Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 12:11 PM JST

PDB ID	:	6ABU / pdb_00006abu
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

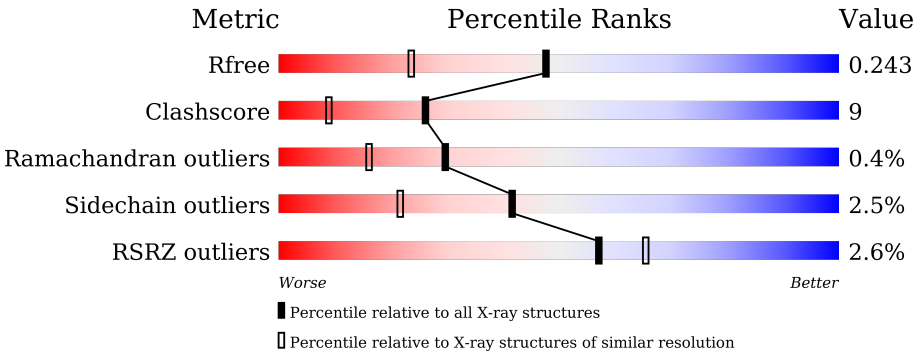
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.77 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 of 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 <=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	3% 82% 14% • •
1	B	1331	2% 82% 14% • •

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)

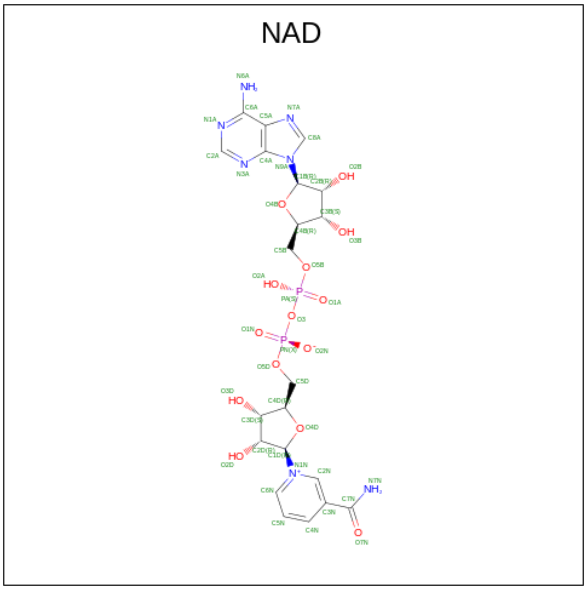
There are 7 unique types of molecules in this entry. The entry contains 21843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

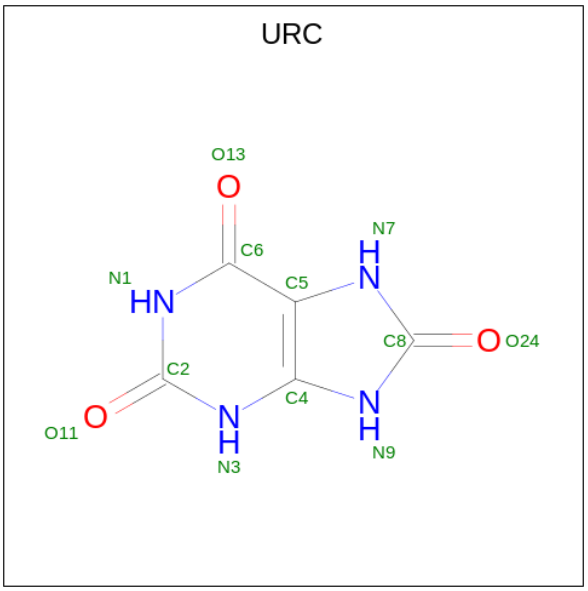
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1304	10076	6383	1735	1893	65	0	0	0
1	B	1291	9971	6320	1716	1871	64	0	0	0

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



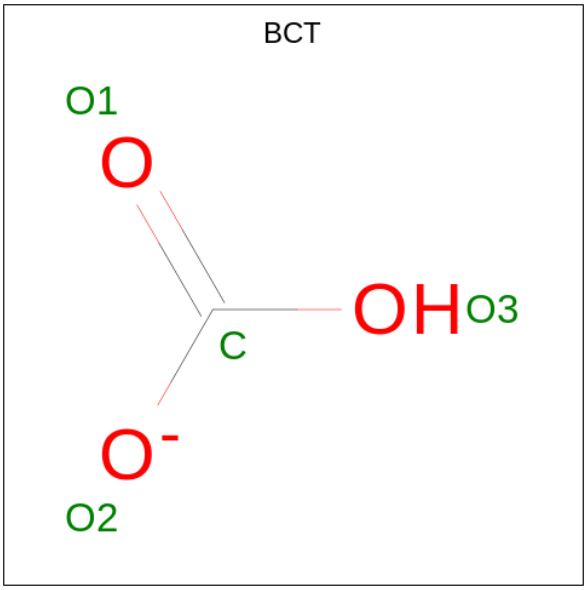
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
2	B	1	23	10	5	7	1	0	0

- Molecule 3 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



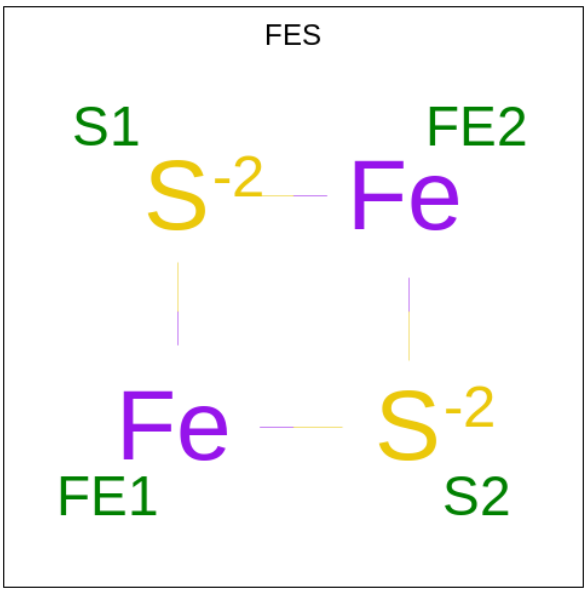
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	5	4	3	0	0
3	B	1	12	5	4	3	0	0

- Molecule 4 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



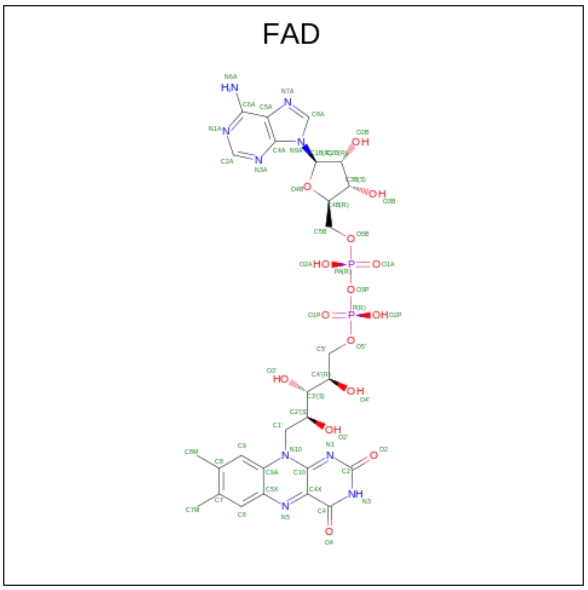
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	4	1	3		0	0
4	B	1	4	1	3		0	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 7 is water.

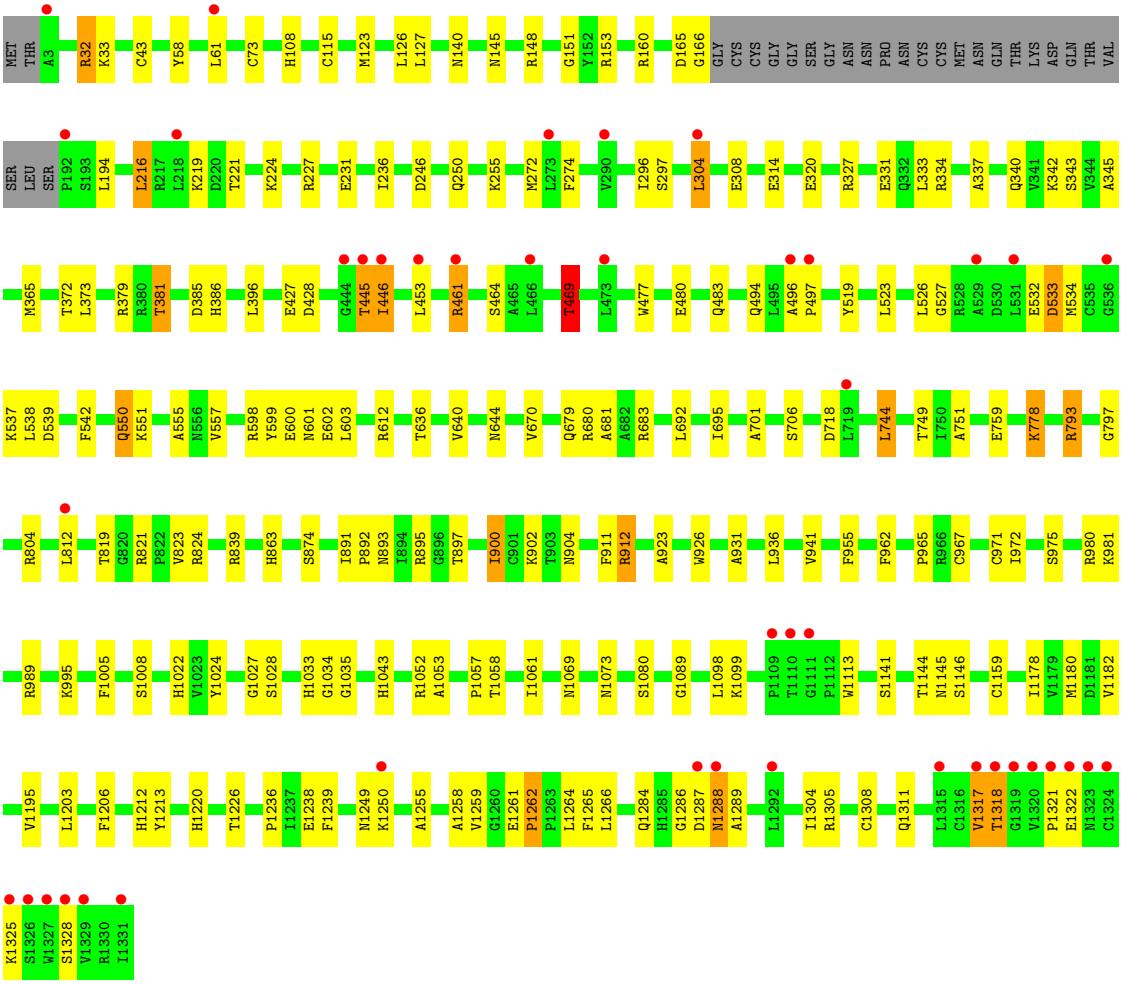
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	727	727	727	0	0
7	B	865	865	865	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

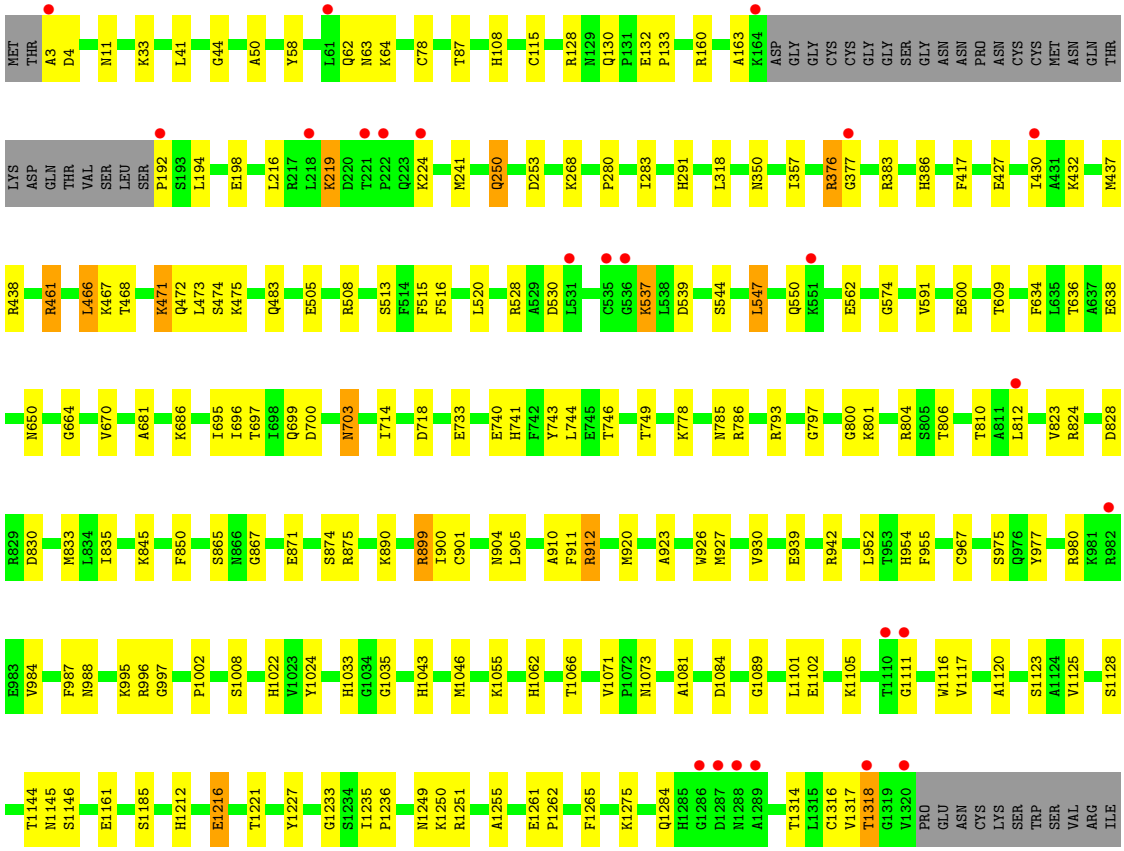
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:


MET THR A3 D4 N11 K33 L41 G44 A50 Y58 L61 Q62 N63 K64 C78 T87 H108 C115 R128 N129 Q130 P131 E132 P133 R160 A163 K164 ASP GLY GLY CYS CYS GLY GLY SER GLY ASN ASN PRO ASN CYS CYS MET ASN GLN THR
LYS ASP GLN THR VAL SER LEU SER P192 S193 L194 E198 L216 R217 L218 K219 D220 T221 P222 Q223 K224 M241 Q250 D253 K268 P280 I283 H291 L318 N350 I357 R376 G377 R383 H386 F417 E427 I430 A431 K432 M437
R438 R461 L466 K467 T468 K471 Q472 L473 S474 K475 Q483 E505 R508 S513 F514 F515 F516 L520 R528 A529 D530 L531 C535 G536 K537 L538 D539 S544 L547 Q550 K551 E562 G574 V591 E600 T609 F634 L635 T636 A637 E638
N650 G664 V670 A681 K686 I695 I696 T697 I698 Q699 D700 N703 I714 D718 E733 E740 H741 F742 Y743 L744 E745 T746 T749 K778 N785 R786 R793 G797 G800 K801 R804 S805 T806 T810 A811 L812 V823 R824 D828
R829 D830 M833 L834 I835 K845 F850 S865 N866 G867 E871 S874 R875 K890 R899 I900 C901 N904 L905 A910 F911 R912 M920 A923 W926 M927 V930 E939 R942 L952 T953 H954 F955 C967 S975 Q976 Y977 R980 K981 R982
E983 V984 F987 N988 K995 R996 G997 P1002 S1008 H1022 V1023 Y1024 H1033 G1034 G1035 H1043 M1046 K1055 H1062 T1066 V1071 P1072 N1073 A1081 D1084 G1089 L1101 E1102 K1105 T1110 G1111 W1116 V1117 A1120 S1123 A1124 V1125 S1128
T1144 N1145 S1146 E1161 S1185 H1212 E1216 T1221 Y1227 G1233 S1234 I1235 P1236 N1249 K1250 R1251 A1255 E1261 P1262 F1265 K1275 Q1284 H1285 G1286 D1287 N1288 A1289 T1314 L1315 C1316 V1317 T1318 G1319 V1320 PRO GLU ASN CYS LYS SER TRP SER VAL ARG ILE

4 Data and refinement statistics (i)

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 30.57 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.57-1.77) 99.8 (30.57-1.77)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	14591 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)	0.35 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAD, FES, URC, FAD, BCT

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	0.86	2/10289 (0.0%)	1.00	5/13923 (0.0%)
1	B	0.88	0/10181	1.00	6/13777 (0.0%)
All	All	0.87	2/20470 (0.0%)	1.00	11/27700 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1005	PHE	N-CA	5.36	1.52	1.46
1	A	1022	HIS	CE1-NE2	5.17	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	700	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	793	ARG	NE-CZ-NH1	6.22	127.72	121.50
1	A	793	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	A	1262	PRO	N-CA-C	5.77	117.73	110.70
1	B	515	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	542	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	830	ASP	CA-CB-CG	5.49	118.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	562	GLU	CB-CG-CD	5.39	121.76	112.60
1	B	899	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	A	469	THR	CB-CA-C	5.21	120.44	110.17
1	B	4	ASP	CA-CB-CG	5.11	117.71	112.60

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10076	0	10079	196	0
1	B	9971	0	9982	188	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	110	1
All	All	21843	0	20155	381	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 (381) 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:HG2	1:A:32:ARG:HH21	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:H	1:A:304:LEU:HD22	1.45	0.82
1:B:130:GLN:HE21	1:B:132:GLU:H	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:365:MET:HE2	1:A:464:SER:HB2	1.67	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:32:ARG:NH2	7:A:1518:HOH:O	2.23	0.71
1:A:236:ILE:HG12	7:A:1588:HOH:O	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:468:THR:O	7:B:3113:HOH:O	2.13	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: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:1250:LYS:HA	7:B:3815:HOH:O	1.96	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:B:241:MET:HE2	1:B:283:ILE:HG21	1.77	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:B:437:MET:C	7:B:3141:HOH:O	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:871:GLU:CD	7:B:3203:HOH:O	2.43	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
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:A:1027:GLY:C	7:A:1502:HOH:O	2.46	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:365:MET:HE3	1:A:386:HIS:N	2.19	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: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:A:165:ASP:O	1:A:166:GLY:C	2.48	0.57
1:B:741:HIS:HD2	7:B:3392:HOH:O	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:432:LYS:HE3	7:B:3565:HOH:O	2.08	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:B:1123:SER:C	7:B:3102:HOH:O	2.50	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:A:1058:THR:C	7:A:1507:HOH:O	2.50	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: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:812:LEU:HD11	1:B:823:VAL:C	2.35	0.51
1:B:108:HIS:HE1	1:B:194:LEU:O	1.92	0.51
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.93	0.51
1:A:1328:SER:HB2	7:A:1581:HOH:O	2.09	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:1203:LEU:HD23	1:A:1203:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:904:ASN:C	7:B:3165:HOH:O	2.54	0.50
1:B:987:PHE:HB3	7:B:3114:HOH:O	2.11	0.50
1:A:1113:TRP:CD1	7:A:1704:HOH:O	2.64	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
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:1264:LEU:C	1:A:1264:LEU:HD23	2.38	0.49
1:A:446:ILE:HD12	1:A:534:MET:HB2	1.94	0.49
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.13	0.49
1:A:523:LEU:HB3	7:A:2138:HOH:O	2.11	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:108:HIS:HD2	7:A:1974:HOH:O	1.95	0.48
1:A:272:MET:HB2	7:A:1719:HOH:O	2.13	0.48
1:A:1033:HIS:CE1	1:A:1043:HIS:CD2	3.01	0.48
1:A:1212:HIS:HB3	7:A:1581:HOH:O	2.11	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:995:LYS:HZ1	1:A:1284:GLN:HE21	1.58	0.48
1:B:219:LYS:HE2	7:B:3223:HOH:O	2.12	0.48
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.96	0.48
1:A:1317:VAL:O	1:A:1318:THR:HG22	2.12	0.48
1:B:911:PHE:O	1:B:912:ARG:C	2.56	0.48
1:A:1308:CYS:N	7:A:1513:HOH:O	2.46	0.48
1:B:749:THR:O	1:B:812:LEU:HD22	2.13	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:A:718:ASP:H	1:A:893:ASN:ND2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:911:PHE:O	1:A:912:ARG:C	2.56	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:396:LEU:C	1:A:396:LEU:HD12	2.39	0.47
1:A:1286:GLY:O	1:A:1287:ASP:HB3	2.15	0.47
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.30	0.47
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.58	0.47
1:A:153:ARG:HD2	1:A:153:ARG:C	2.40	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
1:A:231:GLU:OE2	1:A:680:ARG:NH1	2.47	0.47
1:A:751:ALA:HB3	1:A:812:LEU:CD2	2.44	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: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: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:B:920:MET:HE3	1:B:1265:PHE:CG	2.51	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:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.62	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:1180:MET:HE2	1:A:1180:MET:HB2	1.84	0.45
1:A:1069:ASN:O	1:B:1022:HIS:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:O	1:A:219:LYS:HG2	2.16	0.45
1:A:539:ASP:OD1	1:A:539:ASP:C	2.59	0.45
1:B:696:ILE:C	7:B:3112:HOH:O	2.59	0.45
1:B:1022:HIS:CD2	1:B:1128:SER:OG	2.69	0.45
1:A:1180:MET:HE3	1:A:1195:VAL:HG13	1.98	0.45
1:B:505:GLU:HG3	1:B:1317:VAL:HG22	1.98	0.45
1:B:1046:MET:HE2	1:B:1046:MET:HA	1.99	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:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.99	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:32:ARG:NH2	1:A:32:ARG:CG	2.70	0.44
1:A:304:LEU:HD22	1:A:304:LEU:N	2.23	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:B:539:ASP:CG	7:B:3446:HOH:O	2.60	0.44
1:A:227:ARG:HG3	7:A:1588:HOH:O	2.17	0.44
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.44
1:A:751:ALA:CB	1:A:812:LEU:CD2	2.96	0.44
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: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:A:601:ASN:C	7:A:1505:HOH:O	2.58	0.43
1:A:1178:ILE:CG2	1:A:1180:MET:HE2	2.48	0.43
1:B:438:ARG:NH1	7:B:3151:HOH:O	2.50	0.43
1:B:890:LYS:NZ	7:B:3145:HOH:O	2.49	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:905:LEU:HG	7:B:3165:HOH:O	2.19	0.43
1:B:955:PHE:HA	1:B:1145:ASN:OD1	2.19	0.43
1:A:255:LYS:HE2	1:A:274:PHE:CE1	2.54	0.43
1:B:733:GLU:CD	7:B:3144:HOH:O	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:CE2	1:A:219:LYS:HD2	2.54	0.43
1:A:1265:PHE:C	7:A:1521:HOH:O	2.60	0.43
1:B:50:ALA:N	7:B:3164:HOH:O	2.52	0.43
1:B:417:PHE:CZ	7:B:3141:HOH:O	2.65	0.43
1:A:1220:HIS:CD2	7:A:1581:HOH:O	2.62	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:B:988:ASN:CG	7:B:3114:HOH:O	2.60	0.43
1:B:749:THR:C	1:B:812:LEU:HD22	2.44	0.42
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:373:LEU:N	1:A:373:LEU:HD12	2.34	0.42
1:B:537:LYS:HB2	1:B:537:LYS:HE2	1.63	0.42
1:A:372:THR:C	1:A:373:LEU:HD12	2.44	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:115:CYS:HB3	1:A:744:LEU:CD2	2.46	0.42
1:A:955:PHE:HA	1:A:1145:ASN:OD1	2.19	0.42
1:A:1159:CYS:HB3	7:A:1958:HOH:O	2.19	0.42
1:B:574:GLY:HA2	1:B:1185:SER:O	2.20	0.42
1:A:496:ALA:O	1:A:497:PRO:C	2.61	0.42
1:B:812:LEU:HD11	1:B:823:VAL:HG12	2.01	0.42
1:A:373:LEU:N	1:A:373:LEU:CD1	2.83	0.42
1:A:385:ASP:C	1:A:385:ASP:OD1	2.62	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:N	1:B:900:ILE:HD12	2.35	0.42
1:B:591:VAL:C	7:B:3273:HOH:O	2.62	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:494:GLN:HB2	7:A:1834:HOH:O	2.20	0.41
1:A:1089:GLY:CA	7:A:1678:HOH:O	1.84	0.41
1:B:1216:GLU:CD	7:B:3228:HOH:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:ILE:HG21	1:A:1180:MET:HE2	2.03	0.41
1:A:1239:PHE:HE2	7:A:1501:HOH:O	2.03	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:B:1316:CYS:HB2	7:B:3163:HOH:O	2.21	0.41
1:A:304:LEU:CD2	1:A:342:LYS:HA	2.50	0.41
1:A:308:GLU:HG3	1:A:333:LEU:HD13	2.03	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:1144:THR:OG1	1:B:1146:SER:OG	2.35	0.41
1:B:472:GLN:CG	7:B:3113:HOH:O	2.67	0.41
1:B:939:GLU:CD	1:B:977:TYR:HE2	2.29	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:B:58:TYR:OH	1:B:63:ASN:HA	2.20	0.40
1:B:473:LEU:O	1:B:474:SER:HB2	2.20	0.40
1:B:600:GLU:HG2	7:B:3159:HOH:O	2.20	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:HD12	1:A:216:LEU:HA	1.90	0.40
1:A:1288:ASN:O	1:A:1289:ALA:C	2.64	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 symmetry 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%)	24	11
1	B	1287/1331 (97%)	1246 (97%)	37 (3%)	4 (0%)	36	22
All	All	2587/2662 (97%)	2498 (97%)	79 (3%)	10 (0%)	30	16

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%)	1066 (97%)	35 (3%)	34	13
1	B	1089/1124 (97%)	1070 (98%)	19 (2%)	53	36
All	All	2190/2248 (97%)	2136 (98%)	54 (2%)	42	22

All (54) 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

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Mol	Chain	Res	Type
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	304	LEU
1	A	331	GLU
1	A	343	SER
1	A	381	THR
1	A	445	THR
1	A	446	ILE
1	A	453	LEU
1	A	469	THR
1	A	526	LEU
1	A	533	ASP
1	A	537	LYS
1	A	550	GLN
1	A	551	LYS
1	A	679	GLN
1	A	683	ARG
1	A	692	LEU
1	A	744	LEU
1	A	778	LYS
1	A	900	ILE
1	A	972	ILE
1	A	981	LYS
1	A	1250	LYS
1	A	1288	ASN
1	A	1317	VAL
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

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Mol	Chain	Res	Type
1	B	537	LYS
1	B	547	LEU
1	B	550	GLN
1	B	703	ASN
1	B	899	ARG
1	B	952	LEU
1	B	1002	PRO
1	B	1216	GLU
1	B	1318	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	111	GLN
1	A	143	GLN
1	A	145	ASN
1	A	251	HIS
1	A	449	GLN
1	A	472	GLN
1	A	494	GLN
1	A	585	GLN
1	A	679	GLN
1	A	699	GLN
1	A	703	ASN
1	A	863	HIS
1	A	893	ASN
1	A	904	ASN
1	A	1033	HIS
1	A	1043	HIS
1	A	1073	ASN
1	A	1086	ASN
1	A	1148	ASN
1	A	1212	HIS
1	A	1284	GLN
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

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Mol	Chain	Res	Type
1	B	145	ASN
1	B	207	GLN
1	B	260	ASN
1	B	350	ASN
1	B	386	HIS
1	B	550	GLN
1	B	583	ASN
1	B	699	GLN
1	B	741	HIS
1	B	904	ASN
1	B	1022	HIS
1	B	1043	HIS
1	B	1062	HIS
1	B	1073	ASN
1	B	1086	ASN
1	B	1284	GLN
1	B	1285	HIS

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 oligosaccharides 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	$\#\|Z\| > 2$
5	FES	A	1405	1	0,4,4	-	-	-		
3	URC	B	3004	-	11,13,13	1.72	3 (27%)	12,19,19	3.14	9 (75%)
6	FAD	A	1406	-	56,58,58	1.45	9 (16%)	81,89,89	1.54	15 (18%)
4	BCT	B	3005	-	2,3,3	0.68	0	2,3,3	1.97	1 (50%)
5	FES	B	3001	1	0,4,4	-	-	-		
3	URC	A	1402	-	11,13,13	2.00	5 (45%)	12,19,19	2.61	7 (58%)
2	NAD	A	1401	-	27,29,48	1.56	5 (18%)	42,45,73	2.35	13 (30%)
5	FES	B	3002	7,1	0,4,4	-	-	-		
6	FAD	B	3006	-	56,58,58	1.56	9 (16%)	81,89,89	1.56	19 (23%)
5	FES	A	1404	7,1	0,4,4	-	-	-		
4	BCT	A	1403	-	2,3,3	0.94	0	2,3,3	0.42	0
2	NAD	B	3003	-	25,25,48	1.46	5 (20%)	38,38,73	1.75	10 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FAD	A	1406	-	-	2/34/50/50	0/6/6/6
3	URC	B	3004	-	-	-	0/2/2/2
5	FES	A	1405	1	-	-	0/1/1/1
5	FES	B	3001	1	-	-	0/1/1/1
3	URC	A	1402	-	-	-	0/2/2/2
2	NAD	A	1401	-	-	3/16/32/62	0/3/3/5
5	FES	B	3002	7,1	-	-	0/1/1/1
6	FAD	B	3006	-	-	6/34/50/50	0/6/6/6
5	FES	A	1404	7,1	-	-	0/1/1/1
2	NAD	B	3003	-	-	1/10/26/62	0/3/3/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3006	FAD	C9A-C5X	4.48	1.48	1.41
2	B	3003	NAD	C5A-C4A	4.42	1.47	1.39
2	A	1401	NAD	PN-O1N	4.25	1.64	1.50
6	A	1406	FAD	C9A-C5X	4.15	1.48	1.41
2	A	1401	NAD	C5A-C4A	3.86	1.46	1.39
3	A	1402	URC	O13-C6	3.60	1.30	1.23
6	B	3006	FAD	C8A-N7A	3.45	1.38	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1406	FAD	C5A-C4A	3.25	1.45	1.39
6	B	3006	FAD	C5X-N5	-3.16	1.33	1.39
3	B	3004	URC	C5-C6	2.95	1.49	1.42
6	A	1406	FAD	C8-C7	2.86	1.48	1.40
6	A	1406	FAD	C5A-C6A	2.85	1.49	1.41
6	A	1406	FAD	C4-N3	-2.78	1.33	1.38
6	B	3006	FAD	C5A-C4A	2.77	1.44	1.39
3	A	1402	URC	C8-N7	-2.77	1.33	1.39
3	A	1402	URC	C5-C6	2.75	1.49	1.42
6	B	3006	FAD	C5A-N7A	-2.74	1.33	1.39
2	A	1401	NAD	C5A-C6A	2.70	1.48	1.41
3	B	3004	URC	O24-C8	2.69	1.29	1.23
6	A	1406	FAD	C5X-N5	-2.65	1.34	1.39
2	B	3003	NAD	C8A-N7A	2.58	1.36	1.31
2	B	3003	NAD	C5A-N7A	-2.54	1.34	1.39
6	B	3006	FAD	C4X-N5	2.52	1.35	1.30
3	A	1402	URC	O24-C8	2.52	1.28	1.23
6	B	3006	FAD	C4-N3	-2.51	1.34	1.38
6	A	1406	FAD	C4A-N9A	-2.42	1.32	1.37
6	B	3006	FAD	C8-C7	2.40	1.46	1.40
3	A	1402	URC	C8-N9	-2.38	1.34	1.39
2	B	3003	NAD	C4A-N9A	-2.33	1.32	1.37
6	A	1406	FAD	C4X-N5	2.31	1.35	1.30
2	A	1401	NAD	C5A-N7A	-2.29	1.34	1.39
6	A	1406	FAD	O2-C2	2.28	1.28	1.24
6	B	3006	FAD	C2'-C3'	-2.22	1.49	1.53
2	B	3003	NAD	PA-O3	2.11	1.63	1.54
2	A	1401	NAD	C8A-N7A	2.10	1.35	1.31
3	B	3004	URC	O11-C2	2.04	1.27	1.23

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1401	NAD	C5A-C4A-N3A	-6.95	117.68	126.75
3	B	3004	URC	N7-C8-N9	6.03	116.74	107.19
2	B	3003	NAD	C5A-C4A-N3A	-5.71	119.30	126.75
2	A	1401	NAD	N3A-C4A-N9A	5.67	136.42	127.08
3	A	1402	URC	N7-C8-N9	5.02	115.14	107.19
6	B	3006	FAD	C5A-C4A-N3A	-4.90	120.36	126.75
2	A	1401	NAD	C2A-N3A-C4A	4.67	122.79	111.75
2	A	1401	NAD	O4B-C1B-N9A	4.38	116.69	108.06
3	B	3004	URC	N3-C2-N1	4.21	122.57	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	3006	FAD	N3A-C4A-N9A	4.17	133.95	127.08
2	A	1401	NAD	O5D-PN-O2N	4.16	123.55	107.64
2	B	3003	NAD	N3A-C4A-N9A	3.97	133.63	127.08
2	A	1401	NAD	N3A-C2A-N1A	-3.89	122.51	128.60
6	A	1406	FAD	C4A-N9A-C8A	3.65	109.68	105.73
3	B	3004	URC	O13-C6-C5	-3.58	119.03	127.24
3	B	3004	URC	C6-N1-C2	-3.57	121.19	126.34
3	A	1402	URC	N3-C2-N1	3.56	121.53	115.80
6	A	1406	FAD	C5A-C4A-N3A	-3.41	122.30	126.75
2	A	1401	NAD	C5A-N7A-C8A	3.36	108.29	103.51
6	A	1406	FAD	C2A-N3A-C4A	3.17	119.24	111.75
6	B	3006	FAD	C4A-N9A-C8A	3.16	109.16	105.73
6	A	1406	FAD	C4A-C5A-N7A	-3.13	106.81	110.62
2	A	1401	NAD	C4A-C5A-N7A	-3.12	106.82	110.62
3	A	1402	URC	N9-C4-N3	3.09	135.41	122.78
6	B	3006	FAD	O4B-C1B-N9A	-3.08	101.98	108.06
3	B	3004	URC	N9-C4-N3	3.05	135.25	122.78
6	A	1406	FAD	N3A-C4A-N9A	3.01	132.05	127.08
2	B	3003	NAD	C2A-N3A-C4A	2.97	118.78	111.75
3	A	1402	URC	O13-C6-C5	-2.95	120.47	127.24
2	B	3003	NAD	C4A-C5A-N7A	-2.94	107.04	110.62
6	A	1406	FAD	C5A-N7A-C8A	2.93	107.67	103.51
6	A	1406	FAD	C6A-C5A-N7A	2.93	137.47	132.02
6	B	3006	FAD	C5A-C6A-N6A	-2.86	117.20	123.43
6	A	1406	FAD	N3A-C2A-N1A	-2.85	124.15	128.60
2	A	1401	NAD	C4A-N9A-C8A	2.84	108.81	105.73
6	A	1406	FAD	C2B-C1B-N9A	2.76	120.29	113.30
6	A	1406	FAD	N9A-C8A-N7A	-2.76	110.14	113.91
3	B	3004	URC	O11-C2-N3	-2.74	116.64	121.82
2	A	1401	NAD	N9A-C8A-N7A	-2.73	110.18	113.91
6	B	3006	FAD	C9A-N10-C10	-2.71	116.54	120.77
2	B	3003	NAD	C5A-N7A-C8A	2.69	107.33	103.51
2	A	1401	NAD	C2B-C1B-N9A	-2.69	106.50	113.30
6	B	3006	FAD	N6A-C6A-N1A	2.66	124.18	118.35
6	B	3006	FAD	C2B-C1B-N9A	2.56	119.78	113.30
4	B	3005	BCT	O2-C-O1	2.55	126.17	119.55
3	B	3004	URC	O24-C8-N9	-2.52	120.89	125.39
3	A	1402	URC	O24-C8-N9	-2.50	120.93	125.39
3	B	3004	URC	C5-C6-N1	2.50	119.76	112.31
6	B	3006	FAD	N9A-C8A-N7A	-2.48	110.53	113.91
2	B	3003	NAD	O2A-PA-O1A	2.45	120.27	110.68
6	B	3006	FAD	C4A-N9A-C1B	-2.44	120.77	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	3006	FAD	O4-C4-C4X	-2.44	120.13	126.60
3	B	3004	URC	C6-C5-N7	2.41	137.12	131.96
3	A	1402	URC	C6-C5-N7	2.40	137.11	131.96
2	A	1401	NAD	C5A-C6A-N6A	-2.36	118.29	123.43
6	A	1406	FAD	C10-N1-C2	2.36	121.62	116.90
6	B	3006	FAD	C1'-N10-C9A	2.36	124.45	120.51
2	B	3003	NAD	N9A-C8A-N7A	-2.33	110.72	113.91
6	A	1406	FAD	C4X-C10-N1	-2.32	119.36	124.73
6	A	1406	FAD	C9A-C5X-N5	-2.32	119.92	122.43
6	B	3006	FAD	C5X-C9A-N10	2.28	120.31	117.95
6	B	3006	FAD	C2A-N3A-C4A	2.27	117.12	111.75
6	B	3006	FAD	C10-N1-C2	2.25	121.41	116.90
2	B	3003	NAD	N3A-C2A-N1A	-2.21	125.14	128.60
2	B	3003	NAD	C3B-C2B-C1B	2.18	105.57	101.43
6	B	3006	FAD	C4X-C4-N3	2.17	118.69	113.19
2	A	1401	NAD	C6A-C5A-N7A	2.16	136.04	132.02
6	A	1406	FAD	C6-C7-C8	-2.10	116.66	119.67
2	B	3003	NAD	O2B-C2B-C1B	-2.07	103.10	110.02
6	B	3006	FAD	C4X-C10-N1	-2.07	119.93	124.73
6	A	1406	FAD	O2A-PA-O1A	2.07	122.46	112.24
6	B	3006	FAD	O4'-C4'-C3'	-2.03	104.17	109.10
3	A	1402	URC	C6-N1-C2	-2.03	123.42	126.34
6	B	3006	FAD	N3A-C2A-N1A	-2.00	125.47	128.60

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	NAD	O4B-C4B-C5B-O5B
2	A	1401	NAD	C3B-C4B-C5B-O5B
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	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'

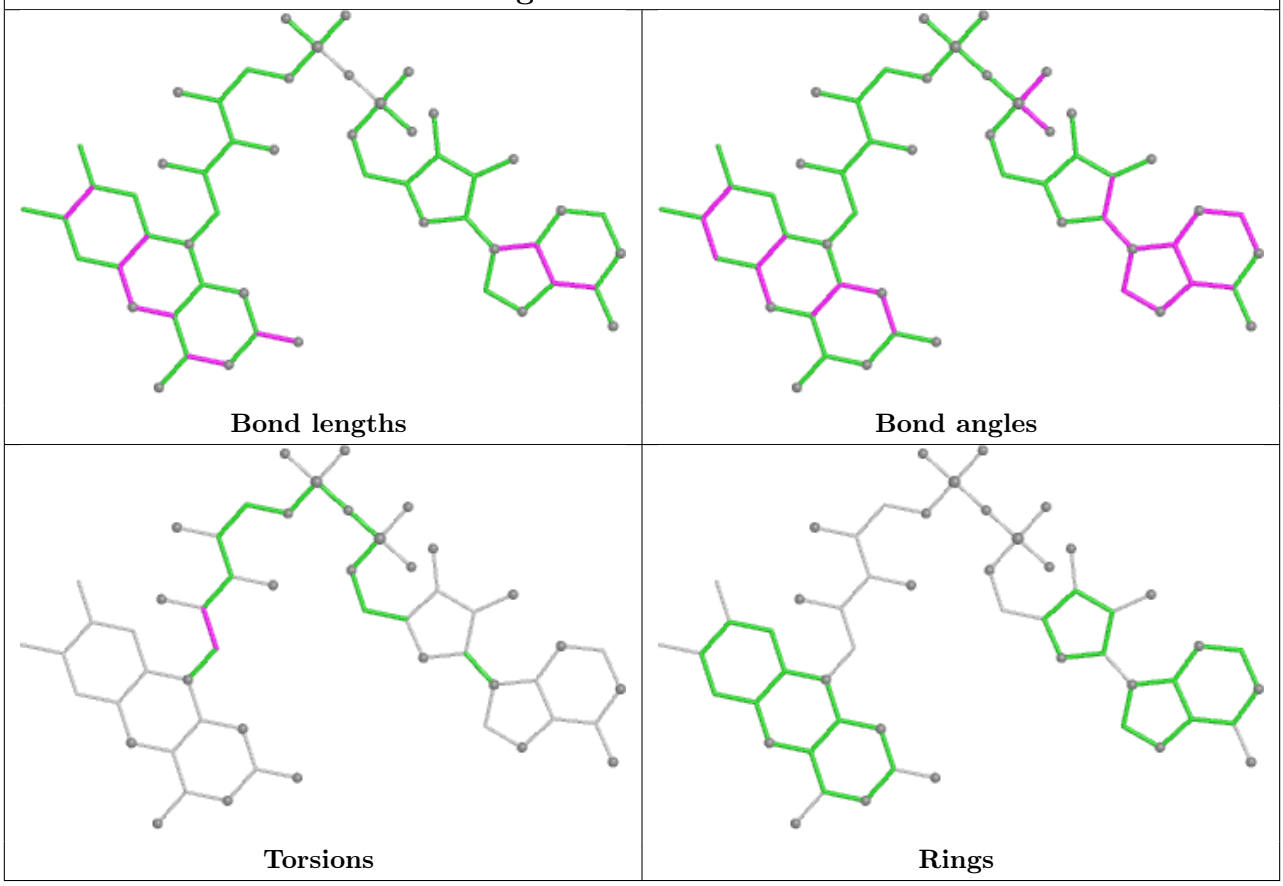
There are no ring outliers.

3 monomers are involved in 4 short contacts:

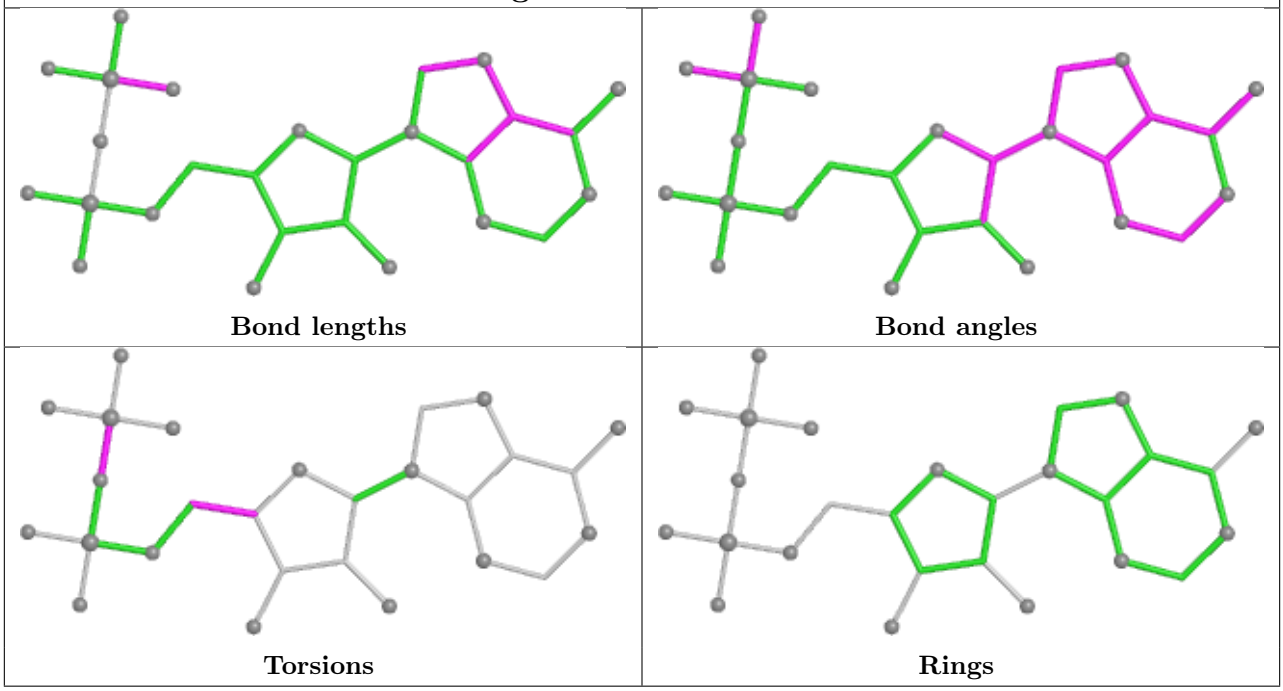
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1406	FAD	1	0
5	B	3001	FES	2	0
5	A	1404	FES	1	0

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 then 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.

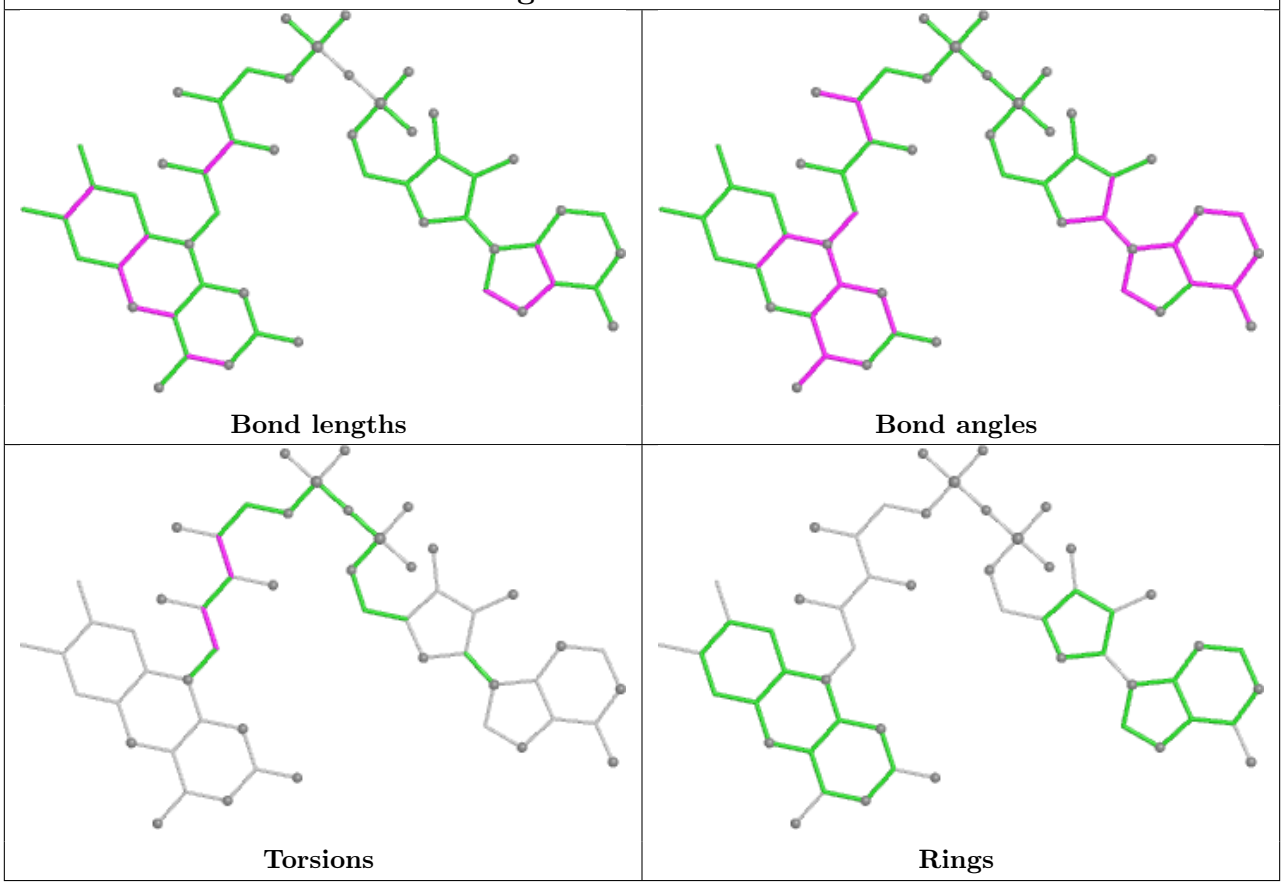
Ligand FAD A 1406

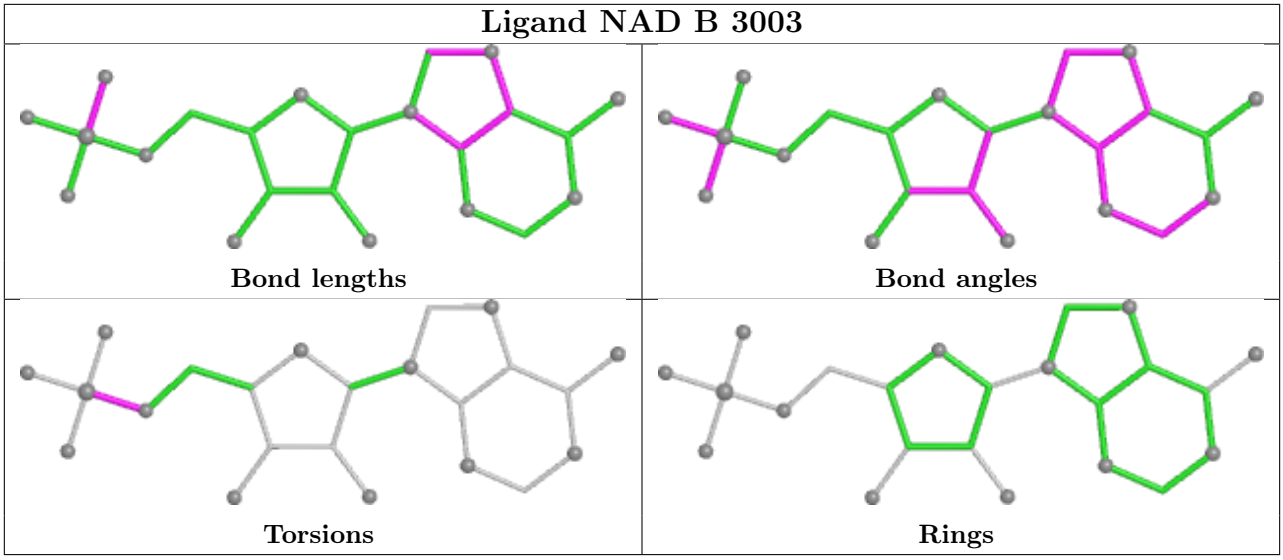


Ligand NAD A 1401



Ligand FAD B 3006





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.24	43 (3%)	49	56	16, 28, 52, 112	0
1	B	1291/1331 (96%)	-0.03	24 (1%)	66	74	16, 23, 44, 84	0
All	All	2595/2662 (97%)	0.10	67 (2%)	57	65	16, 25, 49, 112	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1321	PRO	7.7
1	A	1320	VAL	7.2
1	B	1287	ASP	5.2
1	B	1289	ALA	4.9
1	B	164	LYS	4.7
1	A	1318	THR	4.6
1	A	1110	THR	4.6
1	A	446	ILE	4.5
1	B	1320	VAL	4.5
1	A	192	PRO	4.4
1	A	3	ALA	4.4
1	A	1317	VAL	4.4
1	B	3	ALA	4.2
1	A	1111	GLY	4.0
1	B	218	LEU	3.8
1	B	1111	GLY	3.7
1	A	304	LEU	3.7
1	A	1319	GLY	3.5
1	A	1324	CYS	3.5
1	B	61	LEU	3.5
1	B	1288	ASN	3.5
1	A	1325	LYS	3.4
1	A	444	GLY	3.3
1	A	1323	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1315	LEU	3.3
1	A	531	LEU	3.2
1	A	536	GLY	3.1
1	A	290	VAL	3.1
1	B	1286	GLY	3.0
1	A	61	LEU	2.9
1	A	1331	ILE	2.9
1	A	1322	GLU	2.9
1	B	535	CYS	2.8
1	B	1110	THR	2.8
1	A	496	ALA	2.8
1	A	1250	LYS	2.8
1	A	461	ARG	2.7
1	A	1327	TRP	2.7
1	B	192	PRO	2.6
1	A	1329	VAL	2.6
1	B	536	GLY	2.6
1	B	222	PRO	2.5
1	A	812	LEU	2.5
1	A	1287	ASP	2.5
1	B	1318	THR	2.4
1	A	497	PRO	2.3
1	A	529	ALA	2.3
1	A	1109	PRO	2.3
1	B	221	THR	2.3
1	A	466	LEU	2.3
1	A	719	LEU	2.3
1	B	812	LEU	2.3
1	A	218	LEU	2.2
1	A	453	LEU	2.2
1	A	1292	LEU	2.2
1	B	531	LEU	2.2
1	B	377	GLY	2.2
1	A	1288	ASN	2.2
1	B	551	LYS	2.2
1	A	1328	SER	2.2
1	B	224	LYS	2.1
1	A	273	LEU	2.1
1	A	473	LEU	2.1
1	B	982	ARG	2.1
1	A	445	THR	2.0
1	B	430	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1326	SER	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 oligosaccharides in this entry.

6.4 Ligands (i)

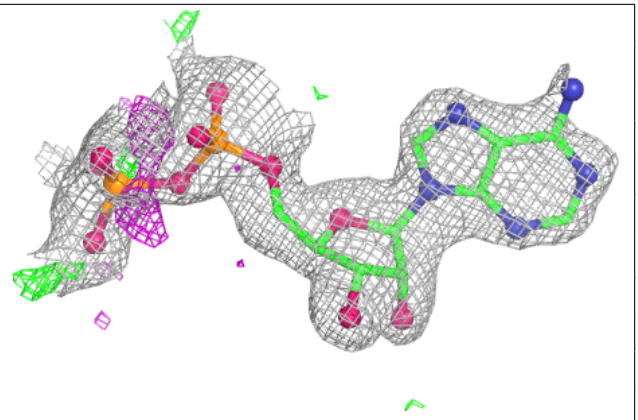
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

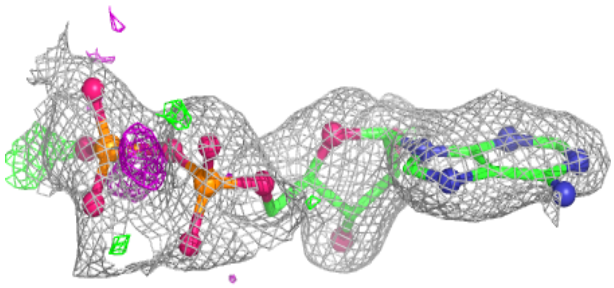
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	1401	27/44	0.81	0.13	43,60,84,86	0
2	NAD	B	3003	23/44	0.85	0.11	35,41,57,71	0
3	URC	A	1402	12/12	0.95	0.06	22,24,26,27	0
3	URC	B	3004	12/12	0.96	0.05	21,21,23,23	0
6	FAD	A	1406	53/53	0.97	0.06	23,27,29,30	0
5	FES	A	1405	4/4	0.98	0.09	29,31,32,35	0
5	FES	B	3001	4/4	0.98	0.10	28,30,32,34	0
4	BCT	A	1403	4/4	0.98	0.07	23,24,24,27	0
6	FAD	B	3006	53/53	0.98	0.05	16,20,22,23	0
4	BCT	B	3005	4/4	0.99	0.04	20,22,22,26	0
5	FES	A	1404	4/4	1.00	0.02	20,20,20,21	0
5	FES	B	3002	4/4	1.00	0.02	17,17,18,18	0

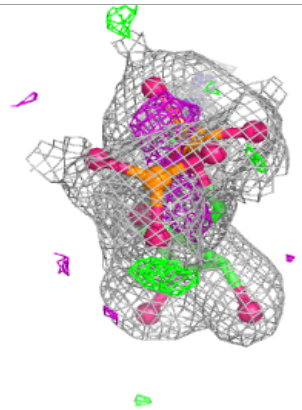
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

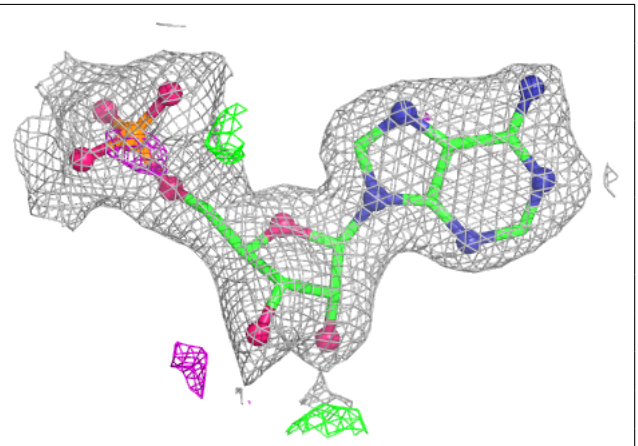


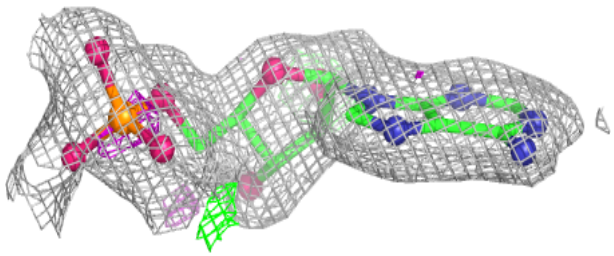


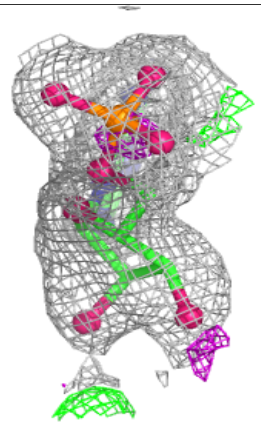


Electron density around NAD B 3003:

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

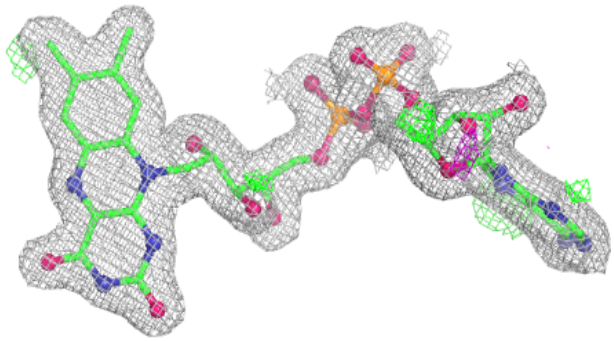


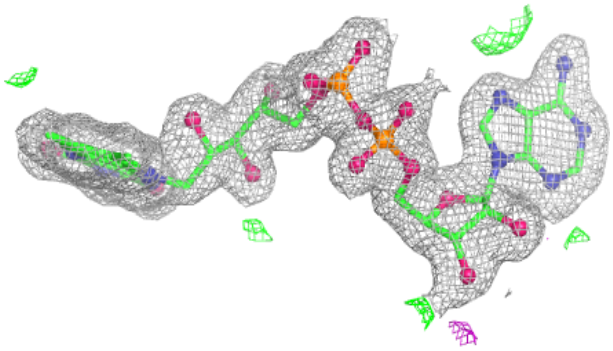


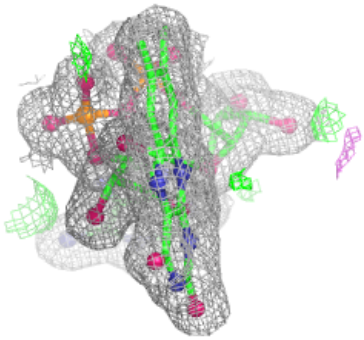


Electron density around FAD A 1406:

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







Electron density around FAD B 3006:

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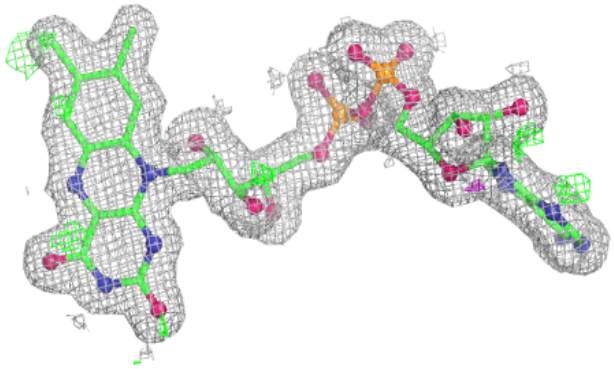
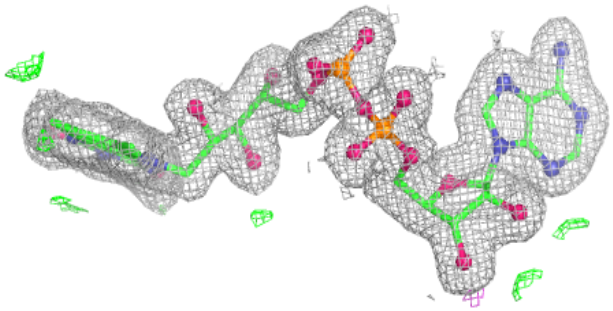
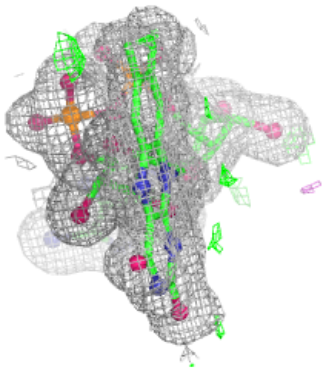
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.