



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:10 pm BST

PDB ID : 6A7X  
Title : Rat Xanthine oxidoreductase, D428A variant, NAD bound form  
Authors : Okamoto, K.; Kawaguchi, Y.  
Deposited on : 2018-07-05  
Resolution : 2.15 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](mailto: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.

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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

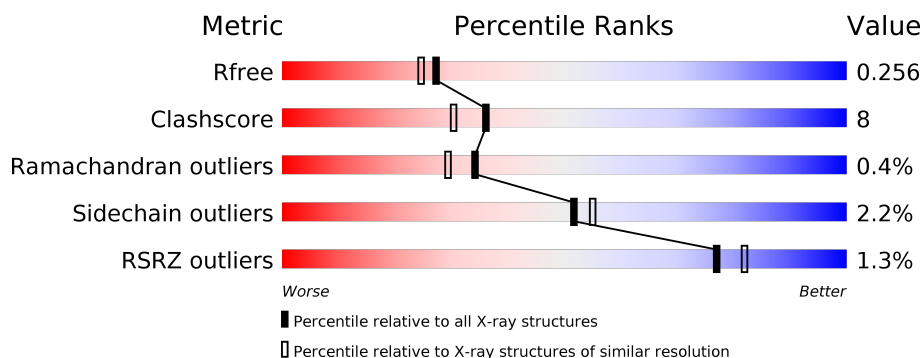
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	1331	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</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:

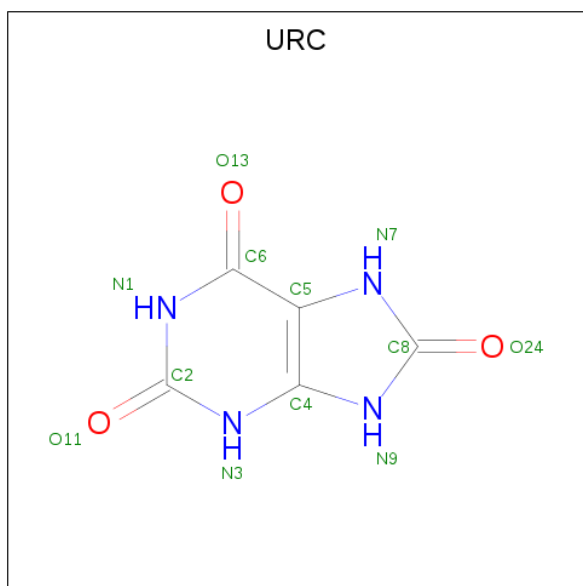
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FES	B	3001	-	-	X	-



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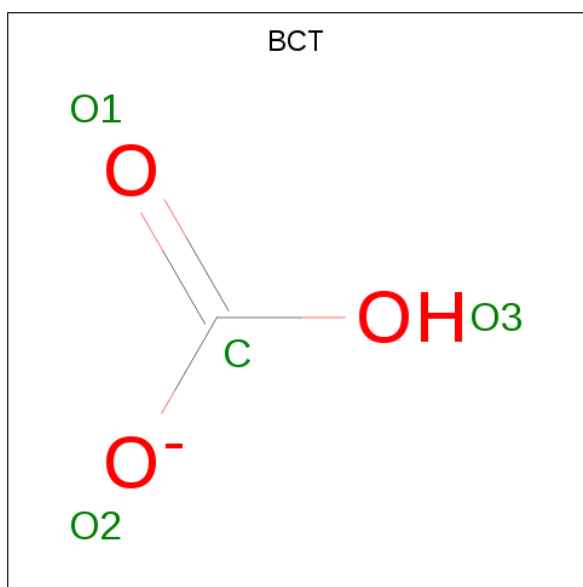
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	
			23	10	5	7	1	
							0	0

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



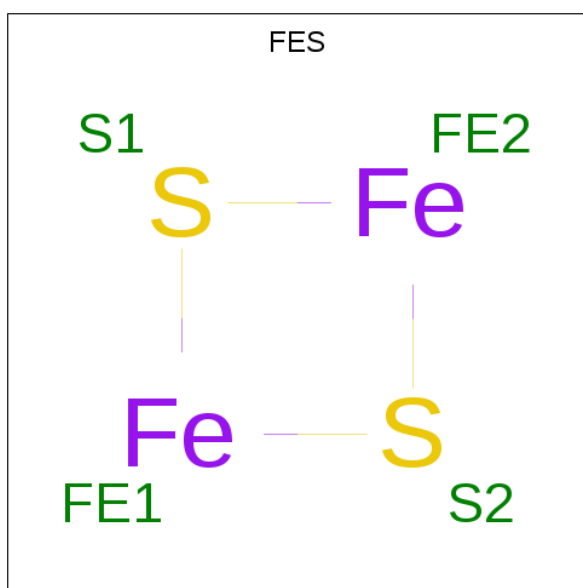
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O		
			12	5	4	3		
							0	0
3	B	1	Total	C	N	O		
			12	5	4	3		
							0	0

- 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:  $\text{Fe}_2\text{S}_2$ ).



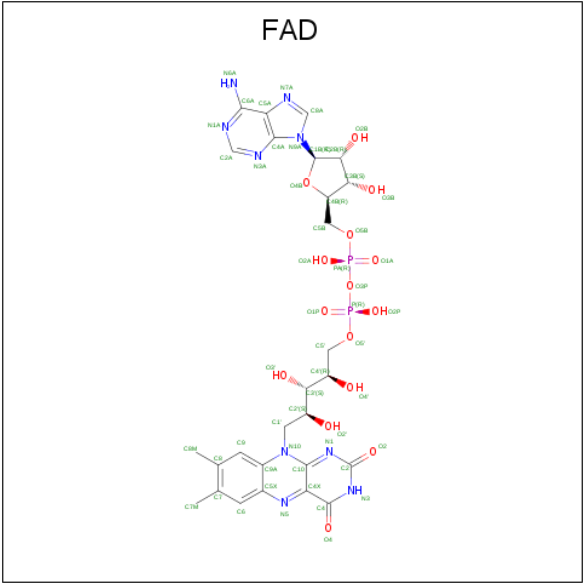
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

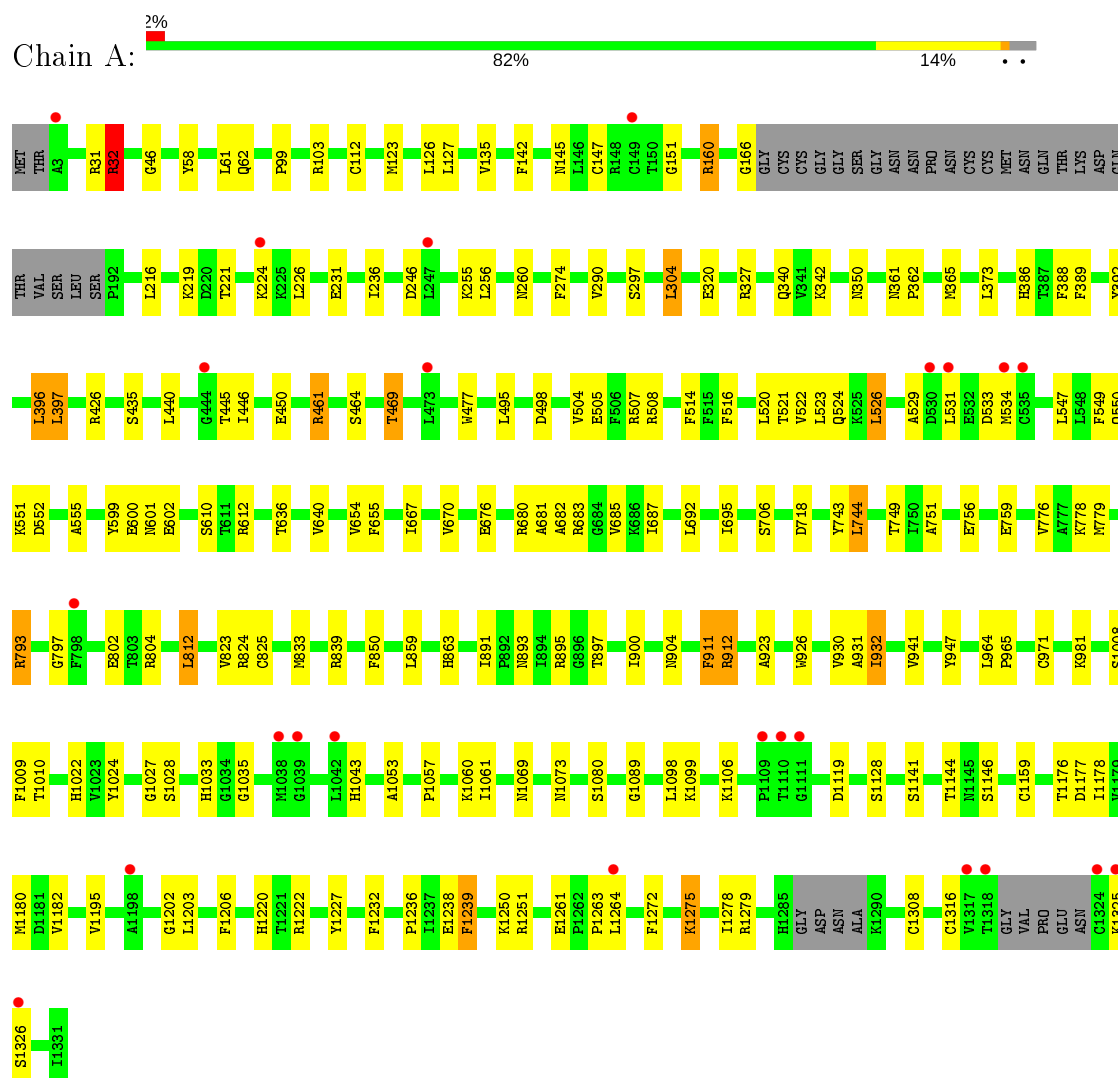
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	721	Total	O	0	0
			721	721		
7	B	872	Total	O	0	0
			872	872		

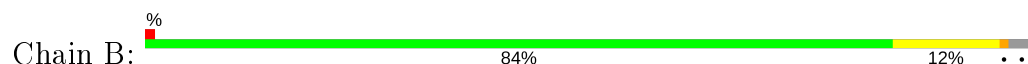
### 3 Residue-property plots [i](#)

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: Xanthine dehydrogenase/oxidase



#### • Molecule 1: Xanthine dehydrogenase/oxidase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.14Å 137.79Å 222.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.63 – 2.15 41.60 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.63-2.15) 99.4 (41.60-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.195 , 0.255 0.200 , 0.256	Depositor DCC
$R_{free}$ test set	8171 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.49	0/10223	0.65	2/13829 (0.0%)
1	B	0.50	0/10178	0.66	0/13773
All	All	0.49	0/20401	0.66	2/27602 (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	6
All	All	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	793	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	793	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1222	ARG	Sidechain
1	A	1251	ARG	Sidechain
1	A	1316	CYS	Peptide
1	A	160	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	32	ARG	Sidechain
1	A	461	ARG	Sidechain
1	A	507	ARG	Sidechain
1	A	804	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	232	ARG	Sidechain
1	B	383	ARG	Sidechain
1	B	461	ARG	Sidechain
1	B	606	ARG	Sidechain
1	B	942	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	10013	0	10029	173	0
1	B	9968	0	9983	155	0
2	A	27	0	12	0	0
2	B	23	0	12	0	0
3	A	12	0	4	1	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	3	0
6	A	53	0	31	2	0
6	B	53	0	31	0	0
7	A	721	0	0	86	0
7	B	872	0	0	89	0
All	All	21778	0	20106	323	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (323) 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:1089:GLY:HA3	7:B:3663:HOH:O	1.29	1.32
1:A:1089:GLY:HA3	7:A:1831:HOH:O	1.26	1.28
1:B:812:LEU:HB2	7:B:3348:HOH:O	1.42	1.18
1:B:366:ALA:HB1	7:B:3120:HOH:O	1.49	1.12
1:A:123:MET:SD	7:A:2164:HOH:O	2.10	1.09
1:A:1308:CYS:SG	7:A:1659:HOH:O	2.15	1.04
1:B:927:MET:SD	7:B:3867:HOH:O	2.16	1.03
1:A:655:PHE:CD2	7:A:2003:HOH:O	2.12	1.01
1:B:927:MET:SD	7:B:3281:HOH:O	2.18	1.01
1:A:260:ASN:ND2	7:A:1503:HOH:O	1.95	1.00
1:A:654:VAL:HG12	7:A:2003:HOH:O	1.62	0.98
1:B:967:CYS:SG	7:B:3117:HOH:O	2.23	0.96
1:B:812:LEU:HD21	1:B:823:VAL:O	1.65	0.94
1:A:812:LEU:HD21	1:A:823:VAL:O	1.69	0.93
1:A:685:VAL:HG23	7:A:1512:HOH:O	1.68	0.93
1:A:1220:HIS:CD2	7:A:1731:HOH:O	2.23	0.92
1:B:900:ILE:HG22	7:B:3101:HOH:O	1.67	0.92
1:A:802:GLU:OE2	7:A:1502:HOH:O	1.90	0.90
1:B:901:CYS:O	7:B:3101:HOH:O	1.89	0.89
1:A:524:GLN:OE1	7:A:1501:HOH:O	1.90	0.89
1:B:1125:VAL:HB	7:B:3148:HOH:O	1.73	0.88
1:B:1280:ALA:HB1	7:B:3264:HOH:O	1.74	0.86
1:B:885:MET:SD	7:B:3639:HOH:O	2.33	0.85
1:B:863:HIS:HE1	7:B:3639:HOH:O	1.59	0.84
1:B:810:THR:HB	7:B:3785:HOH:O	1.78	0.84
1:B:863:HIS:CE1	7:B:3639:HOH:O	2.29	0.84
1:B:995:LYS:HD2	7:B:3264:HOH:O	1.77	0.83
1:B:954:HIS:CD2	7:B:3418:HOH:O	2.30	0.83
1:A:1278:ILE:HG23	7:A:1659:HOH:O	1.78	0.82
1:B:743:TYR:CD2	7:B:3126:HOH:O	2.34	0.81
1:B:1120:ALA:HA	7:B:3148:HOH:O	1.81	0.81
1:B:797:GLY:HA2	7:B:3126:HOH:O	1.81	0.80
1:B:695:ILE:H	1:B:904:ASN:HD22	1.27	0.80
1:A:1057:PRO:O	7:A:1504:HOH:O	2.00	0.79
1:B:1084:ASP:O	7:B:3102:HOH:O	2.01	0.78
1:B:11:ASN:HD21	1:B:87:THR:H	1.31	0.76
5:B:3002:FES:S1	7:B:3327:HOH:O	2.44	0.74
1:B:565:LYS:HB2	7:B:3724:HOH:O	1.85	0.74
1:B:714:ILE:HG21	7:B:3418:HOH:O	1.88	0.73
1:A:1028:SER:O	7:A:1505:HOH:O	2.03	0.73
1:A:602:GLU:N	7:A:1511:HOH:O	2.23	0.72
1:A:971:CYS:SG	7:A:1534:HOH:O	2.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD23	7:A:2164:HOH:O	1.90	0.72
1:A:636:THR:O	7:A:1506:HOH:O	2.07	0.71
1:A:365:MET:HE2	1:A:464:SER:HB2	1.73	0.71
1:B:843:LEU:HG	7:B:3662:HOH:O	1.91	0.70
1:B:793:ARG:HD2	7:B:3183:HOH:O	1.91	0.70
1:B:45:GLU:OE2	7:B:3104:HOH:O	2.09	0.70
1:A:126:LEU:HG	7:A:1699:HOH:O	1.92	0.69
1:A:151:GLY:O	7:A:1508:HOH:O	2.10	0.69
1:B:1236:PRO:O	7:B:3103:HOH:O	2.09	0.69
1:A:839:ARG:CZ	7:A:1553:HOH:O	2.41	0.69
1:B:135:VAL:HG23	1:B:164:LYS:HE2	1.74	0.69
1:A:759:GLU:OE2	1:B:1062:HIS:HE1	1.74	0.69
1:A:32:ARG:HH21	1:A:32:ARG:HG2	1.58	0.68
1:B:357:ILE:HD12	1:B:430:ILE:HG23	1.75	0.68
1:A:1264:LEU:O	7:A:1509:HOH:O	2.13	0.67
1:A:655:PHE:CE2	7:A:2003:HOH:O	2.42	0.67
1:A:1239:PHE:CE1	7:A:2133:HOH:O	2.48	0.67
1:B:386:HIS:HB2	1:B:461:ARG:HH22	1.60	0.66
1:A:932:ILE:HD13	1:A:1279:ARG:NE	2.11	0.66
1:A:744:LEU:HD13	7:A:2053:HOH:O	1.95	0.66
1:B:1280:ALA:CB	7:B:3264:HOH:O	2.36	0.66
1:B:697:THR:O	7:B:3106:HOH:O	2.13	0.66
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	1.79	0.65
1:B:1102:GLU:HG2	1:B:1103:PRO:HD3	1.79	0.65
1:A:304:LEU:HD21	1:A:342:LYS:HA	1.80	0.64
1:B:726:ALA:HB3	7:B:3191:HOH:O	1.98	0.64
1:A:793:ARG:NE	7:A:1507:HOH:O	2.08	0.64
1:B:746:THR:O	7:B:3107:HOH:O	2.15	0.64
1:A:695:ILE:H	1:A:904:ASN:HD22	1.44	0.64
1:B:513:SER:HA	7:B:3827:HOH:O	1.98	0.64
1:A:932:ILE:HD13	1:A:1279:ARG:CZ	2.28	0.64
1:A:1024:TYR:HA	1:B:1073:ASN:HD21	1.63	0.63
1:B:875:ARG:HD2	7:B:3205:HOH:O	1.98	0.63
1:A:833:MET:SD	7:A:1781:HOH:O	2.56	0.63
1:A:166:GLY:HA3	7:A:2070:HOH:O	1.97	0.63
1:B:130:GLN:HE21	1:B:132:GLU:H	1.46	0.62
1:A:1180:MET:HG2	7:A:2185:HOH:O	1.98	0.62
1:B:658:ASP:HB2	7:B:3634:HOH:O	1.98	0.62
1:A:304:LEU:HD22	1:A:304:LEU:H	1.64	0.62
1:B:41:LEU:HD21	7:B:3715:HOH:O	1.99	0.62
1:B:539:ASP:CG	7:B:3185:HOH:O	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.01	0.61
1:A:231:GLU:OE2	1:A:680:ARG:NH1	2.29	0.60
1:B:74:LEU:HD13	7:B:3891:HOH:O	2.01	0.60
1:A:547:LEU:HD12	7:A:2033:HOH:O	2.00	0.60
1:B:1033:HIS:HE2	1:B:1043:HIS:HD2	1.49	0.60
1:B:261:THR:HG22	7:B:3891:HOH:O	2.02	0.60
1:A:1033:HIS:CE1	1:A:1043:HIS:HD2	2.20	0.60
1:A:1206:PHE:CE2	7:A:1509:HOH:O	2.52	0.60
1:A:1009:PHE:HE1	7:A:1502:HOH:O	1.85	0.59
1:B:1250:LYS:HA	7:B:3825:HOH:O	2.00	0.59
1:B:472:GLN:HA	1:B:475:LYS:HD2	1.83	0.59
1:A:1089:GLY:CA	7:A:1831:HOH:O	2.09	0.59
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.99	0.59
1:B:749:THR:HG22	1:B:812:LEU:HD22	1.83	0.58
1:A:1195:VAL:CG2	7:A:2185:HOH:O	2.51	0.58
1:B:1066:THR:O	7:B:3108:HOH:O	2.17	0.58
1:A:749:THR:HG22	1:A:812:LEU:HD22	1.86	0.58
1:B:867:GLY:HA3	7:B:3101:HOH:O	2.04	0.57
1:A:941:VAL:CG2	7:A:1724:HOH:O	2.52	0.57
1:B:942:ARG:HA	7:B:3281:HOH:O	2.04	0.57
1:A:1061:ILE:N	7:A:1504:HOH:O	2.38	0.57
1:A:682:ALA:HA	7:A:1512:HOH:O	2.05	0.57
1:B:537:LYS:NZ	7:B:3105:HOH:O	2.09	0.57
1:A:221:THR:HG22	7:A:1516:HOH:O	2.04	0.56
1:B:145:ASN:ND2	1:B:340:GLN:HE22	2.03	0.56
1:B:376:ARG:O	7:B:3109:HOH:O	2.18	0.56
1:B:357:ILE:CD1	1:B:430:ILE:HG23	2.35	0.56
1:A:516:PHE:CZ	1:A:520:LEU:HD11	2.40	0.56
1:B:438:ARG:N	7:B:3120:HOH:O	2.38	0.56
1:B:470:PRO:O	1:B:473:LEU:HG	2.06	0.56
1:A:1141:SER:HB3	1:A:1144:THR:HG22	1.88	0.56
1:A:931:ALA:HB1	7:A:1724:HOH:O	2.06	0.56
1:B:386:HIS:CD2	1:B:466:LEU:HD21	2.40	0.56
1:B:871:GLU:CD	7:B:3205:HOH:O	2.44	0.55
1:A:612:ARG:N	7:A:1510:HOH:O	2.39	0.55
1:A:640:VAL:HG23	7:A:1506:HOH:O	2.07	0.55
1:A:891:ILE:HA	7:A:1515:HOH:O	2.06	0.55
1:B:429:ASP:OD1	1:B:430:ILE:N	2.38	0.55
1:A:756:GLU:HB3	1:B:584:MET:SD	2.46	0.55
1:B:743:TYR:CG	7:B:3126:HOH:O	2.56	0.55
1:B:812:LEU:CD1	7:B:3348:HOH:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:LEU:HD13	5:B:3001:FES:S1	2.47	0.55
1:B:709:GLY:O	1:B:899:ARG:NH1	2.39	0.55
1:B:995:LYS:NZ	1:B:1284:GLN:NE2	2.54	0.55
1:A:1182:VAL:CG1	7:A:2185:HOH:O	2.55	0.55
1:B:516:PHE:CZ	1:B:520:LEU:HD11	2.42	0.55
1:B:32:ARG:NH2	1:B:676:GLU:OE2	2.39	0.55
1:A:759:GLU:OE2	1:B:1062:HIS:CE1	2.58	0.55
1:B:1101:LEU:HD22	7:B:3169:HOH:O	2.05	0.55
1:B:741:HIS:HE1	1:B:910:ALA:O	1.89	0.55
1:A:1033:HIS:HE1	1:A:1043:HIS:HD2	1.53	0.55
1:A:778:LYS:CE	7:A:1787:HOH:O	2.55	0.54
1:B:438:ARG:HB2	7:B:3120:HOH:O	2.08	0.54
1:B:1275:LYS:HE3	7:B:3476:HOH:O	2.07	0.54
1:B:740:GLU:HG2	1:B:833:MET:HG2	1.90	0.53
1:A:610:SER:OG	7:A:1510:HOH:O	2.19	0.53
1:A:365:MET:CE	1:A:464:SER:HB2	2.39	0.53
1:B:996:ARG:HB2	7:B:3110:HOH:O	2.09	0.53
1:B:1125:VAL:CG2	7:B:3148:HOH:O	2.57	0.53
1:B:785:ASN:OD1	1:B:786:ARG:NH1	2.40	0.53
1:A:670:VAL:HG21	7:A:1512:HOH:O	2.08	0.53
1:A:895:ARG:HD3	7:A:1999:HOH:O	2.09	0.53
1:A:145:ASN:ND2	1:A:340:GLN:HE22	2.07	0.52
1:B:995:LYS:HZ1	1:B:1284:GLN:NE2	2.07	0.52
1:B:987:PHE:HB3	7:B:3110:HOH:O	2.08	0.52
1:A:1236:PRO:HG2	7:A:2133:HOH:O	2.08	0.52
1:A:147:CYS:HA	7:A:2053:HOH:O	2.07	0.52
1:B:216:LEU:O	1:B:219:LYS:HG3	2.09	0.52
1:B:350:ASN:HB2	7:B:3115:HOH:O	2.09	0.52
1:A:1073:ASN:HD21	1:B:1024:TYR:HA	1.74	0.52
1:A:446:ILE:HD12	1:A:534:MET:HB2	1.92	0.52
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.58	0.52
7:A:1507:HOH:O	1:B:756:GLU:OE2	2.19	0.52
1:A:1220:HIS:HD2	7:A:1731:HOH:O	1.75	0.51
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.93	0.51
1:A:932:ILE:CD1	1:A:1279:ARG:NE	2.73	0.51
1:B:145:ASN:HD21	1:B:340:GLN:HE22	1.58	0.51
1:A:599:TYR:HB2	7:A:1511:HOH:O	2.09	0.51
1:A:655:PHE:CG	7:A:2003:HOH:O	2.50	0.51
1:A:31:ARG:HB3	7:A:1977:HOH:O	2.11	0.50
1:A:931:ALA:CB	7:A:1724:HOH:O	2.59	0.50
1:A:1177:ASP:HB3	7:A:2093:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:CYS:HB2	7:A:1534:HOH:O	2.11	0.50
1:A:706:SER:HB3	7:A:1513:HOH:O	2.11	0.50
1:A:290:VAL:CG2	1:A:297:SER:HB3	2.42	0.50
1:A:32:ARG:NH1	1:A:676:GLU:OE2	2.45	0.49
1:A:900:ILE:N	1:A:900:ILE:HD12	2.27	0.49
1:A:440:LEU:HB3	1:A:450:GLU:HB2	1.94	0.49
1:B:696:ILE:HD13	7:B:3122:HOH:O	2.12	0.49
1:B:751:ALA:CB	1:B:812:LEU:HD23	2.42	0.49
1:A:446:ILE:CD1	1:A:534:MET:HB2	2.43	0.49
1:A:1022:HIS:CE1	1:A:1128:SER:HG	2.30	0.49
1:A:135:VAL:HG13	1:A:160:ARG:HH21	1.78	0.49
1:B:1203:LEU:HD23	1:B:1203:LEU:C	2.33	0.49
1:B:1089:GLY:CA	7:B:3663:HOH:O	2.13	0.48
1:B:810:THR:CB	7:B:3785:HOH:O	2.50	0.48
1:A:304:LEU:CD2	1:A:342:LYS:HA	2.42	0.48
1:A:718:ASP:H	1:A:893:ASN:HD22	1.61	0.48
1:A:667:ILE:CD1	1:A:687:ILE:HD13	2.42	0.48
1:B:696:ILE:HA	7:B:3122:HOH:O	2.13	0.48
1:B:911:PHE:O	1:B:912:ARG:C	2.51	0.48
1:A:667:ILE:HD13	1:A:687:ILE:HD13	1.96	0.48
1:A:895:ARG:HB2	7:A:1537:HOH:O	2.13	0.48
1:B:994:LYS:O	1:B:995:LYS:HD3	2.14	0.48
1:A:1227:TYR:HB3	7:A:1781:HOH:O	2.12	0.48
1:B:133:PRO:O	1:B:163:ALA:HA	2.14	0.48
1:A:812:LEU:HD11	1:A:824:ARG:C	2.33	0.48
1:A:31:ARG:CB	7:A:1977:HOH:O	2.62	0.47
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.28	0.47
1:B:1120:ALA:CA	7:B:3148:HOH:O	2.52	0.47
1:A:145:ASN:HD21	1:A:340:GLN:HE22	1.62	0.47
1:B:473:LEU:O	1:B:474:SER:HB2	2.14	0.47
1:A:58:TYR:CE2	1:A:219:LYS:HD2	2.49	0.47
1:A:435:SER:CB	7:A:1899:HOH:O	2.63	0.47
1:B:1071:VAL:HG22	7:B:3218:HOH:O	2.13	0.47
1:A:602:GLU:CA	7:A:1511:HOH:O	2.62	0.47
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.15	0.47
1:B:273:LEU:HA	7:B:3190:HOH:O	2.13	0.47
1:B:253:ASP:HB2	7:B:3628:HOH:O	2.14	0.47
1:B:904:ASN:C	7:B:3122:HOH:O	2.53	0.47
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.18	0.47
1:B:975:SER:O	1:B:980:ARG:HD3	2.15	0.46
1:B:995:LYS:CD	7:B:3264:HOH:O	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:LEU:C	1:A:1203:LEU:HD23	2.36	0.46
1:A:514:PHE:HD2	7:A:1899:HOH:O	1.98	0.46
1:B:955:PHE:HB3	7:B:3418:HOH:O	2.15	0.46
1:A:361:ASN:N	1:A:362:PRO:CD	2.78	0.46
1:B:438:ARG:NH1	7:B:3137:HOH:O	2.49	0.46
1:B:650:ASN:OD1	1:B:778:LYS:NZ	2.49	0.46
1:A:1176:THR:HG21	7:A:2133:HOH:O	2.14	0.46
1:B:1101:LEU:HD22	7:B:3406:HOH:O	2.16	0.45
1:B:1104:PHE:HB2	7:B:3169:HOH:O	2.17	0.45
1:B:1175:ARG:HA	1:B:1238:GLU:O	2.17	0.45
1:A:911:PHE:O	1:A:912:ARG:C	2.54	0.45
1:A:1144:THR:HG23	1:A:1146:SER:OG	2.16	0.45
1:A:1178:ILE:HG21	1:A:1180:MET:HE2	1.98	0.45
1:A:863:HIS:HD2	1:A:897:THR:O	1.99	0.45
1:B:744:LEU:HG	7:B:3675:HOH:O	2.16	0.45
1:B:1057:PRO:HD2	1:B:1060:LYS:HD2	1.98	0.45
1:B:791:VAL:N	7:B:3108:HOH:O	2.50	0.45
1:A:46:GLY:HA2	5:A:1404:FES:S2	2.56	0.45
1:B:241:MET:HE2	1:B:241:MET:HB2	1.71	0.45
1:B:1021:VAL:HG11	7:B:3362:HOH:O	2.17	0.45
1:B:1101:LEU:HD13	7:B:3406:HOH:O	2.15	0.45
1:A:522:VAL:HG12	1:A:526:LEU:HD22	1.99	0.44
1:B:480:GLU:HB3	7:B:3711:HOH:O	2.16	0.44
1:A:1033:HIS:CE1	1:A:1043:HIS:CD2	3.04	0.44
1:A:216:LEU:HA	1:A:216:LEU:HD12	1.88	0.44
1:B:741:HIS:HD2	7:B:3365:HOH:O	2.00	0.44
1:A:1080:SER:OG	1:A:1261:GLU:HG3	2.17	0.44
1:A:941:VAL:HG21	7:A:1724:HOH:O	2.17	0.44
1:A:350:ASN:HB2	6:A:1406:FAD:O4'	2.17	0.44
1:A:521:THR:HA	7:A:1501:HOH:O	2.16	0.44
1:B:149:CYS:HB2	5:B:3001:FES:S2	2.58	0.44
1:B:806:THR:O	1:B:810:THR:HG23	2.17	0.44
1:A:859:LEU:HD22	1:A:926:TRP:CZ2	2.53	0.44
1:A:290:VAL:HG23	1:A:297:SER:HB3	2.00	0.44
1:A:373:LEU:HD21	1:A:397:LEU:HD12	1.99	0.44
1:A:751:ALA:HB3	1:A:812:LEU:HD23	2.00	0.44
1:B:438:ARG:CB	7:B:3120:HOH:O	2.64	0.44
1:A:1069:ASN:O	1:B:1022:HIS:HE1	2.01	0.44
1:A:426:ARG:HD3	1:A:549:PHE:CE1	2.52	0.44
1:A:601:ASN:OD1	7:A:1511:HOH:O	2.21	0.44
1:A:776:VAL:HG23	7:A:1862:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:955:PHE:HA	1:B:1145:ASN:OD1	2.18	0.44
1:B:210:ILE:HG12	1:B:211:PHE:O	2.18	0.44
1:A:1272:PHE:HA	1:A:1275:LYS:HB2	2.00	0.43
1:A:529:ALA:HB1	7:A:1743:HOH:O	2.17	0.43
1:A:1141:SER:CB	1:A:1144:THR:HG22	2.47	0.43
1:A:236:ILE:HG12	7:A:1967:HOH:O	2.19	0.43
1:A:127:LEU:HD23	7:A:1699:HOH:O	2.18	0.43
1:B:153:ARG:N	1:B:154:PRO:HD2	2.33	0.43
1:B:425:ARG:CD	1:B:1208:MET:HE1	2.49	0.43
1:A:226:LEU:HD21	7:A:2056:HOH:O	2.19	0.43
1:A:388:PHE:HA	1:A:396:LEU:HG	2.00	0.43
1:A:706:SER:CB	7:A:1513:HOH:O	2.64	0.43
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.66	0.43
1:B:874:SER:HB3	1:B:900:ILE:HG21	2.01	0.43
1:A:99:PRO:O	1:A:103:ARG:HG3	2.17	0.43
1:A:1239:PHE:HE2	7:A:1508:HOH:O	2.01	0.43
1:A:779:MET:C	1:A:779:MET:SD	2.97	0.43
1:A:304:LEU:HD21	1:A:342:LYS:HG2	1.99	0.43
1:B:425:ARG:HD3	1:B:1208:MET:HE1	2.01	0.43
1:A:256:LEU:O	6:A:1406:FAD:H2B	2.19	0.43
1:A:600:GLU:HB2	7:A:2163:HOH:O	2.17	0.43
1:A:681:ALA:C	7:A:1512:HOH:O	2.56	0.43
1:A:812:LEU:HD11	1:A:825:CYS:N	2.34	0.43
1:B:1125:VAL:CB	7:B:3148:HOH:O	2.46	0.43
1:A:320:GLU:O	1:A:327:ARG:NH2	2.52	0.42
1:B:885:MET:HE1	7:B:3125:HOH:O	2.17	0.42
1:A:793:ARG:NH2	7:A:1507:HOH:O	2.49	0.42
1:A:255:LYS:HE2	1:A:274:PHE:CE1	2.55	0.42
1:B:843:LEU:CG	7:B:3662:HOH:O	2.60	0.42
1:A:1010:THR:HG23	3:A:1402:URC:O11	2.19	0.42
1:A:751:ALA:CB	1:A:812:LEU:HD23	2.50	0.42
1:A:839:ARG:NH1	7:A:1553:HOH:O	2.52	0.42
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.36	0.42
1:A:1061:ILE:HG13	7:A:1504:HOH:O	2.19	0.42
1:A:1326:SER:HB3	7:A:2139:HOH:O	2.19	0.42
1:A:555:ALA:O	1:A:1238:GLU:HA	2.20	0.42
1:B:231:GLU:HB3	7:B:3177:HOH:O	2.20	0.42
1:A:446:ILE:HD11	1:A:531:LEU:HB3	2.02	0.41
1:A:508:ARG:HH11	1:A:508:ARG:HG2	1.85	0.41
1:B:1081:ALA:HB3	7:B:3614:HOH:O	2.20	0.41
1:B:42:GLY:HA3	7:B:3675:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:GLY:HA3	7:A:1509:HOH:O	2.20	0.41
1:B:749:THR:HG21	1:B:809:SER:HA	2.02	0.41
1:B:934:CYS:HB3	1:B:936:LEU:HD12	2.02	0.41
1:A:142:PHE:HB3	1:A:1232:PHE:CE2	2.56	0.41
1:A:446:ILE:HD12	1:A:534:MET:CB	2.50	0.41
1:B:103:ARG:HG2	1:B:200:PHE:CD2	2.56	0.41
1:B:812:LEU:HD11	1:B:824:ARG:C	2.41	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.92	0.41
1:B:882:LEU:HD23	7:B:3639:HOH:O	2.19	0.41
1:A:446:ILE:O	1:A:446:ILE:CG2	2.68	0.41
1:B:267:MET:CG	7:B:3190:HOH:O	2.68	0.41
1:B:469:THR:N	1:B:470:PRO:CD	2.84	0.41
1:B:917:PRO:HG3	7:B:3770:HOH:O	2.21	0.41
1:B:1253:ILE:HB	7:B:3102:HOH:O	2.21	0.41
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.50	0.41
1:A:1180:MET:HE1	1:A:1263:PRO:HB3	2.03	0.41
1:A:1275:LYS:HD2	7:A:1806:HOH:O	2.21	0.41
1:A:964:LEU:N	1:A:965:PRO:CD	2.84	0.41
1:A:1027:GLY:C	7:A:1505:HOH:O	2.58	0.40
1:A:526:LEU:HD12	1:A:526:LEU:HA	1.89	0.40
1:A:1024:TYR:N	7:A:1505:HOH:O	2.54	0.40
1:A:469:THR:HG22	7:A:2081:HOH:O	2.20	0.40
1:B:942:ARG:HD2	7:B:3146:HOH:O	2.19	0.40
1:A:304:LEU:N	1:A:304:LEU:HD22	2.34	0.40
1:A:365:MET:HE3	1:A:386:HIS:N	2.36	0.40
1:A:477:TRP:CD1	1:A:523:LEU:HD12	2.56	0.40
1:A:850:PHE:CD2	1:A:930:VAL:HG22	2.56	0.40
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.85	0.40
1:B:394:LYS:HE2	7:B:3890:HOH:O	2.20	0.40
1:A:446:ILE:HG22	1:A:446:ILE:O	2.22	0.40
1:B:130:GLN:HE21	1:B:132:GLU:N	2.14	0.40
1:B:942:ARG:CA	7:B:3281:HOH:O	2.67	0.40
1:A:1060:LYS:HD3	7:A:1778:HOH:O	2.20	0.40
1:A:389:PHE:O	1:A:461:ARG:NH1	2.54	0.40
1:A:495:LEU:HB2	1:A:504:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1287/1331 (97%)	1239 (96%)	43 (3%)	5 (0%)	34	29
1	B	1287/1331 (97%)	1244 (97%)	38 (3%)	5 (0%)	34	29
All	All	2574/2662 (97%)	2483 (96%)	81 (3%)	10 (0%)	34	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	797	GLY
1	B	912	ARG
1	B	887	ASN
1	A	392	TYR
1	A	947	TYR
1	A	797	GLY
1	B	1111	GLY

### 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	1094/1123 (97%)	1061 (97%)	33 (3%)	41	40
1	B	1088/1123 (97%)	1072 (98%)	16 (2%)	65	69
All	All	2182/2246 (97%)	2133 (98%)	49 (2%)	52	55

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	61	LEU
1	A	62	GLN
1	A	112	CYS
1	A	224	LYS
1	A	246	ASP
1	A	304	LEU
1	A	396	LEU
1	A	397	LEU
1	A	445	THR
1	A	469	THR
1	A	498	ASP
1	A	505	GLU
1	A	526	LEU
1	A	533	ASP
1	A	550	GLN
1	A	551	LYS
1	A	552	ASP
1	A	683	ARG
1	A	692	LEU
1	A	743	TYR
1	A	744	LEU
1	A	812	LEU
1	A	911	PHE
1	A	932	ILE
1	A	981	LYS
1	A	1099	LYS
1	A	1106	LYS
1	A	1119	ASP
1	A	1239	PHE
1	A	1250	LYS
1	A	1275	LYS
1	A	1325	LYS
1	B	224	LYS
1	B	250	GLN
1	B	317	LYS
1	B	466	LEU
1	B	467	LYS
1	B	471	LYS
1	B	483	GLN
1	B	547	LEU
1	B	703	ASN

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Mol	Chain	Res	Type
1	B	743	TYR
1	B	744	LEU
1	B	812	LEU
1	B	899	ARG
1	B	911	PHE
1	B	1239	PHE
1	B	1250	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	111	GLN
1	A	145	ASN
1	A	350	ASN
1	A	585	GLN
1	A	699	GLN
1	A	703	ASN
1	A	863	HIS
1	A	869	ASN
1	A	893	ASN
1	A	904	ASN
1	A	1033	HIS
1	A	1043	HIS
1	A	1073	ASN
1	A	1284	GLN
1	B	11	ASN
1	B	62	GLN
1	B	108	HIS
1	B	111	GLN
1	B	130	GLN
1	B	143	GLN
1	B	145	ASN
1	B	350	ASN
1	B	386	HIS
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

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Mol	Chain	Res	Type
1	B	1073	ASN
1	B	1284	GLN

### 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 ⓘ

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
2	NAD	A	1401	-	24,29,48	1.37	4 (16%)	29,45,73	1.49	4 (13%)
4	BCT	A	1403	-	0,3,3	0.00	-	0,3,3	0.00	-
5	FES	A	1404	1,7	0,4,4	0.00	-	-	-	-
6	FAD	A	1406	-	51,58,58	1.84	6 (11%)	60,89,89	2.03	10 (16%)
6	FAD	B	3006	-	51,58,58	1.85	8 (15%)	60,89,89	2.45	14 (23%)
5	FES	B	3002	1,7	0,4,4	0.00	-	-	-	-
2	NAD	B	3003	-	22,25,48	1.21	4 (18%)	25,38,73	1.35	4 (16%)
5	FES	A	1405	1	0,4,4	0.00	-	-	-	-
3	URC	A	1402	-	13,13,13	3.77	4 (30%)	11,19,19	4.67	8 (72%)
5	FES	B	3001	1	0,4,4	0.00	-	-	-	-
4	BCT	B	3005	-	0,3,3	0.00	-	0,3,3	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	URC	B	3004	-	13,13,13	4.03	5 (38%)	11,19,19	5.40	8 (72%)

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3004	URC	C4-N3	-10.09	1.33	1.46
6	A	1406	FAD	C4X-C10	9.52	1.48	1.38
3	A	1402	URC	C4-N3	-9.08	1.34	1.46
6	B	3006	FAD	C4X-C10	8.60	1.47	1.38
3	A	1402	URC	C4-N9	-7.61	1.35	1.44
3	B	3004	URC	C4-N9	-7.34	1.35	1.44
3	B	3004	URC	C5-N7	-5.61	1.34	1.45
3	A	1402	URC	C5-N7	-5.14	1.35	1.45
6	A	1406	FAD	C4-C4X	4.48	1.49	1.41
6	B	3006	FAD	C4-C4X	4.01	1.48	1.41
2	A	1401	NAD	PN-O1N	3.57	1.62	1.50
3	B	3004	URC	O24-C8	3.25	1.30	1.23
2	A	1401	NAD	O4B-C1B	3.10	1.45	1.41
6	B	3006	FAD	C9A-C5X	3.02	1.48	1.42
6	A	1406	FAD	C9A-C5X	2.94	1.48	1.42
2	B	3003	NAD	C5A-C4A	2.90	1.48	1.40
3	A	1402	URC	O24-C8	2.86	1.29	1.23
6	B	3006	FAD	C6-C5X	-2.82	1.37	1.41
6	A	1406	FAD	C8-C7	2.78	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3006	FAD	C8-C7	2.60	1.47	1.40
6	B	3006	FAD	C9A-N10	2.60	1.42	1.38
2	A	1401	NAD	C5A-C4A	2.53	1.47	1.40
6	B	3006	FAD	C4X-N5	2.47	1.36	1.33
3	B	3004	URC	C5-C6	-2.40	1.48	1.52
6	A	1406	FAD	C9A-N10	2.33	1.41	1.38
2	A	1401	NAD	C2A-N3A	2.33	1.35	1.32
2	B	3003	NAD	O4B-C1B	2.31	1.44	1.41
6	B	3006	FAD	C2B-C1B	-2.24	1.50	1.53
6	A	1406	FAD	C5A-C4A	2.17	1.46	1.40
2	B	3003	NAD	PA-O3	2.04	1.62	1.54
2	B	3003	NAD	C2A-N3A	2.00	1.35	1.32

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3004	URC	C4-N9-C8	-10.83	105.53	112.89
6	B	3006	FAD	C4-N3-C2	9.22	122.93	115.14
3	B	3004	URC	C5-C4-N9	9.04	106.83	102.64
3	A	1402	URC	C4-N9-C8	-8.99	106.78	112.89
6	A	1406	FAD	C4-N3-C2	8.98	122.72	115.14
6	B	3006	FAD	C1'-N10-C9A	7.52	124.21	118.29
6	B	3006	FAD	C4-C4X-C10	-7.28	115.13	119.95
3	A	1402	URC	N1-C2-N3	6.92	123.41	116.12
3	B	3004	URC	N1-C2-N3	6.59	123.06	116.12
3	A	1402	URC	C5-C4-N9	6.38	105.59	102.64
3	B	3004	URC	N7-C8-N9	6.35	114.72	108.76
3	A	1402	URC	N7-C8-N9	6.18	114.56	108.76
6	A	1406	FAD	C4X-N5-C5X	4.61	121.38	116.77
6	A	1406	FAD	C4X-C4-N3	-4.54	117.23	123.43
6	B	3006	FAD	C4-C4X-N5	4.36	123.58	118.60
6	B	3006	FAD	C5X-C9A-N10	4.29	120.83	117.72
6	B	3006	FAD	C9A-N10-C10	-4.27	116.32	121.91
6	A	1406	FAD	C1'-N10-C9A	4.15	121.56	118.29
6	B	3006	FAD	N3A-C2A-N1A	-4.02	122.39	128.68
3	B	3004	URC	C6-N1-C2	-3.90	121.03	126.25
2	A	1401	NAD	O5D-PN-O2N	3.83	122.27	107.64
6	A	1406	FAD	C1B-N9A-C4A	-3.75	120.06	126.64
6	A	1406	FAD	N3A-C2A-N1A	-3.61	123.04	128.68
3	A	1402	URC	C6-N1-C2	-3.53	121.53	126.25
6	B	3006	FAD	C4X-C4-N3	-3.46	118.70	123.43
2	A	1401	NAD	N3A-C2A-N1A	-3.45	123.28	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3006	FAD	C4X-N5-C5X	3.44	120.21	116.77
6	A	1406	FAD	C4-C4X-C10	-3.42	117.69	119.95
2	A	1401	NAD	C4A-C5A-N7A	-3.13	106.14	109.40
3	B	3004	URC	O11-C2-N3	-3.06	116.82	122.92
3	A	1402	URC	O24-C8-N7	-2.96	121.69	125.94
2	B	3003	NAD	O2A-PA-O1A	2.96	122.28	110.68
6	B	3006	FAD	O2A-PA-O1A	2.89	126.54	112.24
2	B	3003	NAD	C4A-C5A-N7A	-2.80	106.48	109.40
6	B	3006	FAD	C1B-N9A-C4A	-2.78	121.75	126.64
2	B	3003	NAD	N3A-C2A-N1A	-2.76	124.37	128.68
2	B	3003	NAD	C3B-C2B-C1B	2.66	104.99	100.98
6	A	1406	FAD	C2A-N1A-C6A	2.55	123.11	118.75
3	B	3004	URC	O24-C8-N7	-2.53	122.31	125.94
6	A	1406	FAD	C9A-N10-C10	-2.52	118.60	121.91
6	A	1406	FAD	C5X-C9A-N10	2.30	119.39	117.72
3	A	1402	URC	O11-C2-N3	-2.17	118.59	122.92
6	B	3006	FAD	O4'-C4'-C3'	-2.15	103.86	109.10
2	A	1401	NAD	C3B-C2B-C1B	2.07	104.09	100.98
6	B	3006	FAD	C5'-C4'-C3'	2.06	116.19	112.20
3	B	3004	URC	O24-C8-N9	-2.06	122.97	125.94
6	B	3006	FAD	C4A-C5A-N7A	-2.06	107.25	109.40
3	A	1402	URC	O11-C2-N1	-2.03	118.00	121.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

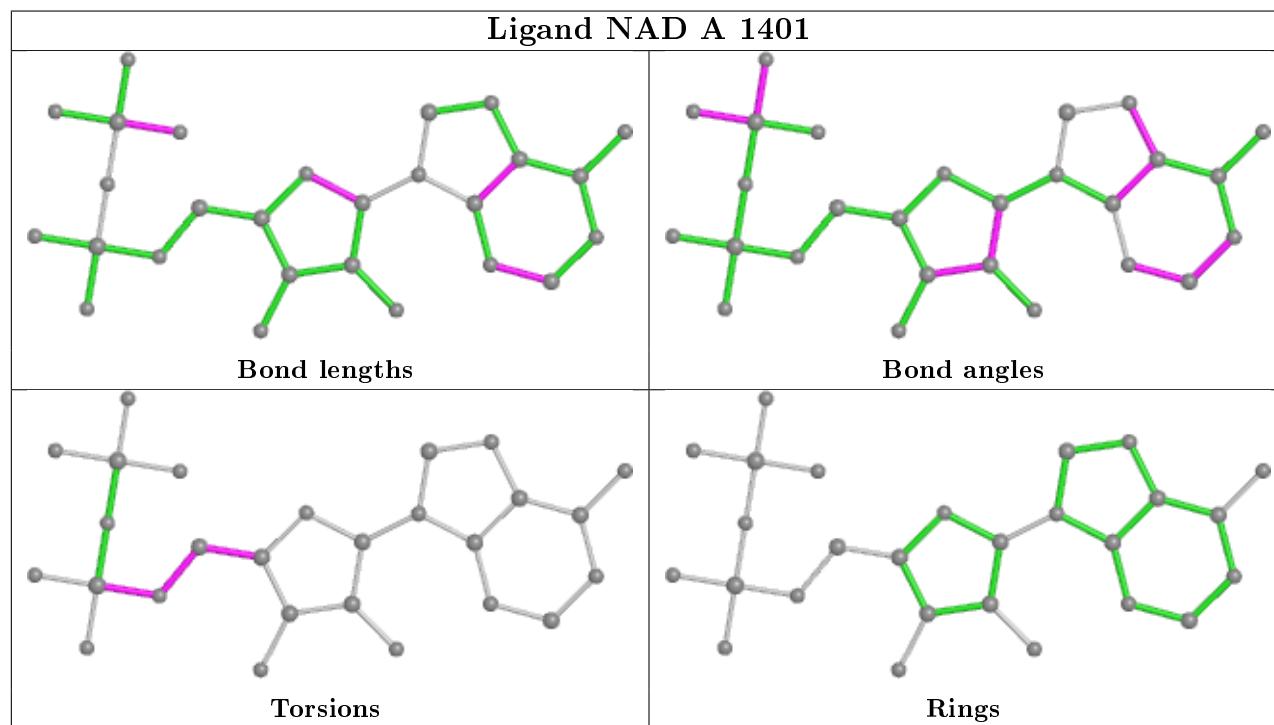
Mol	Chain	Res	Type	Atoms
2	A	1401	NAD	C5B-O5B-PA-O1A
6	A	1406	FAD	N10-C1'-C2'-O2'
6	A	1406	FAD	N10-C1'-C2'-C3'
6	B	3006	FAD	N10-C1'-C2'-O2'
6	B	3006	FAD	N10-C1'-C2'-C3'
2	A	1401	NAD	O4B-C4B-C5B-O5B
2	A	1401	NAD	C3B-C4B-C5B-O5B
6	B	3006	FAD	C2'-C3'-C4'-O4'
6	B	3006	FAD	C2'-C3'-C4'-C5'
2	A	1401	NAD	C5B-O5B-PA-O3
2	A	1401	NAD	C5B-O5B-PA-O2A
6	B	3006	FAD	O3'-C3'-C4'-C5'
2	A	1401	NAD	C4B-C5B-O5B-PA
6	B	3006	FAD	O3'-C3'-C4'-O4'
6	A	1406	FAD	C2'-C3'-C4'-O4'

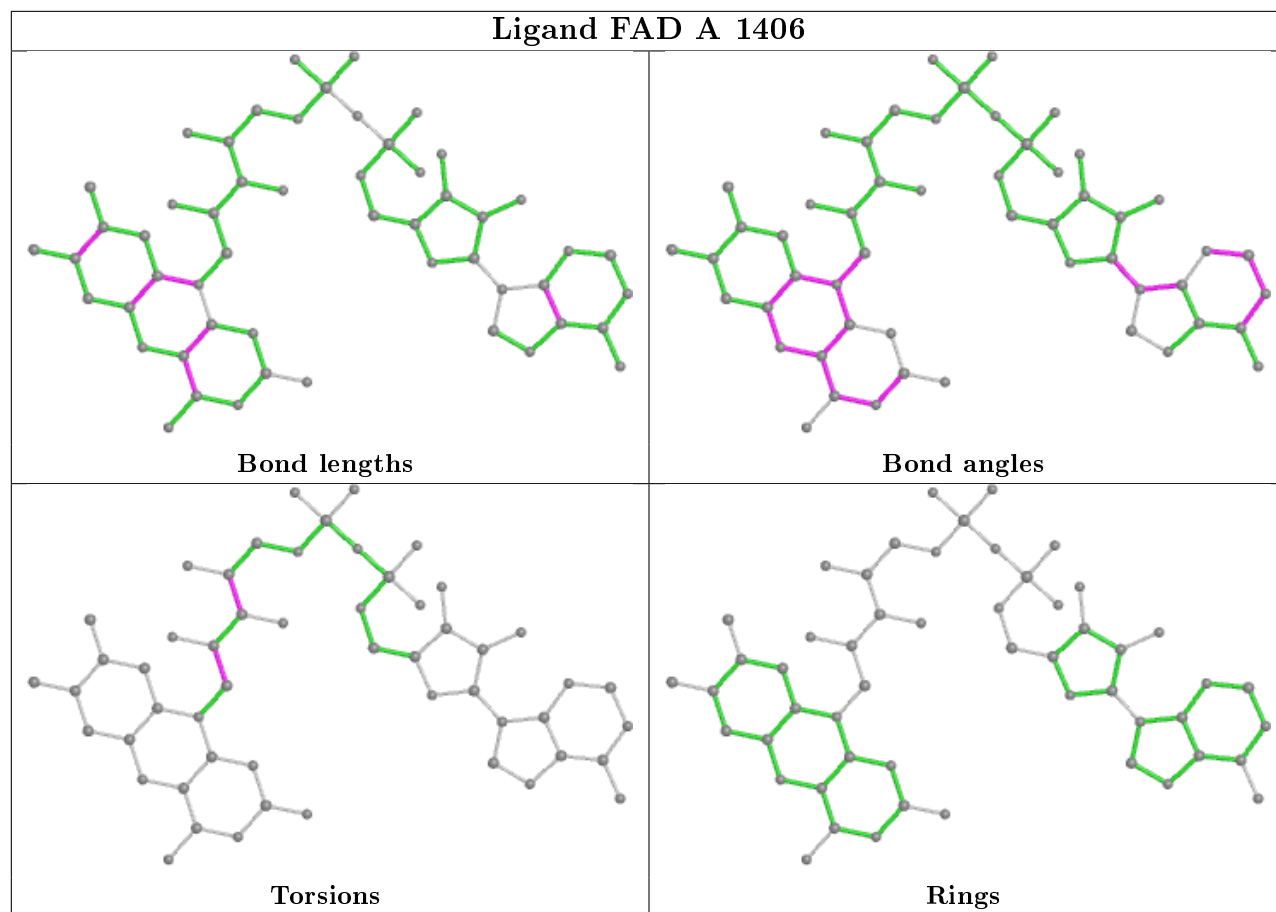
There are no ring outliers.

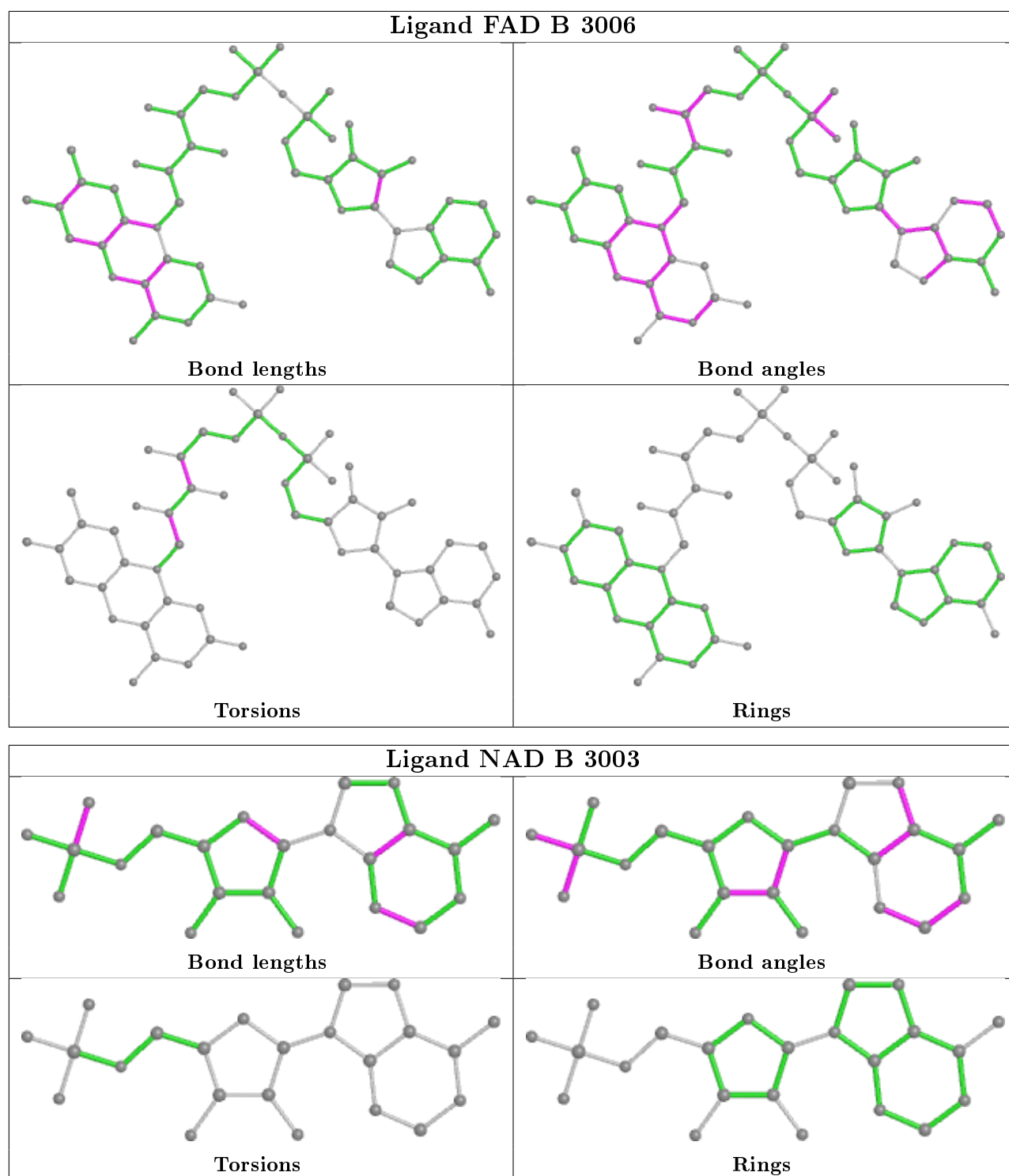
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1404	FES	1	0
6	A	1406	FAD	2	0
5	B	3002	FES	1	0
3	A	1402	URC	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1295/1331 (97%)	-0.08	24 (1%) 66 74	26, 41, 69, 123	0
1	B	1291/1331 (96%)	-0.31	10 (0%) 86 89	24, 35, 59, 102	0
All	All	2586/2662 (97%)	-0.20	34 (1%) 77 82	24, 38, 66, 123	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1324	CYS	8.3
1	B	1111	GLY	4.5
1	A	3	ALA	4.5
1	B	1287	ASP	4.3
1	A	1326	SER	3.6
1	B	1286	GLY	3.3
1	A	1111	GLY	3.1
1	B	218	LEU	3.1
1	A	473	LEU	3.0
1	A	1325	LYS	3.0
1	A	1318	THR	3.0
1	A	535	CYS	2.9
1	A	534	MET	2.8
1	A	531	LEU	2.8
1	A	1110	THR	2.6
1	A	149	CYS	2.5
1	B	1288	ASN	2.5
1	B	565	LYS	2.4
1	A	1039	GLY	2.4
1	A	1198	ALA	2.4
1	A	444	GLY	2.3
1	A	247	LEU	2.3
1	B	61	LEU	2.3
1	A	798	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1042	LEU	2.2
1	A	530	ASP	2.2
1	B	1289	ALA	2.2
1	A	1317	VAL	2.1
1	A	224	LYS	2.1
1	A	1038	MET	2.1
1	B	1106	LYS	2.1
1	A	1109	PRO	2.0
1	B	1110	THR	2.0
1	A	1264	LEU	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](#)

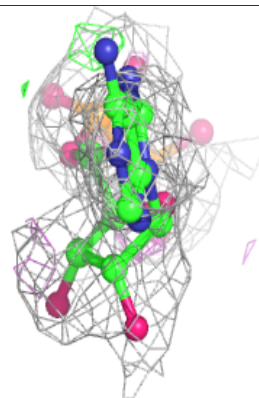
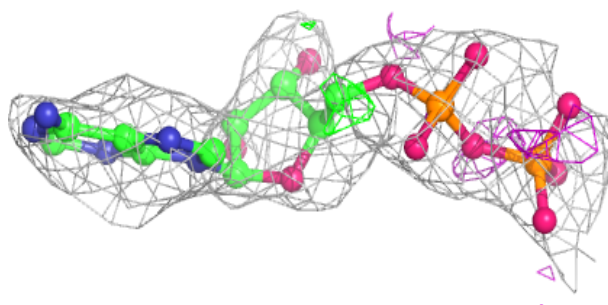
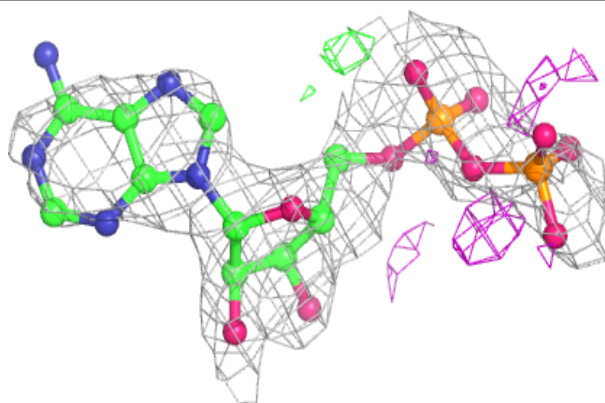
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	A	1401	27/44	0.77	0.19	72,96,117,123	0
2	NAD	B	3003	23/44	0.87	0.15	55,60,76,89	0
3	URC	A	1402	12/12	0.91	0.13	40,45,46,47	0
6	FAD	A	1406	53/53	0.96	0.12	34,40,44,46	0
3	URC	B	3004	12/12	0.96	0.12	35,36,40,41	0
6	FAD	B	3006	53/53	0.97	0.12	26,30,33,34	0
4	BCT	A	1403	4/4	0.98	0.14	37,41,45,45	0
5	FES	B	3001	4/4	0.98	0.06	41,45,45,52	0
4	BCT	B	3005	4/4	0.98	0.10	32,34,36,38	0
5	FES	A	1405	4/4	0.98	0.08	38,43,44,50	0
5	FES	A	1404	4/4	0.99	0.07	29,31,33,33	0
5	FES	B	3002	4/4	0.99	0.08	28,28,29,30	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.

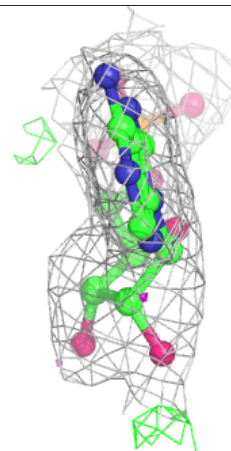
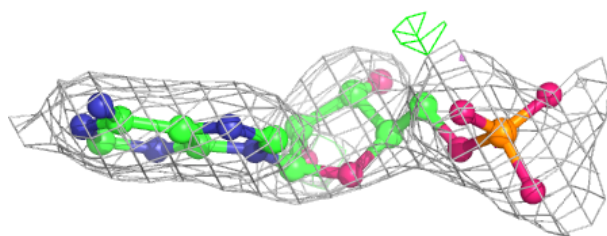
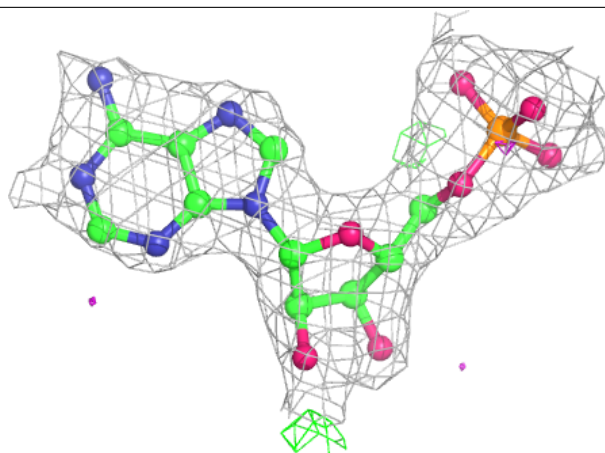
**Electron density around NAD A 1401:**

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

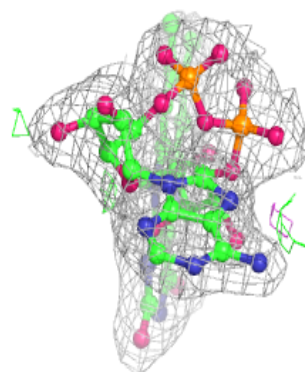
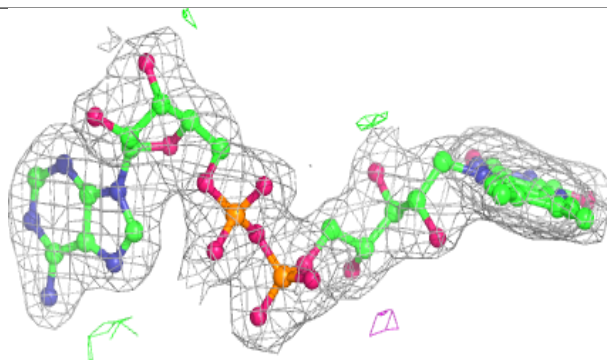
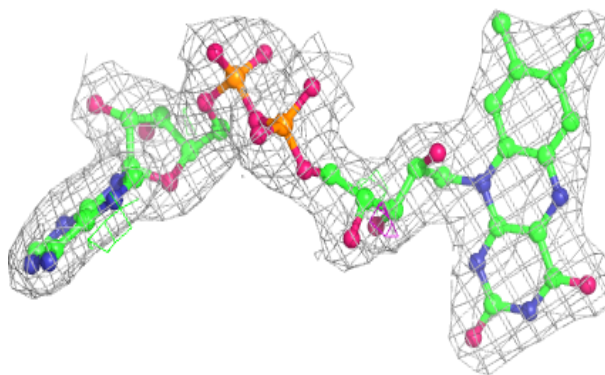


**Electron density around NAD B 3003:**

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

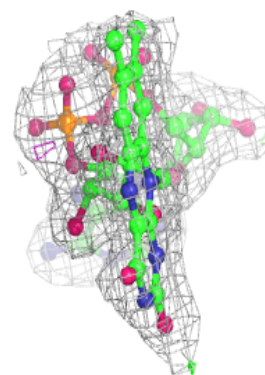
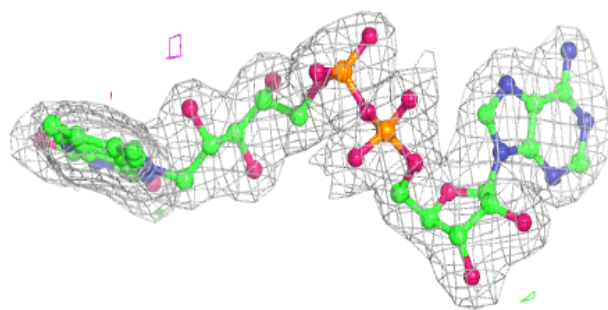
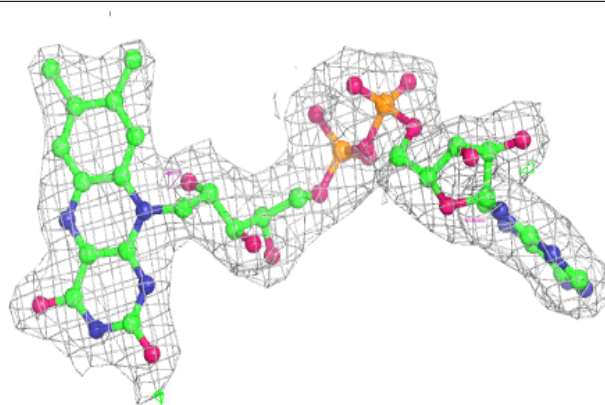
**Electron density around FAD A 1406:**

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



**Electron density around FAD B 3006:**

$2mF_o-DF_c$  (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.