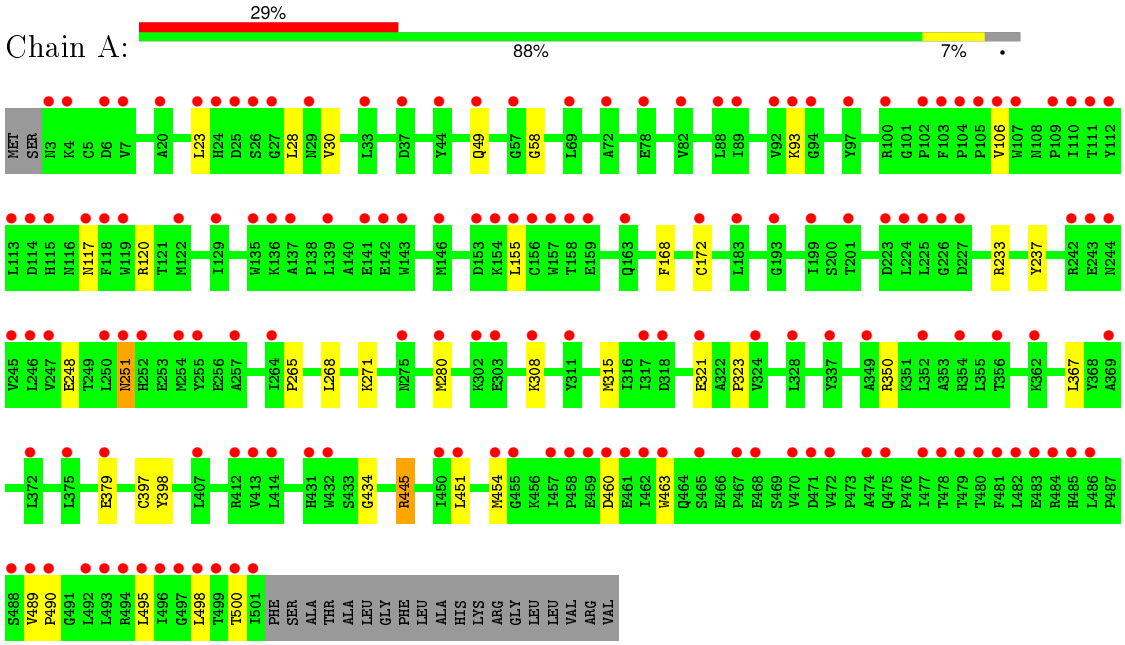
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	376	Total O 376 376	0	0
3	B	443	Total O 443 443	0	0

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 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.

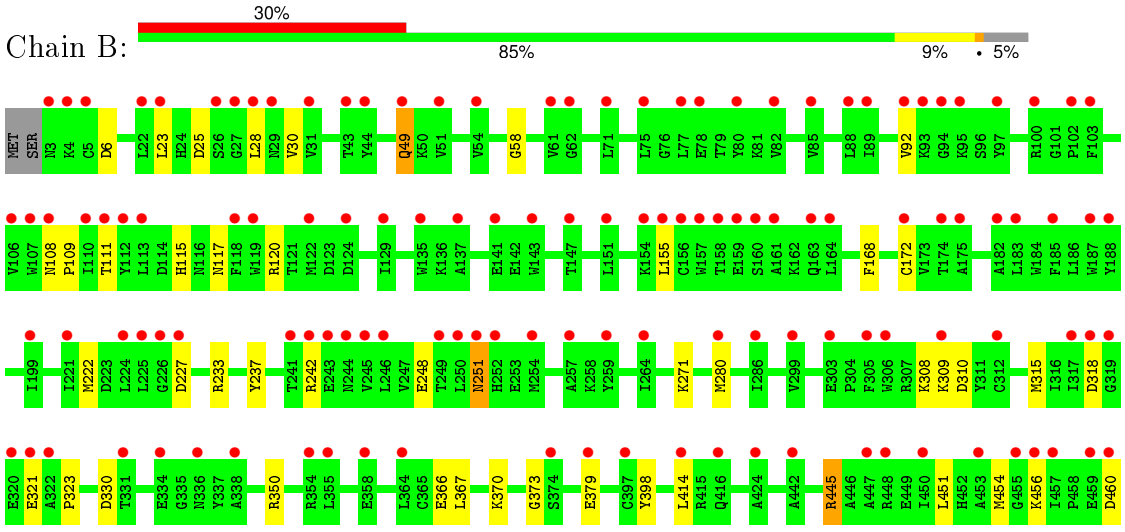
- Molecule 1: Amine oxidase [flavin-containing] B

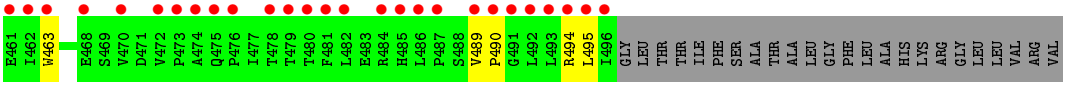
Chain A:



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

Chain B:




E461
I462
W463
E468
S469
V470
D471
V472
P473
A474
Q475
P476
I477
T478
T479
T480
F481
L482
E483
R484
H485
L486
P487
S488
V489
P490
G491
L492
L493
R494
L495
T496
GLY
LEU
THR
THR
ILE
PHE
SER
ALA
THR
ALA
LEU
GLY
PHE
LEU
ALA
HIS
LYS
ARG
GLY
LEU
LEU
VAL
ARG
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	130.76Å 222.91Å 86.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.65 14.96 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-1.65) 98.1 (14.96-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.223 0.208 , 0.226	Depositor DCC
R_{free} test set	3732 reflections (2.59%)	DCC
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 81.0	EDS
Estimated twinning fraction	0.012 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 147566 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8864	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: RMA, 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	0.38	0/4068	0.65	2/5522 (0.0%)
1	B	0.36	0/4037	0.65	7/5479 (0.1%)
All	All	0.37	0/8105	0.65	9/11001 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	445	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	315	MET	CG-SD-CE	5.82	109.51	100.20
1	B	315	MET	CG-SD-CE	5.82	109.51	100.20
1	A	445	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	227	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	445	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	310	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	6	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	330	ASP	CB-CG-OD2	5.08	122.88	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	3971	0	3967	23	0
1	B	3940	0	3937	31	1
2	A	67	0	44	4	0
2	B	67	0	44	2	0
3	A	376	0	0	2	0
3	B	443	0	0	5	0
All	All	8864	0	7992	54	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 3.

All (54) 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	1:B:318:ASP:OD2	1.79	0.83
1:A:28:LEU:HD11	1:A:454:MET:HE1	1.64	0.78
1:B:28:LEU:HD11	1:B:454:MET:HE1	1.67	0.75
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.37	0.72
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.38	0.71
1:B:92:VAL:CG2	1:B:318:ASP:OD2	2.42	0.68
1:B:414:LEU:HD12	3:B:811:HOH:O	1.95	0.67
1:B:251:ASN:H	1:B:251:ASN:HD22	1.44	0.66
1:B:92:VAL:CB	1:B:318:ASP:OD2	2.44	0.65
1:A:251:ASN:H	1:A:251:ASN:HD22	1.43	0.64
1:A:451:LEU:HA	1:A:454:MET:HE2	1.81	0.60
1:B:451:LEU:HA	1:B:454:MET:HE2	1.83	0.60
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.39	0.58
1:B:92:VAL:HG23	1:B:318:ASP:OD2	2.04	0.57
1:B:445:ARG:HD3	3:B:616:HOH:O	2.04	0.56
1:B:445:ARG:HD2	1:B:463:TRP:CH2	2.40	0.56
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.42	0.54
1:A:445:ARG:HD3	3:A:623:HOH:O	2.11	0.50
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.46	0.50
1:A:271:LYS:HE2	3:A:767:HOH:O	2.12	0.50
1:A:233:ARG:HG3	1:A:251:ASN:HD21	1.77	0.50
1:B:233:ARG:HG3	1:B:251:ASN:HD21	1.77	0.50
1:B:168:PHE:CE1	1:B:172:CYS:SG	3.05	0.50
1:A:321:GLU:CD	1:A:321:GLU:H	2.15	0.49
1:B:321:GLU:CD	1:B:321:GLU:H	2.17	0.48
1:A:58:GLY:HA2	2:A:600:FAD:C4X	2.44	0.48
1:A:398:TYR:CZ	2:A:601:RMA:H111	2.48	0.48
1:B:58:GLY:HA2	2:B:600:FAD:C4X	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:MET:HE3	3:B:859:HOH:O	2.15	0.46
1:B:398:TYR:CZ	2:B:601:RMA:H111	2.51	0.45
1:B:237:TYR:HB3	1:B:248:GLU:HB3	1.98	0.45
1:A:168:PHE:CE1	1:A:172:CYS:SG	3.09	0.45
1:B:308:LYS:HE2	1:B:308:LYS:HB2	1.88	0.45
1:B:366:GLU:O	1:B:370:LYS:HG3	2.17	0.44
1:A:237:TYR:HB3	1:A:248:GLU:HB3	1.99	0.44
1:A:265:PRO:HD2	1:A:268:LEU:HD12	2.00	0.44
1:B:111:THR:HG22	1:B:115:HIS:CD2	2.52	0.43
1:B:323:PRO:HD2	1:B:367:LEU:HD22	2.00	0.43
1:A:308:LYS:HB2	1:A:308:LYS:HE2	1.87	0.43
1:A:323:PRO:HD2	1:A:367:LEU:HD22	2.00	0.43
1:A:117:ASN:HD22	1:A:120:ARG:NH2	2.12	0.43
1:B:251:ASN:H	1:B:251:ASN:ND2	2.13	0.43
1:A:251:ASN:ND2	1:A:251:ASN:H	2.13	0.43
1:A:172:CYS:SG	2:A:601:RMA:H6	2.59	0.42
1:B:454:MET:HE3	1:B:456:LYS:HG3	2.02	0.42
1:B:489:VAL:N	1:B:490:PRO:HD2	2.35	0.42
1:B:108:ASN:HA	1:B:109:PRO:HD3	1.87	0.42
1:B:309:LYS:NZ	1:B:373:GLY:O	2.53	0.41
1:B:271:LYS:HE2	3:B:858:HOH:O	2.20	0.41
1:A:489:VAL:N	1:A:490:PRO:HD2	2.35	0.41
1:A:23:LEU:HB2	1:A:30:VAL:HG11	2.03	0.41
1:B:494:ARG:NH1	3:B:926:HOH:O	2.54	0.40
1:A:434:GLY:O	2:A:600:FAD:H1'2	2.21	0.40
1:B:23:LEU:HB2	1:B:30:VAL:HG11	2.02	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]	2.01	0.19

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	497/520 (96%)	486 (98%)	11 (2%)	0	100	100
1	B	492/520 (95%)	480 (98%)	12 (2%)	0	100	100
All	All	989/1040 (95%)	966 (98%)	23 (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	427/444 (96%)	414 (97%)	13 (3%)	48	18
1	B	424/444 (96%)	415 (98%)	9 (2%)	61	34
All	All	851/888 (96%)	829 (97%)	22 (3%)	54	25

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

Mol	Chain	Res	Type
1	A	49	GLN
1	A	93	LYS
1	A	106	VAL
1	A	155	LEU
1	A	251	ASN
1	A	280	MET
1	A	350	ARG
1	A	379	GLU
1	A	397	CYS
1	A	460	ASP
1	A	495	LEU
1	A	498	LEU
1	A	500	THR
1	B	49	GLN
1	B	155	LEU

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Mol	Chain	Res	Type
1	B	242	ARG
1	B	251	ASN
1	B	280	MET
1	B	350	ARG
1	B	379	GLU
1	B	460	ASP
1	B	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	251	ASN
1	B	117	ASN
1	B	170	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	48,58,58	1.20	7 (14%)	54,89,89	2.09	8 (14%)
2	RMA	A	601	2	14,15,15	3.16	3 (21%)	15,20,20	10.83	6 (40%)
2	FAD	B	600	1,2	48,58,58	1.18	6 (12%)	54,89,89	2.15	7 (12%)
2	RMA	B	601	2	14,15,15	3.20	3 (21%)	15,20,20	10.73	7 (46%)

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	-	0/30/50/50	0/6/6/6
2	RMA	A	601	2	-	0/5/16/16	0/2/2/2
2	FAD	B	600	1,2	-	0/30/50/50	0/6/6/6
2	RMA	B	601	2	-	0/5/16/16	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	RMA	C10-N10	-8.89	1.29	1.46
2	A	601	RMA	C10-N10	-8.84	1.29	1.46
2	B	600	FAD	C5X-N5	2.03	1.38	1.35
2	A	600	FAD	C10-N1	2.21	1.39	1.35
2	A	600	FAD	C1'-N10	2.28	1.50	1.48
2	A	600	FAD	C5X-N5	2.30	1.39	1.35
2	A	600	FAD	C2A-N1A	2.39	1.38	1.33
2	B	600	FAD	C2A-N1A	2.40	1.38	1.33
2	B	600	FAD	C4-N3	2.52	1.37	1.33
2	B	600	FAD	C1'-N10	2.62	1.51	1.48
2	A	600	FAD	C4-N3	2.77	1.38	1.33
2	B	600	FAD	C2A-N3A	2.99	1.37	1.32
2	A	600	FAD	C2A-N3A	3.10	1.37	1.32
2	B	600	FAD	C4X-N5	3.56	1.38	1.33
2	A	600	FAD	C4X-N5	3.82	1.39	1.33
2	A	601	RMA	C12-C13	5.29	1.30	1.17
2	A	601	RMA	C11-C12	5.32	1.54	1.47
2	B	601	RMA	C12-C13	5.37	1.30	1.17
2	B	601	RMA	C11-C12	5.48	1.54	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	RMA	C11-C12-C13	-40.51	125.19	177.76
2	B	601	RMA	C11-C12-C13	-40.07	125.76	177.76
2	A	600	FAD	N3A-C2A-N1A	-11.64	119.98	128.89
2	B	600	FAD	N3A-C2A-N1A	-11.59	120.02	128.89
2	A	600	FAD	C1B-N9A-C4A	-2.97	122.46	126.94
2	B	600	FAD	C9A-C5X-N5	-2.94	118.00	122.36
2	B	600	FAD	C4X-C10-N10	-2.80	118.87	120.52
2	B	600	FAD	C4X-C4-N3	-2.71	119.89	123.59
2	B	601	RMA	C6-C7-C8	-2.68	117.53	121.02
2	B	600	FAD	C1B-N9A-C4A	-2.63	122.97	126.94
2	A	601	RMA	C6-C7-C8	-2.52	117.75	121.02
2	A	600	FAD	C4X-C4-N3	-2.44	120.25	123.59
2	A	600	FAD	C9A-C5X-N5	-2.37	118.85	122.36
2	B	601	RMA	C5-C4-C3	-2.13	117.59	120.90
2	A	600	FAD	C4X-C10-N10	-2.05	119.31	120.52
2	A	600	FAD	C4A-C5A-N7A	-2.03	107.61	109.48
2	A	600	FAD	C4-C4X-N5	2.06	121.22	118.72
2	B	600	FAD	C4X-N5-C5X	2.16	119.25	116.76
2	B	601	RMA	C10-N10-C9	2.71	121.16	112.80
2	A	601	RMA	C10-N10-C9	2.80	121.41	112.80
2	B	601	RMA	C11-N10-C9	3.59	118.57	113.65
2	A	601	RMA	C11-N10-C9	3.63	118.63	113.65
2	B	601	RMA	C12-C11-N10	5.23	121.39	111.90
2	A	601	RMA	C12-C11-N10	5.40	121.69	111.90
2	A	600	FAD	C4-N3-C2	5.67	120.15	115.25
2	B	600	FAD	C4-N3-C2	6.44	120.81	115.25
2	A	601	RMA	C10-N10-C11	6.94	119.96	110.15
2	B	601	RMA	C10-N10-C11	7.16	120.27	110.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	2	0
2	A	601	RMA	2	0
2	B	600	FAD	1	0
2	B	601	RMA	1	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, 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	499/520 (95%)	1.86	153 (30%)	1	1	28, 37, 55, 78	0
1	B	494/520 (95%)	1.80	155 (31%)	1	1	28, 37, 52, 72	0
All	All	993/1040 (95%)	1.83	308 (31%)	1	1	28, 37, 53, 78	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	ILE	11.8
1	A	499	THR	11.2
1	A	500	THR	10.3
1	B	496	ILE	8.9
1	A	107	TRP	8.8
1	A	103	PHE	8.5
1	A	496	ILE	8.3
1	A	479	THR	8.3
1	A	498	LEU	8.1
1	A	497	GLY	7.7
1	B	494	ARG	7.7
1	A	480	THR	7.2
1	A	478	THR	7.1
1	B	495	LEU	6.9
1	A	354	ARG	6.7
1	B	107	TRP	6.7
1	B	103	PHE	6.6
1	B	119	TRP	6.6
1	B	157	TRP	6.6
1	A	252	HIS	6.4
1	B	482	LEU	6.3
1	B	492	LEU	6.1
1	A	460	ASP	6.0
1	A	3	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	245	VAL	5.8
1	B	93	LYS	5.8
1	B	242	ARG	5.7
1	B	481	PHE	5.6
1	A	105	PRO	5.4
1	B	252	HIS	5.4
1	A	106	VAL	5.3
1	B	243	GLU	5.2
1	A	242	ARG	5.2
1	A	494	ARG	5.2
1	B	319	GLY	5.2
1	A	102	PRO	5.1
1	B	475	GLN	4.9
1	B	3	ASN	4.8
1	B	89	ILE	4.8
1	A	93	LYS	4.7
1	A	29	ASN	4.7
1	A	243	GLU	4.7
1	B	95	LYS	4.6
1	B	241	THR	4.6
1	A	78	GLU	4.5
1	A	470	VAL	4.4
1	B	110	ILE	4.4
1	A	251	ASN	4.4
1	B	92	VAL	4.3
1	B	470	VAL	4.3
1	A	246	LEU	4.3
1	A	482	LEU	4.3
1	B	244	ASN	4.3
1	A	493	LEU	4.2
1	A	155	LEU	4.2
1	A	454	MET	4.2
1	A	486	LEU	4.2
1	A	159	GLU	4.1
1	A	227	ASP	4.1
1	A	119	TRP	4.1
1	A	110	ILE	4.1
1	B	254	MET	4.1
1	B	85	VAL	4.1
1	B	460	ASP	4.1
1	B	303	GLU	4.0
1	A	321	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	89	ILE	4.0
1	A	459	GLU	4.0
1	B	491	GLY	3.9
1	A	223	ASP	3.9
1	A	163	GLN	3.8
1	A	4	LYS	3.8
1	B	155	LEU	3.8
1	A	472	VAL	3.8
1	B	172	CYS	3.8
1	B	354	ARG	3.8
1	A	154	LYS	3.8
1	B	474	ALA	3.8
1	A	224	LEU	3.8
1	B	490	PRO	3.8
1	A	226	GLY	3.8
1	A	254	MET	3.7
1	A	481	PHE	3.7
1	A	118	PHE	3.7
1	B	4	LYS	3.7
1	B	485	HIS	3.7
1	A	157	TRP	3.7
1	B	225	LEU	3.7
1	A	477	ILE	3.7
1	B	111	THR	3.7
1	A	302	LYS	3.7
1	B	49	GLN	3.7
1	B	227	ASP	3.6
1	B	414	LEU	3.6
1	B	31	VAL	3.6
1	A	142	GLU	3.6
1	A	109	PRO	3.6
1	B	321	GLU	3.6
1	A	49	GLN	3.6
1	A	308	LYS	3.6
1	B	5	CYS	3.5
1	B	455	GLY	3.5
1	A	474	ALA	3.5
1	A	458	PRO	3.5
1	A	44	TYR	3.5
1	A	413	VAL	3.4
1	A	489	VAL	3.4
1	A	250	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	112	TYR	3.4
1	A	483	GLU	3.4
1	A	141	GLU	3.4
1	B	246	LEU	3.4
1	B	97	TYR	3.4
1	A	100	ARG	3.4
1	B	88	LEU	3.3
1	A	465	SER	3.3
1	A	72	ALA	3.3
1	B	493	LEU	3.3
1	A	111	THR	3.3
1	B	468	GLU	3.3
1	A	247	VAL	3.3
1	B	476	PRO	3.3
1	B	459	GLU	3.2
1	B	122	MET	3.2
1	B	478	THR	3.2
1	B	44	TYR	3.2
1	A	156	CYS	3.2
1	B	309	LYS	3.2
1	B	224	LEU	3.2
1	A	112	TYR	3.2
1	B	245	VAL	3.1
1	B	318	ASP	3.1
1	A	485	HIS	3.1
1	A	129	ILE	3.1
1	A	468	GLU	3.1
1	A	97	TYR	3.1
1	A	225	LEU	3.1
1	A	495	LEU	3.1
1	B	113	LEU	3.0
1	B	486	LEU	3.0
1	A	484	ARG	3.0
1	A	135	TRP	3.0
1	B	453	ALA	3.0
1	A	462	ILE	3.0
1	B	118	PHE	3.0
1	B	479	THR	2.9
1	B	374	SER	2.9
1	A	471	ASP	2.9
1	B	251	ASN	2.9
1	B	135	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	153	ASP	2.9
1	B	472	VAL	2.9
1	B	338	ALA	2.8
1	A	362	LYS	2.8
1	B	473	PRO	2.8
1	A	158	THR	2.8
1	B	160	SER	2.8
1	B	484	ARG	2.8
1	A	172	CYS	2.8
1	B	163	GLN	2.8
1	A	37	ASP	2.8
1	A	92	VAL	2.8
1	B	141	GLU	2.8
1	B	71	LEU	2.8
1	A	244	ASN	2.8
1	B	164	LEU	2.7
1	B	29	ASN	2.7
1	B	106	VAL	2.7
1	B	158	THR	2.7
1	B	102	PRO	2.7
1	A	379	GLU	2.7
1	A	328	LEU	2.7
1	A	467	PRO	2.7
1	A	414	LEU	2.7
1	B	22	LEU	2.7
1	B	462	ILE	2.6
1	B	250	LEU	2.6
1	B	336	ASN	2.6
1	B	27	GLY	2.6
1	B	61	VAL	2.6
1	B	183	LEU	2.6
1	A	324	VAL	2.6
1	B	147	THR	2.6
1	A	69	LEU	2.6
1	B	379	GLU	2.6
1	A	455	GLY	2.6
1	B	480	THR	2.6
1	A	457	ILE	2.6
1	B	280	MET	2.6
1	B	457	ILE	2.6
1	A	372	LEU	2.6
1	A	451	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	456	LYS	2.5
1	A	463	TRP	2.5
1	B	129	ILE	2.5
1	B	259	TYR	2.5
1	B	355	LEU	2.5
1	B	182	ALA	2.5
1	A	280	MET	2.5
1	A	88	LEU	2.5
1	A	139	LEU	2.5
1	B	364	LEU	2.5
1	B	80	TYR	2.5
1	A	475	GLN	2.5
1	B	156	CYS	2.5
1	B	78	GLU	2.5
1	B	108	ASN	2.5
1	B	100	ARG	2.5
1	A	311	TYR	2.4
1	A	349	ALA	2.5
1	A	82	VAL	2.4
1	B	175	ALA	2.4
1	B	448	ARG	2.4
1	B	94	GLY	2.4
1	B	299	VAL	2.4
1	A	25	ASP	2.4
1	A	20	ALA	2.4
1	B	424	ALA	2.4
1	B	77	LEU	2.4
1	A	488	SER	2.4
1	A	303	GLU	2.4
1	A	275	ASN	2.4
1	B	320	GLU	2.4
1	A	7	VAL	2.4
1	A	199	ILE	2.3
1	B	322	ALA	2.3
1	B	442	ALA	2.3
1	A	94	GLY	2.3
1	B	489	VAL	2.3
1	A	113	LEU	2.3
1	A	317	ILE	2.3
1	B	264	ILE	2.3
1	A	412	ARG	2.3
1	A	264	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	331	THR	2.3
1	A	146	MET	2.3
1	B	51	VAL	2.3
1	B	26	SER	2.3
1	B	306	TRP	2.3
1	A	33	LEU	2.3
1	A	137	ALA	2.3
1	B	151	LEU	2.3
1	B	221	ILE	2.3
1	A	117	ASN	2.2
1	A	432	TRP	2.2
1	B	312	CYS	2.2
1	A	257	ALA	2.2
1	A	356	THR	2.2
1	A	57	GLY	2.2
1	B	23	LEU	2.2
1	A	450	ILE	2.2
1	B	199	ILE	2.2
1	A	143	TRP	2.2
1	A	337	TYR	2.2
1	B	159	GLU	2.2
1	A	193	GLY	2.2
1	B	226	GLY	2.2
1	A	24	HIS	2.2
1	A	104	PRO	2.2
1	A	490	PRO	2.2
1	B	416	GLN	2.2
1	B	187	TRP	2.2
1	A	136	LYS	2.2
1	B	154	LYS	2.2
1	A	201	THR	2.2
1	A	255	TYR	2.2
1	A	431	HIS	2.2
1	B	463	TRP	2.1
1	B	334	GLU	2.1
1	A	27	GLY	2.1
1	A	183	LEU	2.1
1	A	375	LEU	2.1
1	A	407	LEU	2.1
1	B	397	CYS	2.1
1	B	137	ALA	2.1
1	B	450	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	62	GLY	2.1
1	A	115	HIS	2.1
1	B	257	ALA	2.1
1	A	122	MET	2.1
1	B	185	PHE	2.1
1	B	124	ASP	2.1
1	B	487	PRO	2.1
1	A	352	LEU	2.1
1	A	461	GLU	2.1
1	B	358	GLU	2.1
1	B	82	VAL	2.1
1	B	43	THR	2.1
1	B	188	TYR	2.1
1	B	447	ALA	2.1
1	B	305	PHE	2.1
1	A	23	LEU	2.1
1	B	75	LEU	2.1
1	B	143	TRP	2.1
1	B	461	GLU	2.1
1	B	174	THR	2.0
1	B	28	LEU	2.0
1	A	26	SER	2.0
1	B	249	THR	2.0
1	B	286	ILE	2.0
1	B	317	ILE	2.0
1	A	114	ASP	2.0
1	A	318	ASP	2.0
1	B	54	VAL	2.0
1	A	369	ALA	2.0
1	B	161	ALA	2.0
1	A	492	LEU	2.0
1	A	6	ASP	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

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
2	RMA	A	601	14/14	0.76	0.20	2.65	37,43,44,44	0
2	RMA	B	601	14/14	0.80	0.20	2.13	38,42,43,44	0
2	FAD	A	600	53/53	0.92	0.13	-0.80	29,31,33,33	0
2	FAD	B	600	53/53	0.94	0.13	-1.25	28,31,33,33	0

6.5 Other polymers

There are no such residues in this entry.