



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:27 pm BST

PDB ID : 6ABU
Title : Rat Xanthine oxidoreductase, NAD bound form
Authors : Okamoto, K.; Kawaguchi, Y.
Deposited on : 2018-07-24
Resolution : 1.77 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

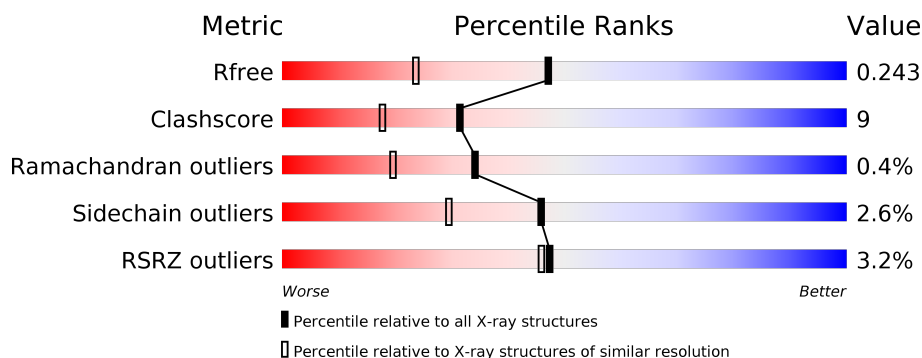
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 respectively. 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	1331	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	1331	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>

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
5	FES	B	3001	-	-	X	-

2 Entry composition [i](#)

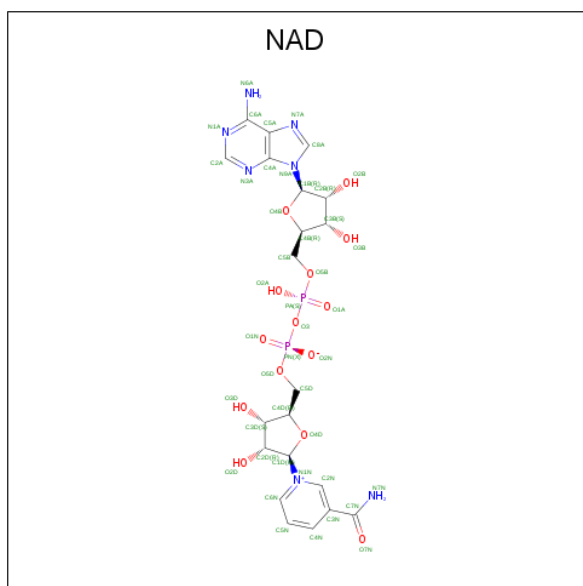
There are 7 unique types of molecules in this entry. The entry contains 21843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

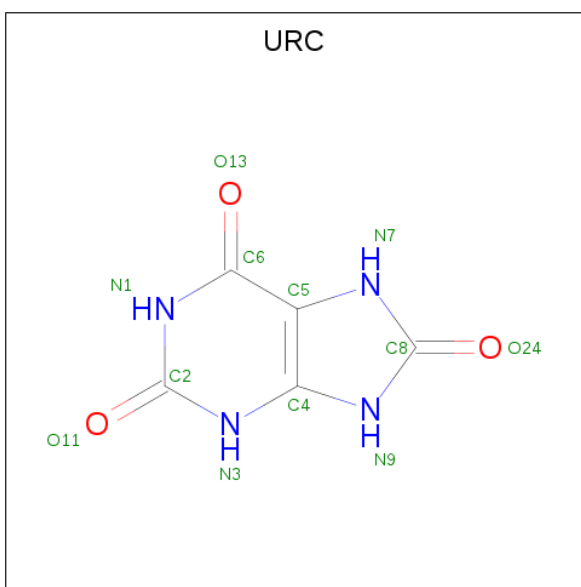
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1304	Total	C	N	O	S	0	0	0
			10076	6383	1735	1893	65			
1	B	1291	Total	C	N	O	S	0	0	0
			9971	6320	1716	1871	64			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



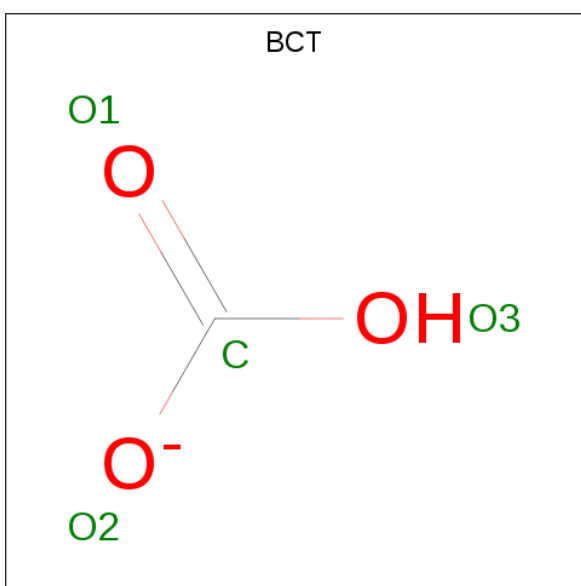
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).



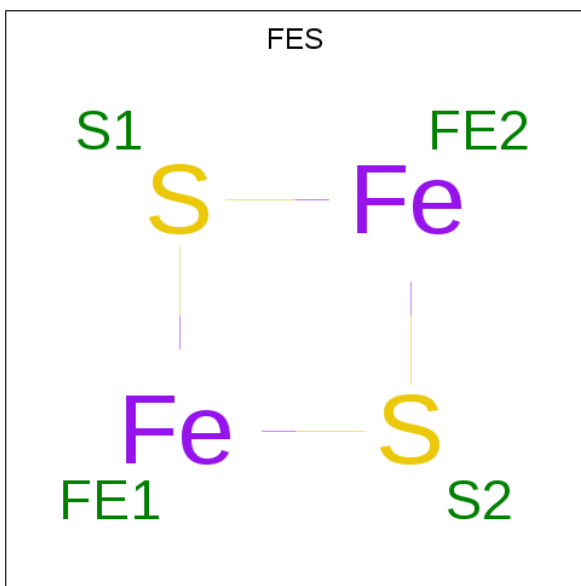
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	5	4	3		
3	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3^-).



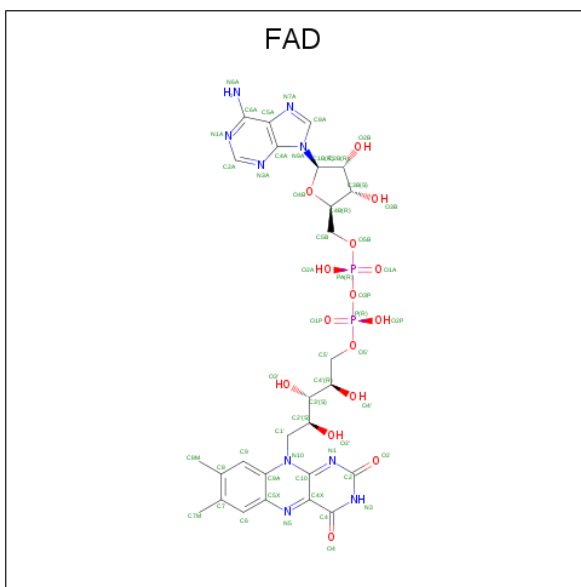
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	B	1	Total	Fe	S	0	0
			4	2	2		
5	B	1	Total	Fe	S	0	0
			4	2	2		

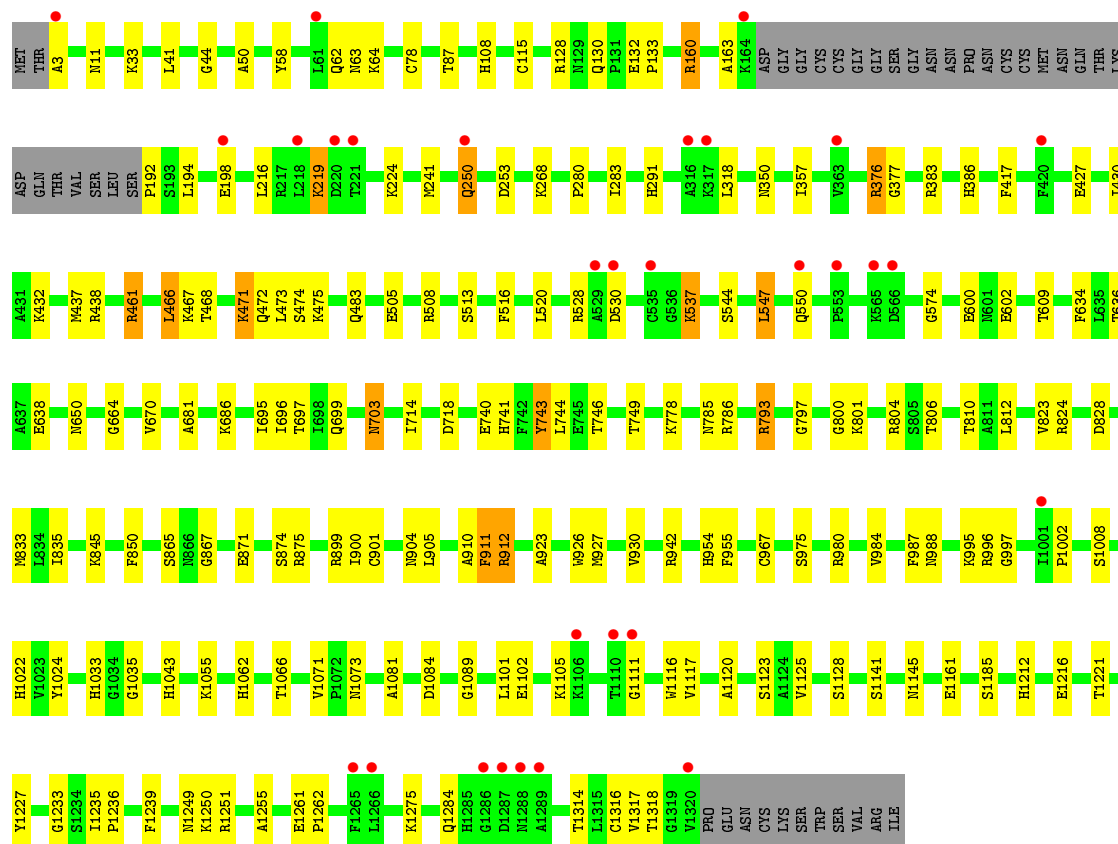
- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	727	Total O 727 727	0	0
7	B	865	Total O 865 865	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.35Å 137.66Å 221.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.57 – 1.77 30.56 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.57-1.77) 99.9 (30.56-1.77)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.199 , 0.237 0.207 , 0.243	Depositor DCC
R_{free} test set	14567 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21843	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: BCT, FAD, FES, NAD, URC

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	0.57	0/10289	0.73	3/13923 (0.0%)
1	B	0.60	1/10181 (0.0%)	0.74	4/13777 (0.0%)
All	All	0.59	1/20470 (0.0%)	0.73	7/27700 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	7
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	602	GLU	CD-OE1	5.39	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	793	ARG	NE-CZ-NH1	14.84	127.72	120.30
1	A	793	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	B	899	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	B	793	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	899	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	B	160	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	793	ARG	CD-NE-CZ	5.12	130.76	123.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	ARG	Sidechain
1	A	1305	ARG	Sidechain
1	A	148	ARG	Sidechain
1	A	160	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	461	ARG	Sidechain
1	A	804	ARG	Sidechain
1	A	989	ARG	Sidechain
1	B	128	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	376	ARG	Sidechain
1	B	383	ARG	Sidechain
1	B	461	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	804	ARG	Sidechain

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	10076	0	10079	190	0
1	B	9971	0	9982	177	0
2	A	27	0	12	0	0
2	B	23	0	12	0	0
3	A	12	0	4	0	0
3	B	12	0	4	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	8	0	0	1	0
5	B	8	0	0	2	0
6	A	53	0	31	1	0
6	B	53	0	31	0	0
7	A	727	0	0	101	1
7	B	865	0	0	104	1
All	All	21843	0	20155	364	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 9.

All (364) 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:744:LEU:HG	7:B:3832:HOH:O	1.24	1.30
1:B:810:THR:HB	7:B:3787:HOH:O	1.30	1.28
1:B:1089:GLY:HA3	7:B:3635:HOH:O	1.03	1.20
1:A:971:CYS:SG	7:A:1958:HOH:O	1.98	1.17
1:B:812:LEU:HB2	7:B:3662:HOH:O	1.00	1.17
1:A:967:CYS:SG	7:A:1529:HOH:O	2.06	1.12
1:A:1089:GLY:HA3	7:A:1678:HOH:O	0.94	1.09
1:A:32:ARG:HH21	1:A:32:ARG:HG2	1.20	1.03
1:B:927:MET:SD	7:B:3345:HOH:O	2.16	1.01
1:B:967:CYS:SG	7:B:3129:HOH:O	2.19	0.99
1:A:123:MET:SD	7:A:2129:HOH:O	2.23	0.97
1:B:801:LYS:N	7:B:3104:HOH:O	1.98	0.95
1:B:1081:ALA:HB3	7:B:3678:HOH:O	1.67	0.94
1:A:812:LEU:HD21	1:A:823:VAL:O	1.70	0.89
1:A:821:ARG:HD3	7:A:1786:HOH:O	1.74	0.88
1:A:151:GLY:O	7:A:1501:HOH:O	1.90	0.87
1:B:357:ILE:CD1	1:B:430:ILE:HG23	2.05	0.85
1:B:743:TYR:OH	7:B:3101:HOH:O	1.94	0.85
1:B:1120:ALA:O	7:B:3102:HOH:O	1.95	0.84
1:A:644:ASN:ND2	7:A:1504:HOH:O	2.08	0.83
1:B:11:ASN:HD21	1:B:87:THR:H	1.26	0.83
1:B:417:PHE:CE2	7:B:3141:HOH:O	2.31	0.83
1:B:996:ARG:O	7:B:3103:HOH:O	1.95	0.83
1:A:532:GLU:HB2	7:A:1585:HOH:O	1.78	0.82
1:B:695:ILE:H	1:B:904:ASN:HD22	1.24	0.82
1:A:304:LEU:HD22	1:A:304:LEU:H	1.45	0.82
1:B:130:GLN:HE21	1:B:132:GLU:H	1.28	0.81
1:A:1144:THR:HG21	7:A:2086:HOH:O	1.80	0.80
1:A:227:ARG:HA	7:A:1588:HOH:O	1.80	0.80
1:A:483:GLN:HE22	1:A:1311:GLN:HE22	1.26	0.80
1:B:357:ILE:HD12	1:B:430:ILE:HG23	1.63	0.78
1:A:695:ILE:H	1:A:904:ASN:HD22	1.29	0.78
1:B:954:HIS:CD2	7:B:3424:HOH:O	2.36	0.78
1:B:746:THR:O	7:B:3107:HOH:O	2.02	0.78
1:A:365:MET:HE2	1:A:464:SER:HB2	1.65	0.78
1:A:839:ARG:CZ	7:A:1514:HOH:O	2.30	0.77
1:B:1084:ASP:O	7:B:3106:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HB2	7:A:1786:HOH:O	1.83	0.77
1:B:115:CYS:HB3	1:B:744:LEU:HD22	1.67	0.77
1:A:891:ILE:HG23	7:A:1523:HOH:O	1.84	0.76
1:A:469:THR:CG2	7:A:2066:HOH:O	2.32	0.76
1:A:1239:PHE:CE1	7:A:2127:HOH:O	2.37	0.76
1:A:32:ARG:HG2	1:A:32:ARG:NH2	1.94	0.76
1:B:1251:ARG:NH2	7:B:3116:HOH:O	2.18	0.76
1:A:1028:SER:O	7:A:1502:HOH:O	2.03	0.75
1:A:602:GLU:N	7:A:1505:HOH:O	2.19	0.75
1:A:603:LEU:HD11	7:A:1786:HOH:O	1.87	0.75
1:B:714:ILE:HG21	7:B:3424:HOH:O	1.86	0.74
1:A:126:LEU:HG	7:A:2029:HOH:O	1.88	0.74
1:A:812:LEU:HB2	7:A:2022:HOH:O	1.86	0.74
1:B:696:ILE:HA	7:B:3165:HOH:O	1.88	0.73
1:B:828:ASP:HA	7:B:3335:HOH:O	1.88	0.73
1:A:115:CYS:HB3	1:A:744:LEU:HD22	1.71	0.73
1:A:839:ARG:NH2	7:A:1514:HOH:O	2.22	0.73
1:B:468:THR:HG22	7:B:3113:HOH:O	1.88	0.72
1:A:1308:CYS:SG	7:A:1513:HOH:O	2.48	0.71
1:B:1236:PRO:O	7:B:3108:HOH:O	2.08	0.71
1:A:236:ILE:HG12	7:A:1588:HOH:O	1.90	0.71
1:A:32:ARG:NH2	7:A:1518:HOH:O	2.23	0.71
1:A:73:CYS:SG	7:A:1646:HOH:O	2.49	0.71
1:B:812:LEU:HD21	1:B:823:VAL:O	1.90	0.71
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.88	0.71
1:B:1066:THR:O	7:B:3109:HOH:O	2.09	0.70
1:B:78:CYS:SG	7:B:3872:HOH:O	2.48	0.70
1:A:533:ASP:HB3	7:A:2150:HOH:O	1.91	0.70
1:A:601:ASN:OD1	7:A:1505:HOH:O	2.08	0.70
1:B:1250:LYS:HE2	7:B:3116:HOH:O	1.92	0.70
1:A:603:LEU:CD1	7:A:1786:HOH:O	2.40	0.70
1:A:902:LYS:O	7:A:1506:HOH:O	2.09	0.69
1:A:1057:PRO:O	7:A:1507:HOH:O	2.11	0.69
1:A:1287:ASP:O	1:A:1288:ASN:HB2	1.92	0.69
1:B:749:THR:HG22	1:B:812:LEU:CD2	2.23	0.69
1:B:600:GLU:OE2	7:B:3110:HOH:O	2.11	0.68
1:B:1125:VAL:HG23	7:B:3102:HOH:O	1.95	0.67
1:B:115:CYS:HB3	1:B:744:LEU:CD2	2.25	0.67
1:B:812:LEU:CD1	7:B:3662:HOH:O	2.41	0.67
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.92	0.67
1:A:793:ARG:NE	7:A:1503:HOH:O	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:THR:O	7:B:3113:HOH:O	2.13	0.67
1:A:610:SER:OG	7:A:1508:HOH:O	2.13	0.67
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.77	0.67
1:B:995:LYS:HB3	7:B:3103:HOH:O	1.93	0.66
1:B:988:ASN:OD1	7:B:3114:HOH:O	2.14	0.66
1:A:778:LYS:HE3	7:A:1780:HOH:O	1.95	0.66
1:B:513:SER:HA	7:B:3827:HOH:O	1.95	0.66
1:B:793:ARG:HD2	7:B:3273:HOH:O	1.96	0.66
1:A:1061:ILE:N	7:A:1507:HOH:O	2.27	0.66
1:B:1250:LYS:HA	7:B:3815:HOH:O	1.96	0.66
1:B:41:LEU:HD21	7:B:3335:HOH:O	1.96	0.66
1:B:697:THR:O	7:B:3112:HOH:O	2.13	0.66
1:B:386:HIS:HE1	7:B:3831:HOH:O	1.79	0.65
1:A:1144:THR:HG23	1:A:1146:SER:OG	1.96	0.65
1:B:812:LEU:HD13	7:B:3662:HOH:O	1.97	0.65
1:A:480:GLU:OE2	7:A:1512:HOH:O	2.15	0.65
1:A:636:THR:O	7:A:1509:HOH:O	2.14	0.64
1:A:706:SER:O	7:A:1506:HOH:O	2.13	0.64
1:A:1226:THR:OG1	7:A:1510:HOH:O	2.14	0.64
1:A:936:LEU:O	7:A:1511:HOH:O	2.14	0.64
1:B:530:ASP:N	7:B:3111:HOH:O	2.12	0.64
1:B:216:LEU:O	1:B:219:LYS:HG3	1.97	0.64
1:B:749:THR:HG22	1:B:812:LEU:HD23	1.78	0.64
1:A:1220:HIS:HD2	7:A:1581:HOH:O	1.80	0.64
1:A:612:ARG:N	7:A:1508:HOH:O	2.27	0.63
1:B:699:GLN:HE21	1:B:703:ASN:HD22	1.47	0.63
1:A:1206:PHE:HE2	7:A:1521:HOH:O	1.81	0.63
1:A:1099:LYS:HG2	7:A:2092:HOH:O	1.99	0.63
1:B:867:GLY:N	7:B:3115:HOH:O	2.32	0.62
1:A:365:MET:CE	1:A:464:SER:HB2	2.30	0.62
1:A:469:THR:HG22	7:A:2066:HOH:O	1.97	0.62
1:A:469:THR:HG23	7:A:2066:HOH:O	1.99	0.61
1:A:931:ALA:HB1	7:A:1511:HOH:O	2.00	0.61
1:A:599:TYR:HB2	7:A:1505:HOH:O	1.99	0.61
1:B:1123:SER:HB2	7:B:3102:HOH:O	2.01	0.60
1:A:778:LYS:CE	7:A:1780:HOH:O	2.48	0.60
1:B:44:GLY:N	7:B:3128:HOH:O	2.34	0.59
1:B:609:THR:HG21	7:B:3725:HOH:O	2.01	0.59
1:A:598:ARG:NH1	7:A:1518:HOH:O	2.36	0.59
1:B:806:THR:O	1:B:810:THR:HG23	2.02	0.59
1:A:304:LEU:HD21	1:A:345:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:HIS:HE1	1:A:1043:HIS:HD2	1.50	0.59
1:B:1161:GLU:HG3	7:B:3125:HOH:O	2.01	0.59
1:B:1314:THR:O	1:B:1318:THR:HB	2.03	0.59
1:B:1033:HIS:HD1	1:B:1035:GLY:H	1.49	0.58
1:B:437:MET:C	7:B:3141:HOH:O	2.42	0.58
1:B:357:ILE:HD13	1:B:430:ILE:HG23	1.85	0.58
1:B:744:LEU:CG	7:B:3832:HOH:O	2.06	0.58
1:A:751:ALA:HB3	1:A:812:LEU:HD23	1.85	0.58
1:A:304:LEU:HD23	1:A:342:LYS:HA	1.85	0.57
1:A:819:THR:HB	7:A:1786:HOH:O	2.04	0.57
1:A:1073:ASN:HD21	1:B:1024:TYR:HA	1.68	0.57
1:A:365:MET:HE3	1:A:386:HIS:N	2.19	0.57
1:A:749:THR:O	1:A:812:LEU:HD13	2.05	0.57
1:A:1024:TYR:HA	1:B:1073:ASN:HD21	1.69	0.57
1:B:130:GLN:HE21	1:B:132:GLU:N	2.00	0.57
1:B:130:GLN:NE2	1:B:132:GLU:H	1.99	0.57
1:A:1236:PRO:HG2	7:A:2127:HOH:O	2.05	0.57
1:B:192:PRO:CB	7:B:3818:HOH:O	2.53	0.57
1:B:741:HIS:HD2	7:B:3392:HOH:O	1.88	0.56
1:B:871:GLU:CD	7:B:3203:HOH:O	2.43	0.56
1:A:127:LEU:HD23	7:A:2029:HOH:O	2.05	0.56
1:A:236:ILE:HA	7:A:1588:HOH:O	2.05	0.56
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.05	0.56
1:A:600:GLU:HG3	7:A:2139:HOH:O	2.05	0.56
1:A:1144:THR:CG2	7:A:2086:HOH:O	2.46	0.56
1:B:686:LYS:NZ	7:B:3133:HOH:O	2.37	0.56
1:A:1055:LYS:NZ	7:A:1539:HOH:O	2.38	0.55
1:A:1178:ILE:CG2	1:A:1180:MET:HE2	2.36	0.55
1:A:1182:VAL:HA	7:A:1519:HOH:O	2.04	0.55
1:B:1275:LYS:HE3	7:B:3539:HOH:O	2.06	0.55
1:A:1033:HIS:CE1	1:A:1043:HIS:HD2	2.24	0.55
1:B:1081:ALA:CB	7:B:3321:HOH:O	2.53	0.55
1:B:253:ASP:HB2	7:B:3496:HOH:O	2.05	0.55
1:B:942:ARG:HA	7:B:3345:HOH:O	2.06	0.55
1:A:345:ALA:HB1	6:A:1406:FAD:H4'	1.88	0.55
1:B:1102:GLU:HB2	7:B:3876:HOH:O	2.07	0.55
1:B:664:GLY:HA2	7:B:3725:HOH:O	2.07	0.54
1:A:812:LEU:HD11	1:A:824:ARG:HA	1.89	0.54
1:B:350:ASN:HB2	7:B:3135:HOH:O	2.06	0.54
1:A:337:ALA:HA	1:A:428:ASP:OD1	2.08	0.54
1:A:975:SER:O	1:A:980:ARG:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LYS:HE3	7:B:3565:HOH:O	2.08	0.54
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.55	0.54
1:B:865:SER:O	7:B:3115:HOH:O	2.17	0.54
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.55	0.54
1:A:1027:GLY:C	7:A:1502:HOH:O	2.46	0.54
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	1.89	0.53
1:B:1125:VAL:N	7:B:3102:HOH:O	2.41	0.53
1:B:1212:HIS:HB3	7:B:3738:HOH:O	2.06	0.53
1:A:892:PRO:HD2	7:A:1523:HOH:O	2.08	0.53
1:B:955:PHE:HB3	7:B:3424:HOH:O	2.08	0.53
1:B:508:ARG:NH1	1:B:1316:CYS:O	2.37	0.53
1:B:1022:HIS:HD2	1:B:1128:SER:OG	1.92	0.53
1:A:695:ILE:H	1:A:904:ASN:ND2	2.03	0.52
1:A:900:ILE:N	1:A:900:ILE:HD12	2.24	0.52
5:A:1404:FES:S2	7:A:1646:HOH:O	2.60	0.52
1:A:165:ASP:O	1:A:166:GLY:C	2.48	0.52
1:A:1028:SER:N	7:A:1502:HOH:O	2.43	0.52
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.56	0.52
1:B:749:THR:HG22	1:B:812:LEU:HD22	1.92	0.51
1:A:718:ASP:H	1:A:893:ASN:HD22	1.58	0.51
1:B:108:HIS:HE1	1:B:194:LEU:O	1.92	0.51
1:A:1328:SER:HB2	7:A:1581:HOH:O	2.09	0.51
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.93	0.51
1:A:1141:SER:HB3	1:A:1144:THR:HG22	1.91	0.51
1:B:544:SER:HA	1:B:547:LEU:HD22	1.93	0.51
1:B:812:LEU:CB	7:B:3662:HOH:O	1.87	0.51
1:B:427:GLU:OE2	1:B:1233:GLY:HA3	2.10	0.51
1:A:895:ARG:HD2	7:A:1605:HOH:O	2.10	0.51
1:B:386:HIS:HB2	1:B:461:ARG:HH22	1.75	0.51
1:B:472:GLN:HG2	7:B:3113:HOH:O	2.09	0.51
1:A:749:THR:O	1:A:812:LEU:CD1	2.59	0.51
1:B:437:MET:N	7:B:3141:HOH:O	2.44	0.50
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.93	0.50
1:B:133:PRO:O	1:B:163:ALA:HA	2.11	0.50
1:B:987:PHE:HB3	7:B:3114:HOH:O	2.11	0.50
1:A:108:HIS:HE1	1:A:194:LEU:O	1.95	0.50
1:A:759:GLU:OE2	1:B:1062:HIS:HE1	1.95	0.50
1:B:62:GLN:NE2	1:B:64:LYS:HE2	2.27	0.50
1:B:718:ASP:OD2	7:B:3117:HOH:O	2.19	0.50
1:B:318:LEU:O	7:B:3118:HOH:O	2.19	0.50
1:B:744:LEU:HD13	5:B:3001:FES:S1	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:CYS:N	7:B:3115:HOH:O	2.44	0.49
1:A:1328:SER:CB	7:A:1581:HOH:O	2.60	0.49
1:A:812:LEU:CB	7:A:2022:HOH:O	2.55	0.49
1:B:996:ARG:HB3	7:B:3125:HOH:O	2.12	0.49
1:B:1055:LYS:HD2	7:B:3926:HOH:O	2.12	0.49
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.13	0.49
1:A:446:ILE:HD12	1:A:534:MET:HB2	1.94	0.49
1:B:1123:SER:C	7:B:3102:HOH:O	2.50	0.49
1:A:523:LEU:HB3	7:A:2138:HOH:O	2.11	0.49
1:A:1058:THR:C	7:A:1507:HOH:O	2.50	0.49
1:A:477:TRP:CD1	1:A:523:LEU:HD12	2.47	0.48
1:A:895:ARG:CD	7:A:2021:HOH:O	2.60	0.48
1:B:638:GLU:CB	7:B:3893:HOH:O	2.60	0.48
1:A:1033:HIS:CE1	1:A:1043:HIS:CD2	3.01	0.48
1:A:108:HIS:HD2	7:A:1974:HOH:O	1.95	0.48
1:A:1212:HIS:HB3	7:A:1581:HOH:O	2.11	0.48
1:A:272:MET:HB2	7:A:1719:HOH:O	2.13	0.48
1:B:695:ILE:H	1:B:904:ASN:ND2	2.01	0.48
1:B:975:SER:O	1:B:980:ARG:HD3	2.13	0.48
1:B:984:VAL:O	7:B:3114:HOH:O	2.20	0.48
1:A:1178:ILE:HG21	1:A:1180:MET:HE2	1.93	0.48
1:B:219:LYS:HE2	7:B:3223:HOH:O	2.12	0.48
1:A:1317:VAL:O	1:A:1318:THR:HG22	2.12	0.48
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.96	0.48
1:A:57:LYS:NZ	7:A:1561:HOH:O	2.46	0.48
1:A:1308:CYS:N	7:A:1513:HOH:O	2.46	0.48
1:B:1101:LEU:HD13	7:B:3305:HOH:O	2.14	0.48
1:B:1117:VAL:HG23	7:B:3305:HOH:O	2.13	0.48
1:B:749:THR:O	1:B:812:LEU:HD22	2.13	0.48
1:A:718:ASP:H	1:A:893:ASN:ND2	2.12	0.48
1:B:988:ASN:ND2	7:B:3103:HOH:O	2.44	0.48
1:B:875:ARG:HD2	7:B:3203:HOH:O	2.13	0.47
1:B:291:HIS:CE1	7:B:3683:HOH:O	2.66	0.47
1:B:835:ILE:HG12	7:B:3725:HOH:O	2.14	0.47
1:A:895:ARG:HD3	7:A:2021:HOH:O	2.13	0.47
1:A:751:ALA:H	1:A:812:LEU:HD21	1.79	0.47
1:A:1286:GLY:O	1:A:1287:ASP:HB3	2.15	0.47
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.58	0.47
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.30	0.47
1:B:268:LYS:HG2	7:B:3713:HOH:O	2.14	0.47
1:B:800:GLY:N	7:B:3104:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLU:OE2	1:A:680:ARG:NH1	2.47	0.47
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.31	0.47
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.15	0.47
1:A:751:ALA:HB3	1:A:812:LEU:CD2	2.44	0.47
1:B:812:LEU:HD11	1:B:823:VAL:C	2.35	0.47
1:B:1105:LYS:HG3	1:B:1116:TRP:CZ2	2.50	0.47
1:B:1216:GLU:CG	7:B:3228:HOH:O	2.63	0.47
1:A:640:VAL:HG23	7:A:1509:HOH:O	2.14	0.46
1:B:250:GLN:HG2	7:B:3914:HOH:O	2.15	0.46
1:A:427:GLU:HG2	7:A:2041:HOH:O	2.16	0.46
1:B:1235:ILE:HG13	7:B:3108:HOH:O	2.16	0.46
1:A:941:VAL:CG2	7:A:1511:HOH:O	2.63	0.46
1:A:1203:LEU:C	1:A:1203:LEU:HD23	2.36	0.46
1:A:1317:VAL:HG12	7:A:1524:HOH:O	2.15	0.46
1:B:650:ASN:OD1	1:B:778:LYS:NZ	2.48	0.46
1:A:527:GLY:HA3	7:A:1603:HOH:O	2.15	0.46
1:B:741:HIS:HE1	1:B:910:ALA:O	1.98	0.46
1:B:744:LEU:HD22	5:B:3001:FES:S1	2.56	0.46
1:B:1250:LYS:CE	7:B:3116:HOH:O	2.57	0.46
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.16	0.46
1:B:812:LEU:CD1	1:B:823:VAL:HG12	2.46	0.46
1:B:904:ASN:C	7:B:3165:HOH:O	2.54	0.46
1:B:1033:HIS:NE2	1:B:1043:HIS:HD2	2.14	0.46
1:A:863:HIS:HD2	1:A:897:THR:O	1.99	0.45
1:A:1144:THR:CG2	1:A:1146:SER:OG	2.64	0.45
1:B:386:HIS:CD2	1:B:466:LEU:HD21	2.52	0.45
1:A:1069:ASN:O	1:B:1022:HIS:HE1	1.99	0.45
1:A:216:LEU:O	1:A:219:LYS:HG2	2.16	0.45
1:B:1022:HIS:CD2	1:B:1128:SER:OG	2.69	0.45
1:B:505:GLU:HG3	1:B:1317:VAL:HG22	1.98	0.45
1:A:296:ILE:HD11	1:A:314:GLU:HG2	1.97	0.45
1:A:446:ILE:HD12	1:A:534:MET:CB	2.47	0.45
1:B:376:ARG:HA	7:B:3105:HOH:O	2.16	0.45
1:B:845:LYS:HE2	7:B:3144:HOH:O	2.17	0.44
1:A:304:LEU:HD22	1:A:304:LEU:N	2.23	0.44
1:A:32:ARG:NH2	1:A:32:ARG:CG	2.70	0.44
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.31	0.44
1:A:445:THR:HG22	1:A:446:ILE:H	1.81	0.44
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.44
1:A:227:ARG:HG3	7:A:1588:HOH:O	2.17	0.44
1:A:751:ALA:CB	1:A:812:LEU:CD2	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:PHE:CD2	1:B:930:VAL:HG13	2.52	0.44
1:A:1141:SER:CB	1:A:1144:THR:HG22	2.47	0.44
1:A:381:THR:HG21	7:A:2174:HOH:O	2.17	0.44
1:A:461:ARG:NH2	7:A:1573:HOH:O	2.50	0.44
1:A:538:LEU:HD13	7:A:2138:HOH:O	2.17	0.44
1:B:516:PHE:CZ	1:B:520:LEU:HD11	2.52	0.44
1:A:1264:LEU:HD23	1:A:1264:LEU:C	2.38	0.44
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.81	0.43
1:A:221:THR:HB	7:A:1928:HOH:O	2.16	0.43
1:B:438:ARG:NH1	7:B:3151:HOH:O	2.50	0.43
1:A:701:ALA:HB1	7:A:1506:HOH:O	2.17	0.43
1:A:1304:ILE:O	7:A:1513:HOH:O	2.20	0.43
1:A:555:ALA:O	1:A:1238:GLU:HA	2.17	0.43
1:B:955:PHE:HA	1:B:1145:ASN:OD1	2.19	0.43
1:B:905:LEU:HG	7:B:3165:HOH:O	2.19	0.43
1:B:911:PHE:O	1:B:912:ARG:C	2.56	0.43
1:A:255:LYS:HE2	1:A:274:PHE:CE1	2.54	0.43
1:B:996:ARG:HB2	7:B:3114:HOH:O	2.18	0.43
1:B:695:ILE:HG22	7:B:3112:HOH:O	2.19	0.43
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.65	0.43
1:A:58:TYR:CE2	1:A:219:LYS:HD2	2.54	0.43
1:B:417:PHE:CZ	7:B:3141:HOH:O	2.65	0.43
1:B:50:ALA:N	7:B:3164:HOH:O	2.52	0.43
1:A:1220:HIS:CD2	7:A:1581:HOH:O	2.62	0.43
1:A:911:PHE:O	1:A:912:ARG:C	2.56	0.43
1:B:377:GLY:N	7:B:3105:HOH:O	1.98	0.43
1:A:1024:TYR:O	7:A:1502:HOH:O	2.22	0.43
1:A:1033:HIS:HE1	1:A:1043:HIS:CD2	2.32	0.43
1:A:1080:SER:O	1:A:1258:ALA:HB1	2.18	0.43
1:A:379:ARG:NH1	7:A:1549:HOH:O	2.42	0.42
1:B:1081:ALA:HB1	7:B:3321:HOH:O	2.17	0.42
1:A:145:ASN:ND2	1:A:340:GLN:HE22	2.18	0.42
1:A:153:ARG:HD2	1:A:153:ARG:C	2.40	0.42
1:A:373:LEU:HD12	1:A:373:LEU:N	2.34	0.42
1:B:537:LYS:HB2	1:B:537:LYS:HE2	1.63	0.42
1:A:1213:TYR:N	7:A:1581:HOH:O	2.52	0.42
1:B:1071:VAL:HG22	7:B:3250:HOH:O	2.17	0.42
1:B:812:LEU:HD11	1:B:824:ARG:N	2.34	0.42
1:B:874:SER:HB3	1:B:900:ILE:HG21	2.01	0.42
1:A:1159:CYS:HB3	7:A:1958:HOH:O	2.19	0.42
1:A:115:CYS:HB3	1:A:744:LEU:CD2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:PHE:HA	1:A:1145:ASN:OD1	2.19	0.42
1:B:574:GLY:HA2	1:B:1185:SER:O	2.20	0.42
1:B:812:LEU:HD11	1:B:823:VAL:HG12	2.01	0.42
1:A:1180:MET:HE3	1:A:1195:VAL:HG13	2.00	0.42
1:A:373:LEU:CD1	1:A:373:LEU:N	2.83	0.42
1:A:941:VAL:HG21	7:A:1511:HOH:O	2.19	0.42
1:A:557:VAL:O	7:A:1515:HOH:O	2.22	0.42
1:A:603:LEU:HD12	7:A:1786:HOH:O	2.16	0.42
1:B:785:ASN:OD1	1:B:786:ARG:NH1	2.49	0.42
1:B:900:ILE:HD12	1:B:900:ILE:N	2.35	0.42
1:B:473:LEU:O	1:B:474:SER:HB2	2.20	0.41
1:A:602:GLU:CA	7:A:1505:HOH:O	2.66	0.41
1:A:751:ALA:H	1:A:812:LEU:CD2	2.34	0.41
1:A:519:TYR:O	1:A:523:LEU:HD13	2.21	0.41
1:A:1089:GLY:CA	7:A:1678:HOH:O	1.84	0.41
1:A:396:LEU:HD12	1:A:396:LEU:C	2.39	0.41
1:A:494:GLN:HB2	7:A:1834:HOH:O	2.20	0.41
1:A:1239:PHE:HE2	7:A:1501:HOH:O	2.03	0.41
1:B:1316:CYS:HB2	7:B:3163:HOH:O	2.21	0.41
1:B:471:LYS:O	1:B:475:LYS:HE3	2.21	0.41
1:B:699:GLN:HE21	1:B:703:ASN:ND2	2.16	0.41
1:A:308:GLU:HG3	1:A:333:LEU:HD13	2.03	0.41
1:A:304:LEU:CD2	1:A:342:LYS:HA	2.50	0.41
1:B:634:PHE:CE2	1:B:636:THR:CG2	3.04	0.41
1:B:995:LYS:NZ	1:B:1284:GLN:NE2	2.63	0.41
1:A:497:PRO:HD3	7:A:1562:HOH:O	2.19	0.41
1:B:472:GLN:CG	7:B:3113:HOH:O	2.67	0.41
1:B:1033:HIS:NE2	1:B:1043:HIS:CD2	2.89	0.40
1:A:1034:GLY:HA3	7:A:1725:HOH:O	2.21	0.40
1:A:539:ASP:C	1:A:539:ASP:OD1	2.59	0.40
1:B:58:TYR:OH	1:B:63:ASN:HA	2.20	0.40
1:B:600:GLU:HG2	7:B:3159:HOH:O	2.20	0.40
1:B:696:ILE:C	7:B:3112:HOH:O	2.59	0.40
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.56	0.40
1:B:740:GLU:HG2	1:B:833:MET:HG2	2.03	0.40
1:A:216:LEU:HA	1:A:216:LEU:HD12	1.90	0.40
1:B:997:GLY:N	7:B:3125:HOH:O	2.53	0.40
1:A:320:GLU:O	1:A:327:ARG:NH2	2.54	0.40
1:A:550:GLN:HG2	7:A:2016:HOH:O	2.22	0.40
1:B:3:ALA:HA	7:B:3801:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1925:HOH:O	7:B:3704:HOH:O[2_554]	1.74	0.46

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	1300/1331 (98%)	1252 (96%)	42 (3%)	6 (0%)	29	14
1	B	1287/1331 (97%)	1246 (97%)	37 (3%)	4 (0%)	41	25
All	All	2587/2662 (97%)	2498 (97%)	79 (3%)	10 (0%)	34	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	A	1318	THR
1	B	912	ARG
1	B	797	GLY
1	B	1111	GLY
1	A	797	GLY
1	A	43	CYS
1	A	1321	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1101/1124 (98%)	1064 (97%)	37 (3%)	37	20
1	B	1089/1124 (97%)	1070 (98%)	19 (2%)	60	48
All	All	2190/2248 (97%)	2134 (97%)	56 (3%)	46	29

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	33	LYS
1	A	61	LEU
1	A	112	CYS
1	A	140	ASN
1	A	216	LEU
1	A	224	LYS
1	A	246	ASP
1	A	250	GLN
1	A	297	SER
1	A	303	PRO
1	A	304	LEU
1	A	331	GLU
1	A	343	SER
1	A	396	LEU
1	A	445	THR
1	A	446	ILE
1	A	453	LEU
1	A	469	THR
1	A	526	LEU
1	A	537	LYS
1	A	550	GLN
1	A	679	GLN
1	A	683	ARG
1	A	692	LEU
1	A	743	TYR
1	A	744	LEU
1	A	899	ARG
1	A	911	PHE
1	A	972	ILE
1	A	981	LYS
1	A	1239	PHE
1	A	1250	LYS
1	A	1288	ASN
1	A	1317	VAL

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Mol	Chain	Res	Type
1	A	1322	GLU
1	A	1325	LYS
1	B	33	LYS
1	B	198	GLU
1	B	219	LYS
1	B	224	LYS
1	B	250	GLN
1	B	280	PRO
1	B	466	LEU
1	B	467	LYS
1	B	471	LYS
1	B	483	GLN
1	B	537	LYS
1	B	547	LEU
1	B	550	GLN
1	B	703	ASN
1	B	743	TYR
1	B	911	PHE
1	B	1002	PRO
1	B	1141	SER
1	B	1239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	111	GLN
1	A	145	ASN
1	A	207	GLN
1	A	350	ASN
1	A	585	GLN
1	A	699	GLN
1	A	703	ASN
1	A	863	HIS
1	A	893	ASN
1	A	904	ASN
1	A	1016	GLN
1	A	1033	HIS
1	A	1043	HIS
1	A	1073	ASN
1	A	1148	ASN
1	A	1284	GLN

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Mol	Chain	Res	Type
1	A	1288	ASN
1	A	1311	GLN
1	B	11	ASN
1	B	62	GLN
1	B	108	HIS
1	B	111	GLN
1	B	130	GLN
1	B	145	ASN
1	B	350	ASN
1	B	386	HIS
1	B	550	GLN
1	B	585	GLN
1	B	703	ASN
1	B	741	HIS
1	B	904	ASN
1	B	1016	GLN
1	B	1022	HIS
1	B	1043	HIS
1	B	1062	HIS
1	B	1073	ASN
1	B	1194	GLN
1	B	1284	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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
4	BCT	B	3005	-	0,3,3	0.00	-	0,3,3	0.00	-
5	FES	A	1405	1	0,4,4	0.00	-	-	-	-
3	URC	A	1402	-	13,13,13	3.66	5 (38%)	11,19,19	3.82	6 (54%)
6	FAD	A	1406	-	51,58,58	1.75	7 (13%)	60,89,89	2.22	13 (21%)
4	BCT	A	1403	-	0,3,3	0.00	-	0,3,3	0.00	-
2	NAD	B	3003	-	22,25,48	1.17	3 (13%)	25,38,73	1.30	5 (20%)
5	FES	A	1404	1,7	0,4,4	0.00	-	-	-	-
5	FES	B	3001	1	0,4,4	0.00	-	-	-	-
5	FES	B	3002	1,7	0,4,4	0.00	-	-	-	-
3	URC	B	3004	-	13,13,13	3.27	5 (38%)	11,19,19	5.59	8 (72%)
6	FAD	B	3006	-	51,58,58	1.75	11 (21%)	60,89,89	2.35	13 (21%)
2	NAD	A	1401	-	24,29,48	1.49	4 (16%)	29,45,73	1.51	3 (10%)

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
6	FAD	A	1406	-	-	2/30/50/50	0/6/6/6
5	FES	A	1405	1	-	-	0/1/1/1
3	URC	A	1402	-	-	-	0/2/2/2
2	NAD	B	3003	-	-	1/6/26/62	0/3/3/5
5	FES	A	1404	1,7	-	-	0/1/1/1
2	NAD	A	1401	-	-	3/12/32/62	0/3/3/5
5	FES	B	3001	1	-	-	0/1/1/1
5	FES	B	3002	1,7	-	-	0/1/1/1
3	URC	B	3004	-	-	-	0/2/2/2
6	FAD	B	3006	-	-	6/30/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	URC	C4-N9	-8.31	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	URC	C4-N3	-7.98	1.36	1.46
3	B	3004	URC	C4-N3	-7.92	1.36	1.46
6	A	1406	FAD	C4X-C10	7.67	1.46	1.38
3	B	3004	URC	C4-N9	-6.51	1.36	1.44
6	B	3006	FAD	C4X-C10	5.70	1.44	1.38
2	A	1401	NAD	PN-O1N	4.25	1.64	1.50
6	A	1406	FAD	C4-C4X	4.14	1.48	1.41
3	A	1402	URC	C5-N7	-3.97	1.37	1.45
6	B	3006	FAD	O4B-C1B	3.78	1.46	1.41
6	A	1406	FAD	C9A-N10	3.76	1.43	1.38
3	B	3004	URC	C5-N7	-3.59	1.38	1.45
3	A	1402	URC	O13-C6	3.54	1.30	1.23
6	B	3006	FAD	C9A-N10	3.46	1.43	1.38
6	B	3006	FAD	C10-N1	3.11	1.37	1.33
6	B	3006	FAD	C4-C4X	3.10	1.46	1.41
6	A	1406	FAD	O4B-C1B	3.10	1.45	1.41
2	A	1401	NAD	O4B-C1B	3.07	1.45	1.41
6	B	3006	FAD	C9A-C5X	3.06	1.48	1.42
6	A	1406	FAD	C8-C7	2.86	1.48	1.40
2	B	3003	NAD	O4B-C1B	2.84	1.45	1.41
6	A	1406	FAD	C9A-C5X	2.78	1.48	1.42
6	B	3006	FAD	C2B-C1B	-2.77	1.49	1.53
3	B	3004	URC	O24-C8	2.69	1.29	1.23
6	B	3006	FAD	C6-C5X	-2.66	1.37	1.41
2	A	1401	NAD	C2A-N3A	2.54	1.36	1.32
3	A	1402	URC	O24-C8	2.52	1.28	1.23
6	B	3006	FAD	C8-C7	2.40	1.46	1.40
2	B	3003	NAD	C5A-C4A	2.39	1.47	1.40
2	A	1401	NAD	C2B-C1B	-2.34	1.50	1.53
6	B	3006	FAD	C2'-C3'	-2.22	1.49	1.53
6	A	1406	FAD	C2B-C1B	-2.21	1.50	1.53
2	B	3003	NAD	PA-O3	2.11	1.63	1.54
6	B	3006	FAD	C2-N1	-2.06	1.34	1.38
3	B	3004	URC	O11-C2	2.04	1.27	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3004	URC	C4-N9-C8	-11.03	105.39	112.89
6	A	1406	FAD	C4-N3-C2	10.85	124.30	115.14
6	B	3006	FAD	C4-N3-C2	9.94	123.53	115.14
3	B	3004	URC	N7-C8-N9	8.50	116.74	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3004	URC	C5-C4-N9	8.29	106.48	102.64
6	B	3006	FAD	C1'-N10-C9A	7.82	124.45	118.29
3	A	1402	URC	C4-N9-C8	-7.04	108.10	112.89
3	A	1402	URC	N7-C8-N9	6.80	115.14	108.76
6	B	3006	FAD	C4-C4X-C10	-6.35	115.75	119.95
3	B	3004	URC	N1-C2-N3	6.13	122.57	116.12
3	A	1402	URC	N1-C2-N3	5.14	121.53	116.12
6	A	1406	FAD	C4-C4X-C10	-4.82	116.76	119.95
6	A	1406	FAD	C4X-C4-N3	-4.57	117.19	123.43
2	A	1401	NAD	O5D-PN-O2N	4.16	123.55	107.64
6	B	3006	FAD	C9A-N10-C10	-4.10	116.54	121.91
6	A	1406	FAD	C4X-N5-C5X	4.01	120.78	116.77
2	A	1401	NAD	N3A-C2A-N1A	-3.95	122.51	128.68
6	A	1406	FAD	C1'-N10-C9A	3.87	121.34	118.29
6	B	3006	FAD	C10-C4X-N5	3.81	123.89	121.26
3	A	1402	URC	C5-C4-N9	3.81	104.41	102.64
3	B	3004	URC	C6-N1-C2	-3.78	121.19	126.25
6	B	3006	FAD	C5X-C9A-N10	3.58	120.31	117.72
3	B	3004	URC	O24-C8-N9	-3.51	120.89	125.94
3	A	1402	URC	O24-C8-N9	-3.49	120.93	125.94
6	B	3006	FAD	C4X-C4-N3	-3.46	118.69	123.43
6	B	3006	FAD	C1B-N9A-C4A	-3.34	120.77	126.64
3	B	3004	URC	O11-C2-N3	-3.15	116.64	122.92
2	B	3003	NAD	C3B-C2B-C1B	3.05	105.57	100.98
6	A	1406	FAD	N3A-C2A-N1A	-2.90	124.15	128.68
6	A	1406	FAD	C9A-N10-C10	-2.88	118.14	121.91
6	A	1406	FAD	C5X-C9A-N10	2.86	119.79	117.72
6	B	3006	FAD	N6A-C6A-N1A	2.70	124.18	118.57
6	B	3006	FAD	C4X-N5-C5X	2.54	119.31	116.77
3	B	3004	URC	O24-C8-N7	-2.49	122.36	125.94
6	A	1406	FAD	C4A-C5A-N7A	-2.48	106.81	109.40
2	A	1401	NAD	C4A-C5A-N7A	-2.47	106.82	109.40
2	B	3003	NAD	O2A-PA-O1A	2.45	120.27	110.68
6	A	1406	FAD	C1B-N9A-C4A	-2.33	122.55	126.64
6	A	1406	FAD	C1'-N10-C10	2.31	120.48	118.41
2	B	3003	NAD	N3A-C2A-N1A	-2.26	125.14	128.68
2	B	3003	NAD	C4A-C5A-N7A	-2.26	107.04	109.40
3	A	1402	URC	C6-N1-C2	-2.11	123.42	126.25
2	B	3003	NAD	O2B-C2B-C1B	-2.10	103.10	110.85
6	B	3006	FAD	C5A-C6A-N6A	-2.07	117.20	120.35
6	A	1406	FAD	O2A-PA-O1A	2.07	122.46	112.24
6	B	3006	FAD	N3A-C2A-N1A	-2.05	125.47	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1406	FAD	C10-C4X-N5	2.05	122.67	121.26
6	B	3006	FAD	O4'-C4'-C3'	-2.03	104.17	109.10

There are no chirality outliers.

All (12) torsion outliers are listed below:

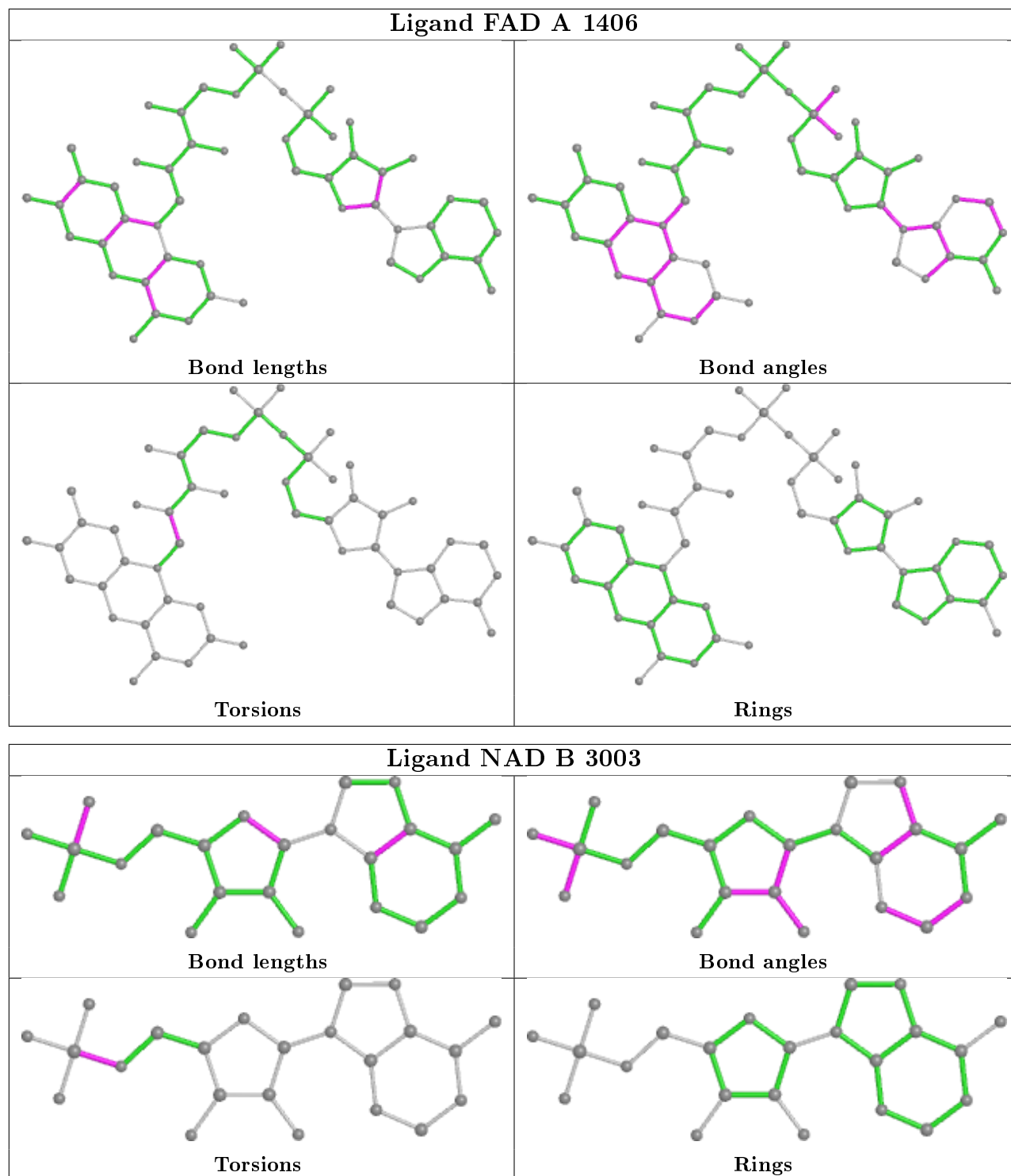
Mol	Chain	Res	Type	Atoms
6	A	1406	FAD	N10-C1'-C2'-O2'
6	A	1406	FAD	N10-C1'-C2'-C3'
2	A	1401	NAD	O4B-C4B-C5B-O5B
2	A	1401	NAD	C3B-C4B-C5B-O5B
6	B	3006	FAD	N10-C1'-C2'-O2'
6	B	3006	FAD	N10-C1'-C2'-C3'
2	B	3003	NAD	C5B-O5B-PA-O1A
6	B	3006	FAD	C2'-C3'-C4'-C5'
2	A	1401	NAD	PA-O3-PN-O1N
6	B	3006	FAD	C2'-C3'-C4'-O4'
6	B	3006	FAD	O3'-C3'-C4'-O4'
6	B	3006	FAD	O3'-C3'-C4'-C5'

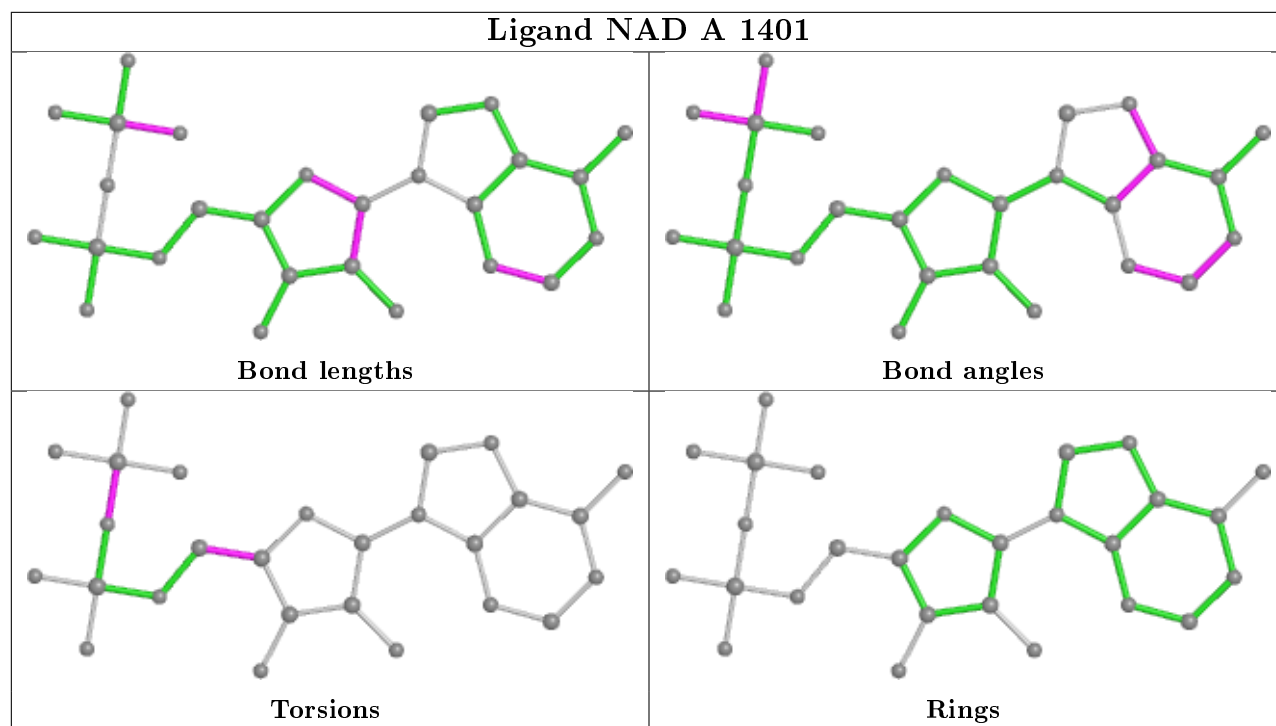
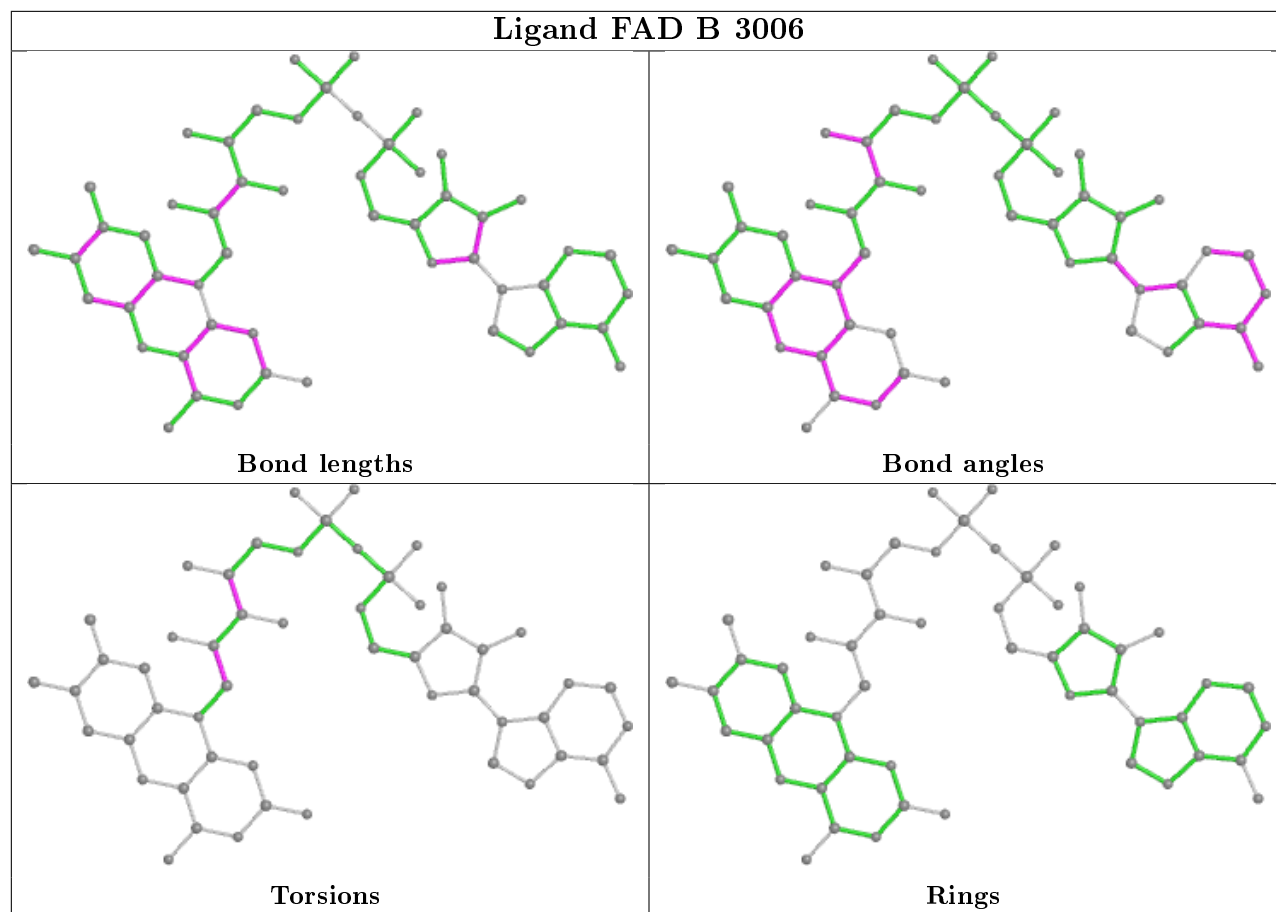
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1406	FAD	1	0
5	A	1404	FES	1	0
5	B	3001	FES	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	1304/1331 (97%)	0.18	54 (4%) 37 35	16, 28, 52, 112	0
1	B	1291/1331 (96%)	-0.00	30 (2%) 60 60	16, 23, 44, 84	0
All	All	2595/2662 (97%)	0.09	84 (3%) 47 46	16, 25, 49, 112	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1323	ASN	10.3
1	A	1320	VAL	8.7
1	A	1319	GLY	6.6
1	A	1324	CYS	6.4
1	A	1318	THR	6.3
1	A	1321	PRO	6.1
1	A	1322	GLU	5.2
1	B	1287	ASP	5.1
1	B	1286	GLY	5.0
1	A	1317	VAL	5.0
1	A	1288	ASN	4.9
1	B	1289	ALA	4.8
1	A	3	ALA	4.6
1	B	1288	ASN	4.5
1	A	1287	ASP	4.4
1	B	1111	GLY	4.3
1	A	290	VAL	4.2
1	B	218	LEU	4.2
1	A	1111	GLY	4.0
1	A	1325	LYS	3.6
1	B	535	CYS	3.6
1	A	220	ASP	3.6
1	A	453	LEU	3.6
1	A	1327	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	565	LYS	3.4
1	A	566	ASP	3.4
1	B	1320	VAL	3.3
1	B	3	ALA	3.1
1	A	1110	THR	3.1
1	A	250	GLN	3.0
1	B	1110	THR	2.9
1	A	192	PRO	2.9
1	A	217	ARG	2.9
1	A	316	ALA	2.9
1	B	1106	LYS	2.8
1	A	377	GLY	2.7
1	A	530	ASP	2.7
1	B	198	GLU	2.7
1	A	1331	ILE	2.7
1	B	1266	LEU	2.7
1	A	1326	SER	2.7
1	A	1107	LYS	2.6
1	B	530	ASP	2.6
1	B	1001	ILE	2.6
1	A	1109	PRO	2.6
1	A	318	LEU	2.6
1	B	61	LEU	2.5
1	A	473	LEU	2.5
1	B	317	LYS	2.5
1	B	220	ASP	2.4
1	B	553	PRO	2.4
1	B	566	ASP	2.4
1	A	1314	THR	2.4
1	A	218	LEU	2.4
1	A	198	GLU	2.4
1	B	221	THR	2.4
1	A	528	ARG	2.4
1	A	533	ASP	2.4
1	A	396	LEU	2.3
1	A	446	ILE	2.3
1	B	250	GLN	2.3
1	A	720	LYS	2.3
1	B	316	ALA	2.3
1	A	319	PRO	2.3
1	A	1328	SER	2.3
1	A	565	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	529	ALA	2.3
1	B	363	VAL	2.2
1	B	1265	PHE	2.2
1	A	293	PRO	2.2
1	A	435	SER	2.2
1	A	498	ASP	2.2
1	B	550	GLN	2.2
1	A	923	ALA	2.2
1	A	496	ALA	2.2
1	A	304	LEU	2.2
1	A	61	LEU	2.1
1	B	420	PHE	2.1
1	A	1315	LEU	2.1
1	B	164	LYS	2.1
1	A	392	TYR	2.1
1	A	686	LYS	2.1
1	A	724	SER	2.0
1	A	439	VAL	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. 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	B-factors(\AA^2)	Q<0.9
2	NAD	A	1401	27/44	0.82	0.20	43,60,84,86	0
2	NAD	B	3003	23/44	0.89	0.17	35,41,57,71	0
3	URC	A	1402	12/12	0.96	0.07	22,24,26,27	0
6	FAD	A	1406	53/53	0.97	0.09	23,27,29,30	0
3	URC	B	3004	12/12	0.97	0.06	21,21,23,23	0

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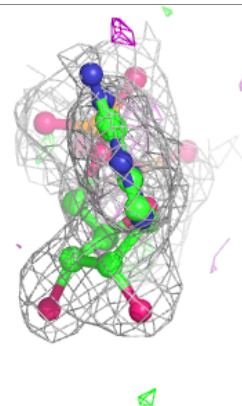
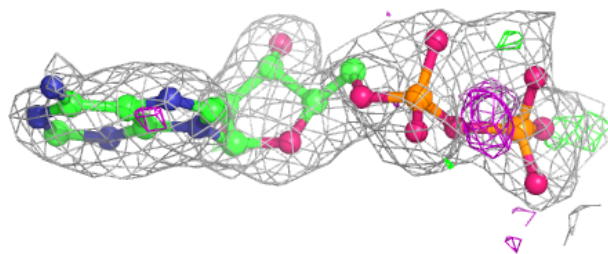
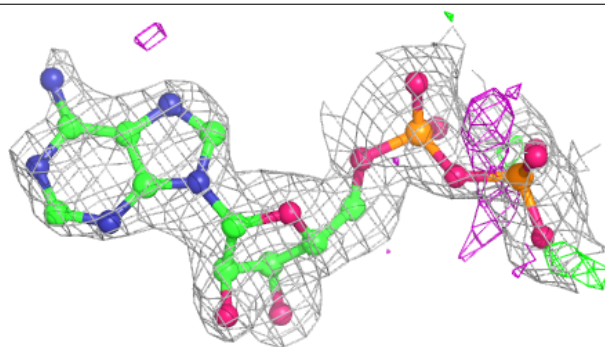
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FES	B	3001	4/4	0.98	0.05	28,30,32,34	0
5	FES	A	1405	4/4	0.98	0.04	29,31,32,35	0
6	FAD	B	3006	53/53	0.98	0.07	16,20,22,23	0
4	BCT	A	1403	4/4	0.99	0.05	23,24,24,27	0
4	BCT	B	3005	4/4	0.99	0.07	20,22,22,26	0
5	FES	A	1404	4/4	1.00	0.04	20,20,20,21	0
5	FES	B	3002	4/4	1.00	0.04	17,17,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

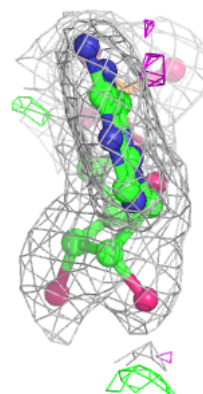
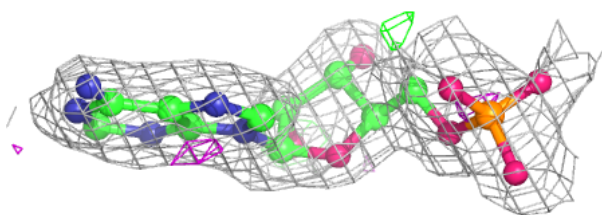
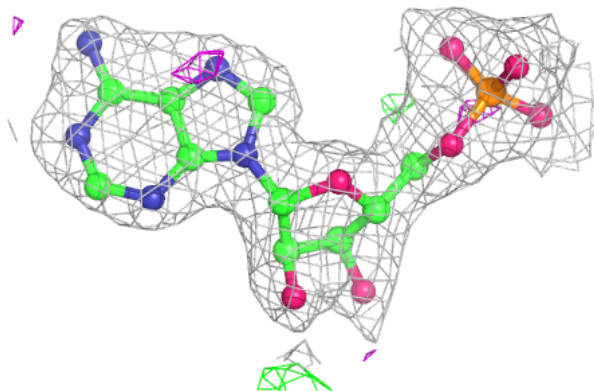
Electron density around NAD A 1401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

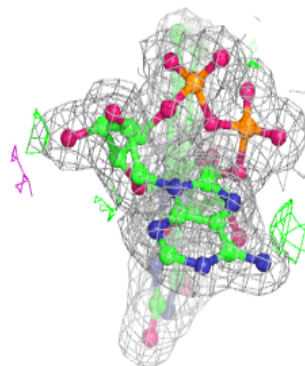
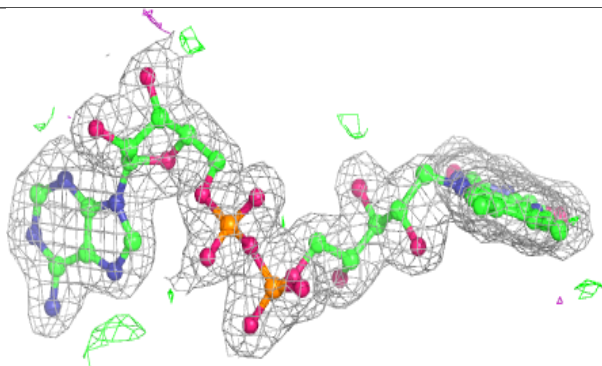
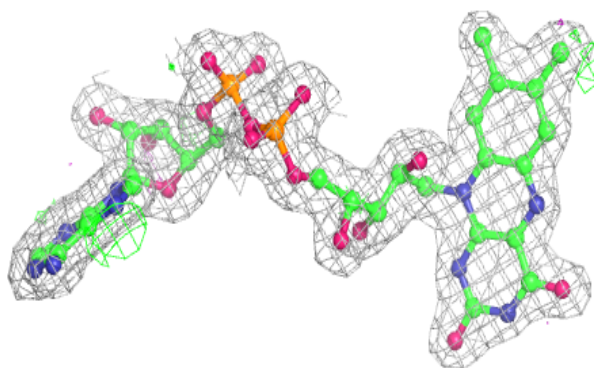


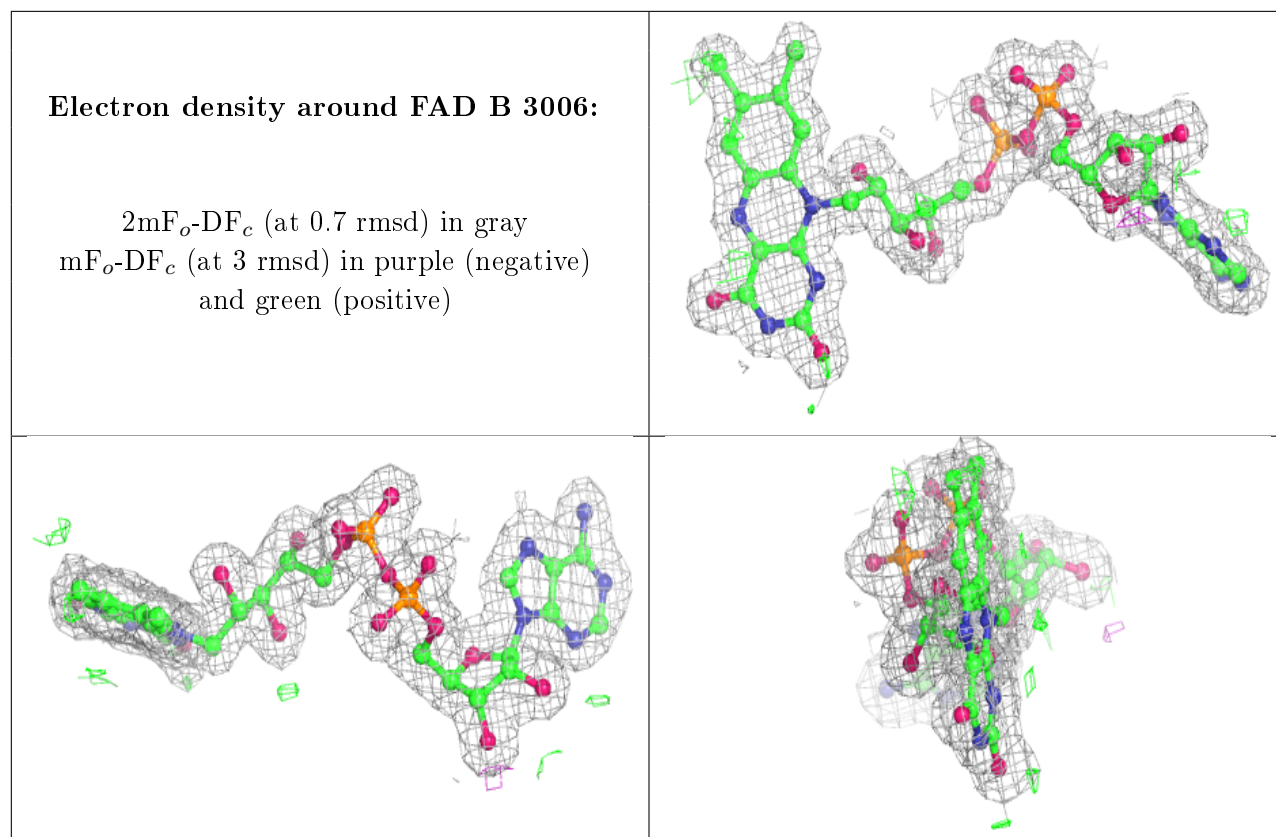
Electron density around NAD B 3003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD A 1406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.