Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 02:57 PM JST

PDB ID	:	6AC1 / pdb_00006ac1
Title	:	Rat Xanthine oxidoreductase, NADH 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:

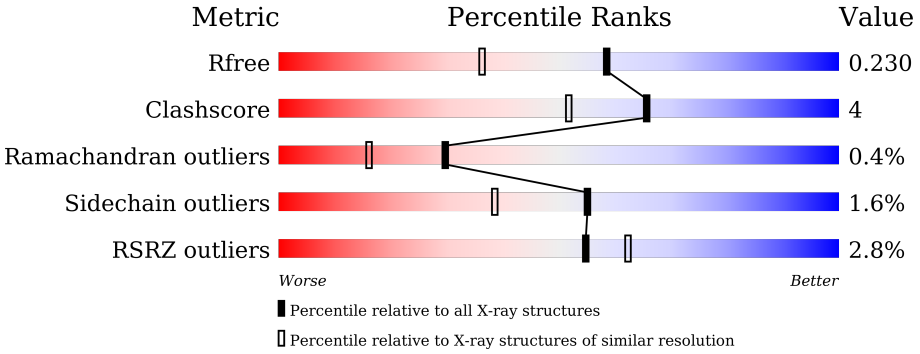
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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	4% 89% 8%
1	B	1331	2% 89% 8%

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
4	FES	B	3001	-	-	X	-

2 Entry composition (i)

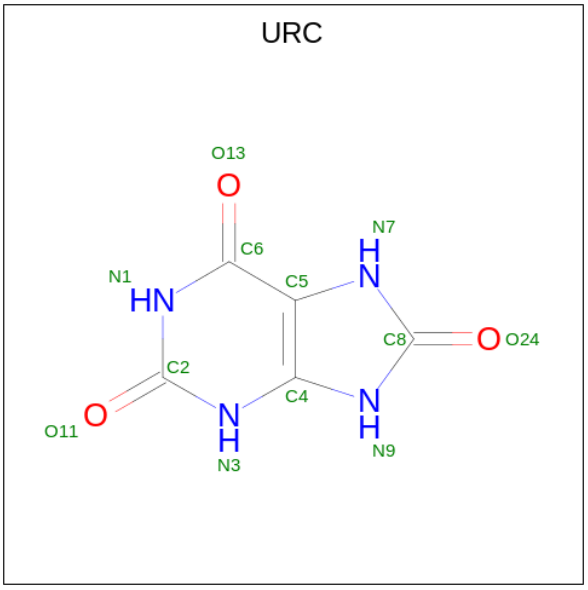
There are 7 unique types of molecules in this entry. The entry contains 21345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

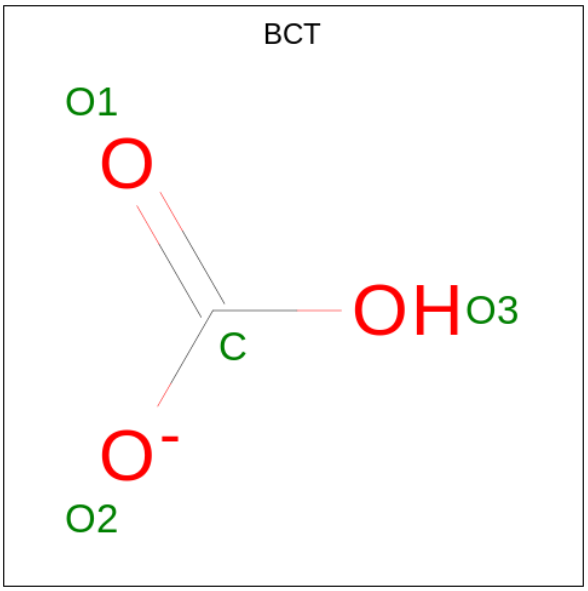
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1297	10033	6359	1727	1882	65	0	0	0
1	B	1291	9971	6320	1716	1871	64	0	0	0

- Molecule 2 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



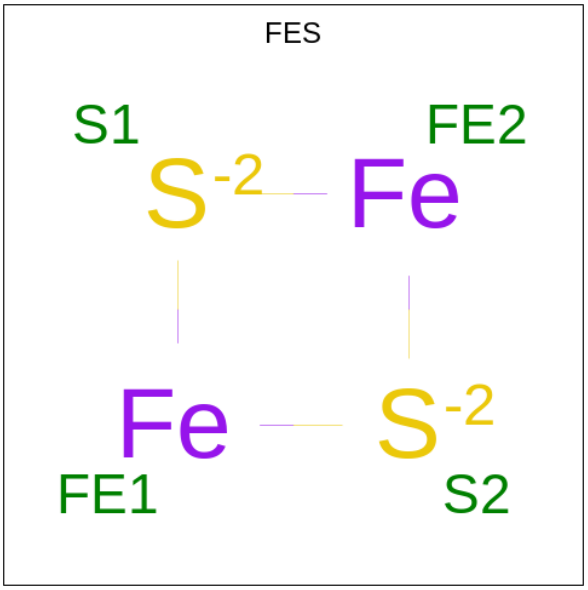
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	5	4	3	0	0
2	B	1	12	5	4	3	0	0

- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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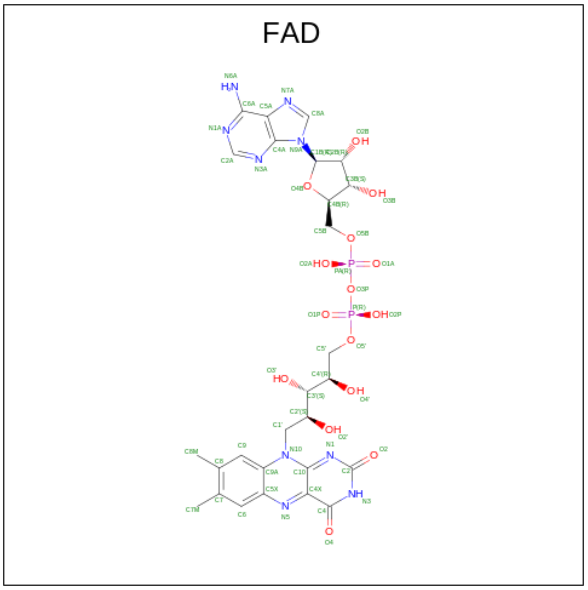
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	S			
4	B	1	4	2	2		0	0
			Total	Fe	S			
4	B	1	4	2	2		0	0

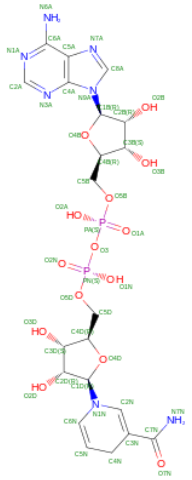
- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

NAI



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
6	B	1	44	21	7	14	2	0	0

- Molecule 7 is water.

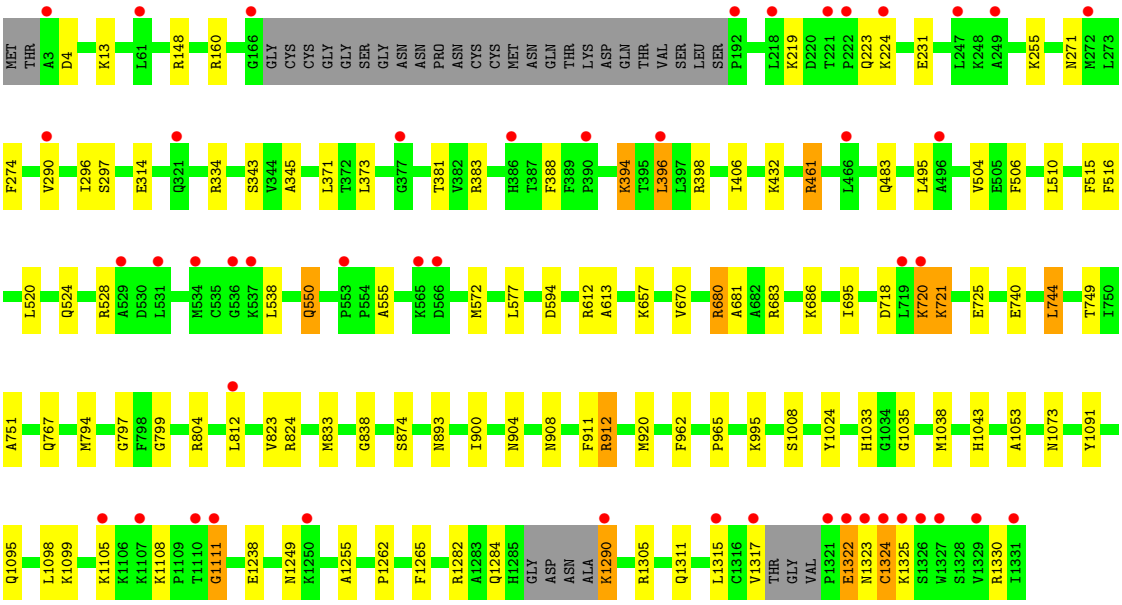
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	486	486	486	0	0
			Total	O		
7	B	613	613	613	0	0

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.

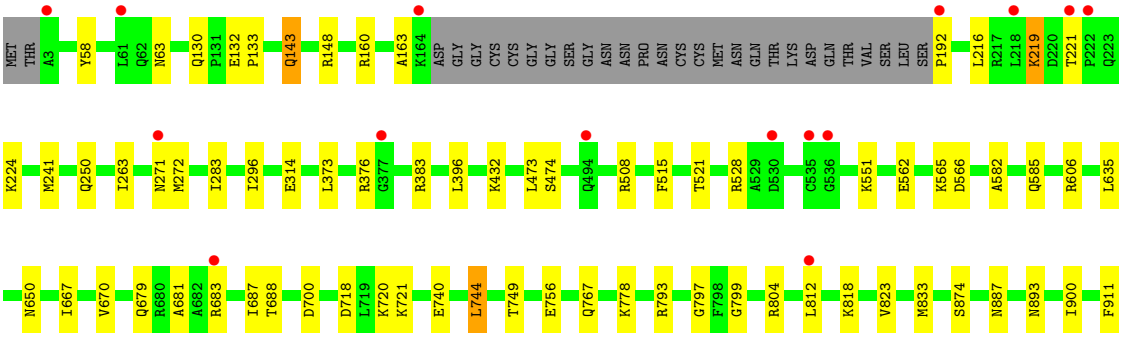
• Molecule 1: Xanthine dehydrogenase/oxidase

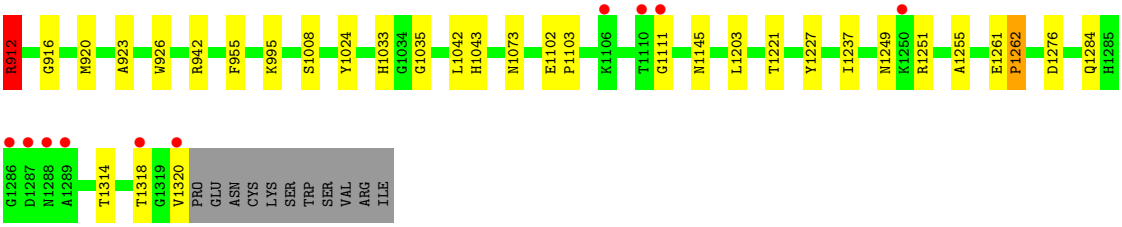
Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:




R912
G916
M920
A923
W926
R942
F955
K995
S1008
Y1024
H1033
G1034
G1035
L1042
H1043
N1073
E1102
P1103
K1106
T1110
G1111
N1145
L1203
T1221
Y1227
I1237
N1249
K1250
R1251
A1255
E1261
P1262
D1276
Q1284
H1285

G1286
D1287
N1288
A1289
T1314
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	98.80Å 137.55Å 222.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.19 – 1.77 32.19 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.19-1.77) 99.6 (32.19-1.77)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.188 , 0.222 0.196 , 0.230	Depositor DCC
R_{free} test set	14756 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.5	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	21345	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: FES, BCT, FAD, URC, NAI

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	0.89	2/10244 (0.0%)	1.00	2/13857 (0.0%)
1	B	0.92	3/10181 (0.0%)	1.01	8/13777 (0.1%)
All	All	0.90	5/20425 (0.0%)	1.00	10/27634 (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	10
1	B	0	9
All	All	0	19

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	ALA	N-CA	5.67	1.53	1.46
1	B	585	GLN	N-CA	5.47	1.53	1.46
1	A	1111	GLY	N-CA	5.45	1.52	1.44
1	B	521	THR	N-CA	5.32	1.52	1.46
1	A	1322	GLU	N-CA	5.08	1.52	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	793	ARG	NE-CZ-NH2	-9.49	110.66	119.20
1	B	793	ARG	NE-CZ-NH1	8.57	130.07	121.50
1	B	1276	ASP	CA-CB-CG	7.17	119.77	112.60
1	B	562	GLU	CB-CG-CD	6.25	123.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1262	PRO	N-CA-C	6.11	118.15	110.70
1	B	756	GLU	CB-CA-C	-5.98	100.57	110.14
1	B	700	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	515	PHE	CA-CB-CG	-5.50	108.30	113.80
1	B	515	PHE	CA-CB-CG	-5.29	108.51	113.80
1	B	1262	PRO	N-CA-C	5.13	116.96	110.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1305	ARG	Sidechain
1	A	1330	ARG	Sidechain
1	A	148	ARG	Sidechain
1	A	160	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	461	ARG	Sidechain
1	A	528	ARG	Sidechain
1	A	612	ARG	Sidechain
1	A	680	ARG	Sidechain
1	A	804	ARG	Sidechain
1	B	1251	ARG	Sidechain
1	B	148	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	376	ARG	Sidechain
1	B	383	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	804	ARG	Sidechain
1	B	912	ARG	Sidechain
1	B	942	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	10033	0	10041	78	0
1	B	9971	0	9982	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	4	0	0
2	B	12	0	4	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	8	0	0	1	0
4	B	8	0	0	2	0
5	A	53	0	31	3	0
5	B	53	0	31	2	0
6	A	44	0	27	2	0
6	B	44	0	27	1	0
7	A	486	0	0	0	0
7	B	613	0	0	4	0
All	All	21345	0	20147	154	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 4.

All (154) 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:812:LEU:HB2	7:B:3633:HOH:O	0.92	1.07
1:B:749:THR:HG22	1:B:812:LEU:HD23	1.39	1.04
1:B:718:ASP:H	1:B:893:ASN:HD22	1.16	0.93
1:B:1318:THR:HG21	1:B:1320:VAL:HG22	1.55	0.86
1:A:720:LYS:HA	1:A:720:LYS:CE	2.04	0.85
1:A:720:LYS:HA	1:A:720:LYS:HE3	1.60	0.84
1:A:695:ILE:H	1:A:904:ASN:HD22	1.28	0.80
1:B:130:GLN:HE21	1:B:132:GLU:H	1.30	0.78
1:A:812:LEU:HD21	1:A:823:VAL:O	1.85	0.77
1:B:272:MET:HE2	1:B:272:MET:HA	1.69	0.75
1:B:143:GLN:NE2	7:B:3101:HOH:O	2.21	0.73
1:B:192:PRO:HD2	7:B:3518:HOH:O	1.89	0.73
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.36	0.72
1:B:271:ASN:OD1	1:B:683:ARG:NH1	2.21	0.71
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.87	0.71
1:A:812:LEU:HD11	1:A:824:ARG:CA	2.19	0.71
1:B:812:LEU:HD11	1:B:823:VAL:C	2.17	0.70
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.74	0.70
1:B:718:ASP:H	1:B:893:ASN:ND2	1.90	0.69
1:B:1318:THR:CG2	1:B:1320:VAL:HG22	2.21	0.69
1:A:1323:ASN:HA	1:A:1324:CYS:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	1.78	0.66
1:A:1033:HIS:HE1	1:A:1043:HIS:HD2	1.43	0.65
1:A:718:ASP:H	1:A:893:ASN:HD22	1.45	0.65
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.28	0.64
1:A:1024:TYR:HA	1:B:1073:ASN:HD21	1.63	0.64
1:A:1323:ASN:HA	1:A:1324:CYS:CB	2.28	0.64
1:A:767:GLN:HE22	1:A:799:GLY:H	1.44	0.64
1:B:749:THR:CG2	1:B:812:LEU:HD23	2.23	0.64
1:B:812:LEU:HD11	1:B:823:VAL:HB	1.80	0.63
1:B:749:THR:O	1:B:812:LEU:HD22	1.97	0.63
1:A:483:GLN:HE22	1:A:1311:GLN:HE22	1.45	0.63
1:A:838:GLY:H	1:A:908:ASN:HD22	1.48	0.62
1:A:388:PHE:HA	1:A:396:LEU:HD13	1.83	0.61
1:B:688:THR:HG23	7:B:3303:HOH:O	2.01	0.61
1:A:495:LEU:HB2	1:A:504:VAL:HG13	1.83	0.60
1:A:695:ILE:H	1:A:904:ASN:ND2	1.99	0.60
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.83	0.60
1:A:1033:HIS:CE1	1:A:1043:HIS:HD2	2.21	0.59
1:B:744:LEU:HD13	4:B:3001:FES:S1	2.43	0.58
1:A:396:LEU:C	1:A:396:LEU:HD23	2.29	0.58
1:A:1073:ASN:HD21	1:B:1024:TYR:HA	1.67	0.58
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.49	0.58
1:A:751:ALA:HB3	1:A:812:LEU:HD23	1.85	0.58
1:B:749:THR:O	1:B:812:LEU:CD2	2.52	0.58
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.01	0.57
1:A:812:LEU:HD11	1:A:824:ARG:HA	1.85	0.57
1:B:767:GLN:HE22	1:B:799:GLY:H	1.53	0.56
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.06	0.56
1:B:812:LEU:CD1	1:B:823:VAL:HB	2.36	0.56
1:A:290:VAL:HG23	1:A:297:SER:HB2	1.88	0.56
1:B:271:ASN:CG	1:B:683:ARG:HH11	2.13	0.56
1:B:812:LEU:HD11	1:B:823:VAL:CB	2.35	0.56
1:A:718:ASP:H	1:A:893:ASN:ND2	2.04	0.55
1:B:1102:GLU:HG2	1:B:1103:PRO:HD3	1.90	0.54
1:A:720:LYS:HA	1:A:720:LYS:HE2	1.88	0.53
1:A:751:ALA:CB	1:A:812:LEU:HD23	2.39	0.53
1:B:1033:HIS:HD1	1:B:1035:GLY:H	1.55	0.53
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.91	0.52
1:A:371:LEU:HD21	1:A:406:ILE:HD12	1.92	0.52
5:A:1505:FAD:C4X	6:A:1506:NAI:C5N	2.87	0.52
1:B:812:LEU:HD21	1:B:823:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:O	1:B:219:LYS:CG	2.58	0.52
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.10	0.51
1:A:231:GLU:OE2	1:A:680:ARG:NH1	2.43	0.51
1:A:1033:HIS:CE1	1:A:1043:HIS:CD2	2.99	0.51
1:A:749:THR:HG22	1:A:812:LEU:HD22	1.93	0.51
1:A:516:PHE:CZ	1:A:520:LEU:HD11	2.46	0.51
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.94	0.50
1:A:911:PHE:O	1:A:912:ARG:C	2.54	0.50
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.28	0.50
1:A:812:LEU:HD11	1:A:824:ARG:C	2.37	0.50
1:A:751:ALA:H	1:A:812:LEU:HD21	1.76	0.50
1:B:1318:THR:HG22	1:B:1320:VAL:HG13	1.95	0.49
1:B:216:LEU:O	1:B:219:LYS:HG2	2.11	0.49
1:A:1033:HIS:HE1	1:A:1043:HIS:CD2	2.28	0.49
1:B:911:PHE:O	1:B:912:ARG:C	2.55	0.49
1:B:1033:HIS:NE2	1:B:1043:HIS:HD2	2.11	0.49
1:A:555:ALA:HB3	1:A:1238:GLU:HG2	1.94	0.49
1:B:130:GLN:NE2	1:B:132:GLU:H	2.06	0.48
5:A:1505:FAD:C4X	6:A:1506:NAI:C6N	2.92	0.48
1:B:812:LEU:CD1	1:B:823:VAL:HG12	2.43	0.48
1:B:900:ILE:HD12	1:B:900:ILE:N	2.30	0.47
1:A:740:GLU:HG2	1:A:833:MET:HE3	1.97	0.47
1:B:740:GLU:HG2	1:B:833:MET:HE3	1.96	0.47
1:A:721:LYS:HE2	1:A:725:GLU:OE2	2.15	0.47
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.96	0.46
1:B:271:ASN:CG	1:B:683:ARG:HD3	2.40	0.46
1:B:1314:THR:O	1:B:1318:THR:HB	2.15	0.46
1:A:751:ALA:CB	1:A:812:LEU:CD2	2.94	0.46
5:B:3005:FAD:C4X	6:B:3006:NAI:C5N	2.94	0.46
1:B:263:ILE:HD11	5:B:3005:FAD:H3B	1.98	0.46
1:B:874:SER:HB3	1:B:900:ILE:HG21	1.98	0.46
1:A:920:MET:HE3	1:A:1265:PHE:CG	2.52	0.45
1:B:635:LEU:HD21	1:B:818:LYS:HD3	1.97	0.45
1:B:955:PHE:HA	1:B:1145:ASN:OD1	2.17	0.45
1:B:995:LYS:NZ	1:B:1284:GLN:NE2	2.64	0.45
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.46	0.45
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.16	0.45
1:B:812:LEU:HD11	1:B:823:VAL:O	2.16	0.45
1:B:1318:THR:HG21	1:B:1320:VAL:CG2	2.36	0.45
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	0.45
1:A:900:ILE:HD12	1:A:900:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:ASN:OD1	1:B:778:LYS:NZ	2.50	0.44
1:A:812:LEU:HD23	1:A:812:LEU:C	2.43	0.43
1:A:255:LYS:HE2	1:A:274:PHE:CE1	2.53	0.43
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.53	0.43
1:A:555:ALA:O	1:A:1238:GLU:HA	2.19	0.43
1:A:720:LYS:HE3	1:A:720:LYS:CA	2.40	0.43
1:A:572:MET:HE2	1:A:577:LEU:HD13	2.00	0.43
1:B:744:LEU:CD1	4:B:3001:FES:S1	3.06	0.43
1:A:613:ALA:O	1:A:904:ASN:HB3	2.19	0.43
1:B:916:GLY:C	1:B:920:MET:HE3	2.43	0.43
1:A:657:LYS:HA	1:A:657:LYS:HD3	1.78	0.43
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.82	0.43
1:A:812:LEU:CD1	1:A:824:ARG:C	2.92	0.43
1:B:58:TYR:OH	1:B:63:ASN:HA	2.19	0.43
1:B:667:ILE:CD1	1:B:687:ILE:HD13	2.49	0.43
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.19	0.42
1:B:130:GLN:HE21	1:B:132:GLU:N	2.07	0.42
1:B:216:LEU:O	1:B:219:LYS:HG3	2.20	0.42
1:B:812:LEU:CD1	1:B:823:VAL:CG1	2.97	0.42
1:A:749:THR:O	1:A:812:LEU:HD13	2.19	0.42
1:A:290:VAL:HG22	1:A:297:SER:HB2	2.00	0.42
1:A:550:GLN:CA	1:A:550:GLN:HE21	2.33	0.42
1:B:508:ARG:HH11	1:B:508:ARG:HD3	1.69	0.42
1:A:271:ASN:CG	1:A:683:ARG:HD2	2.45	0.42
1:A:555:ALA:HB3	1:A:1238:GLU:CG	2.50	0.42
1:B:718:ASP:N	1:B:893:ASN:HD22	1.99	0.42
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.66	0.42
1:B:1035:GLY:HA3	1:B:1042:LEU:HD21	2.02	0.42
1:B:749:THR:C	1:B:812:LEU:CD2	2.93	0.41
1:B:1033:HIS:NE2	1:B:1043:HIS:CD2	2.88	0.41
1:A:751:ALA:HB3	1:A:812:LEU:CD2	2.49	0.41
1:A:550:GLN:HE21	1:A:550:GLN:HA	1.86	0.41
1:A:1322:GLU:HA	1:A:1323:ASN:HA	1.94	0.41
1:B:396:LEU:C	1:B:396:LEU:HD12	2.44	0.41
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.44	0.41
1:A:524:GLN:HG3	1:A:538:LEU:HD22	2.03	0.41
1:B:133:PRO:O	1:B:163:ALA:HA	2.21	0.41
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.50	0.41
1:A:394:LYS:HE3	1:A:394:LYS:HA	2.03	0.41
1:A:345:ALA:HB1	5:A:1505:FAD:H4'	2.03	0.41
1:A:506:PHE:CZ	1:A:510:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ASP:OD1	1:A:824:ARG:HD3	2.21	0.41
1:A:794:MET:HE3	1:A:1038:MET:HB3	2.02	0.41
1:A:388:PHE:CD1	1:A:396:LEU:HD22	2.56	0.40
1:A:744:LEU:HD13	4:A:1504:FES:S1	2.61	0.40
1:A:1282:ARG:NH2	1:A:1290:LYS:HB3	2.36	0.40
1:B:551:LYS:HD2	1:B:1237:ILE:HD11	2.02	0.40
1:B:1221:THR:CG2	1:B:1227:TYR:HB2	2.48	0.40
1:A:767:GLN:HE22	1:A:799:GLY:N	2.14	0.40
1:B:566:ASP:OD1	1:B:566:ASP:N	2.50	0.40
1:B:473:LEU:O	1:B:474:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

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	1289/1331 (97%)	1243 (96%)	40 (3%)	6 (0%)	24	11
1	B	1287/1331 (97%)	1253 (97%)	29 (2%)	5 (0%)	30	16
All	All	2576/2662 (97%)	2496 (97%)	69 (3%)	11 (0%)	30	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	A	1324	CYS
1	B	1008	SER
1	B	912	ARG
1	A	4	ASP
1	A	797	GLY
1	A	912	ARG
1	B	797	GLY

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Mol	Chain	Res	Type
1	A	1111	GLY
1	B	887	ASN
1	B	1111	GLY

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	1097/1124 (98%)	1072 (98%)	25 (2%)	44	25
1	B	1089/1124 (97%)	1078 (99%)	11 (1%)	68	55
All	All	2186/2248 (97%)	2150 (98%)	36 (2%)	55	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	219	LYS
1	A	223	GLN
1	A	224	LYS
1	A	343	SER
1	A	373	LEU
1	A	381	THR
1	A	383	ARG
1	A	394	LYS
1	A	396	LEU
1	A	398	ARG
1	A	432	LYS
1	A	461	ARG
1	A	550	GLN
1	A	686	LYS
1	A	720	LYS
1	A	721	LYS
1	A	744	LEU
1	A	1099	LYS
1	A	1105	LYS

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Mol	Chain	Res	Type
1	A	1108	LYS
1	A	1290	LYS
1	A	1315	LEU
1	A	1317	VAL
1	A	1325	LYS
1	B	143	GLN
1	B	219	LYS
1	B	221	THR
1	B	224	LYS
1	B	250	GLN
1	B	373	LEU
1	B	432	LYS
1	B	565	LYS
1	B	720	LYS
1	B	721	LYS
1	B	744	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	81	HIS
1	A	95	GLN
1	A	111	GLN
1	A	129	ASN
1	A	145	ASN
1	A	223	GLN
1	A	251	HIS
1	A	291	HIS
1	A	350	ASN
1	A	483	GLN
1	A	524	GLN
1	A	550	GLN
1	A	585	GLN
1	A	699	GLN
1	A	767	GLN
1	A	893	ASN
1	A	904	ASN
1	A	908	ASN
1	A	956	ASN
1	A	1016	GLN
1	A	1033	HIS

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Mol	Chain	Res	Type
1	A	1043	HIS
1	A	1073	ASN
1	A	1086	ASN
1	A	1137	ASN
1	A	1148	ASN
1	A	1284	GLN
1	B	62	GLN
1	B	63	ASN
1	B	130	GLN
1	B	143	GLN
1	B	145	ASN
1	B	207	GLN
1	B	350	ASN
1	B	524	GLN
1	B	556	ASN
1	B	585	GLN
1	B	704	ASN
1	B	767	GLN
1	B	869	ASN
1	B	893	ASN
1	B	956	ASN
1	B	1043	HIS
1	B	1073	ASN
1	B	1086	ASN
1	B	1137	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	$\#\|Z\| > 2$
4	FES	B	3002	1	0,4,4	-	-	-		
6	NAI	B	3006	-	45,48,48	1.24	3 (6%)	60,73,73	1.65	9 (15%)
3	BCT	A	1502	-	2,3,3	0.95	0	2,3,3	0.28	0
5	FAD	A	1505	-	56,58,58	1.39	9 (16%)	81,89,89	1.53	15 (18%)
3	BCT	B	3004	-	2,3,3	0.75	0	2,3,3	1.96	1 (50%)
6	NAI	A	1506	-	45,48,48	1.30	6 (13%)	60,73,73	1.87	13 (21%)
5	FAD	B	3005	-	56,58,58	1.49	9 (16%)	81,89,89	1.66	13 (16%)
2	URC	A	1501	-	11,13,13	2.42	5 (45%)	12,19,19	2.24	5 (41%)
4	FES	A	1503	1	0,4,4	-	-	-		
4	FES	A	1504	1	0,4,4	-	-	-		
4	FES	B	3001	1	0,4,4	-	-	-		
2	URC	B	3003	-	11,13,13	2.30	5 (45%)	12,19,19	2.18	5 (41%)

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
4	FES	B	3002	1	-	-	0/1/1/1
6	NAI	B	3006	-	-	4/29/72/72	0/5/5/5
5	FAD	A	1505	-	-	7/34/50/50	0/6/6/6
6	NAI	A	1506	-	-	4/29/72/72	0/5/5/5
5	FAD	B	3005	-	-	3/34/50/50	0/6/6/6
2	URC	A	1501	-	-	-	0/2/2/2
4	FES	A	1503	1	-	-	0/1/1/1
4	FES	A	1504	1	-	-	0/1/1/1
4	FES	B	3001	1	-	-	0/1/1/1
2	URC	B	3003	-	-	-	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3005	FAD	C9A-C5X	5.69	1.50	1.41
6	B	3006	NAI	C5A-C4A	4.37	1.47	1.39
6	A	1506	NAI	C5A-C4A	4.22	1.46	1.39
2	A	1501	URC	O13-C6	4.18	1.31	1.23
2	B	3003	URC	O13-C6	3.98	1.31	1.23
5	A	1505	FAD	C5A-C4A	3.86	1.46	1.39
6	A	1506	NAI	C6N-C5N	3.85	1.40	1.33
2	A	1501	URC	O24-C8	3.51	1.30	1.23
5	B	3005	FAD	C5X-N5	-3.44	1.32	1.39
5	A	1505	FAD	C9A-C5X	3.34	1.46	1.41
5	A	1505	FAD	C5A-N7A	-3.32	1.32	1.39
2	A	1501	URC	C5-C6	3.24	1.50	1.42
2	B	3003	URC	O24-C8	3.10	1.29	1.23
6	B	3006	NAI	C6N-C5N	3.04	1.38	1.33
5	A	1505	FAD	C1'-C2'	2.89	1.56	1.52
5	B	3005	FAD	C8-C7	2.84	1.48	1.40
5	A	1505	FAD	C4A-N9A	-2.80	1.31	1.37
2	A	1501	URC	C8-N9	-2.78	1.33	1.39
2	B	3003	URC	C5-C6	2.74	1.49	1.42
5	B	3005	FAD	C5A-C4A	2.69	1.44	1.39
5	A	1505	FAD	C4X-N5	2.59	1.35	1.30
2	B	3003	URC	O11-C2	2.59	1.28	1.23
6	A	1506	NAI	C7N-C3N	2.51	1.54	1.48
6	A	1506	NAI	C4A-N9A	-2.44	1.32	1.37
5	B	3005	FAD	C8A-N7A	2.43	1.36	1.31
2	A	1501	URC	C8-N7	-2.42	1.34	1.39
6	B	3006	NAI	C4A-N9A	-2.37	1.32	1.37
5	A	1505	FAD	O2-C2	2.37	1.28	1.24
2	B	3003	URC	C8-N9	-2.33	1.34	1.39
5	B	3005	FAD	C6-C7	2.26	1.42	1.39
5	B	3005	FAD	C4X-N5	2.26	1.35	1.30
5	A	1505	FAD	C8-C7	2.25	1.46	1.40
5	B	3005	FAD	C1'-C2'	2.22	1.55	1.52
6	A	1506	NAI	C5A-C6A	2.22	1.47	1.41
5	A	1505	FAD	C5A-C6A	2.16	1.47	1.41
5	B	3005	FAD	O3'-C3'	2.11	1.47	1.43
6	A	1506	NAI	C5A-N7A	-2.08	1.35	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1506	NAI	N3A-C4A-N9A	5.62	136.35	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1506	NAI	C5A-C4A-N3A	-5.50	119.58	126.75
6	B	3006	NAI	C5A-C4A-N3A	-5.45	119.64	126.75
5	B	3005	FAD	N3A-C4A-N9A	4.65	134.74	127.08
2	B	3003	URC	N7-C8-N9	4.50	114.31	107.19
5	B	3005	FAD	C5A-C4A-N3A	-4.42	120.98	126.75
6	A	1506	NAI	C4A-N9A-C8A	4.34	110.43	105.73
6	B	3006	NAI	N3A-C4A-N9A	4.33	134.22	127.08
6	A	1506	NAI	C2A-N3A-C4A	4.25	121.78	111.75
5	B	3005	FAD	C4A-N9A-C8A	4.21	110.29	105.73
5	B	3005	FAD	N3A-C2A-N1A	-4.18	122.07	128.60
5	A	1505	FAD	C4A-N9A-C8A	4.03	110.10	105.73
6	A	1506	NAI	N3A-C2A-N1A	-3.95	122.43	128.60
2	A	1501	URC	N7-C8-N9	3.92	113.40	107.19
6	B	3006	NAI	N3A-C2A-N1A	-3.86	122.56	128.60
6	B	3006	NAI	C2A-N3A-C4A	3.80	120.73	111.75
5	B	3005	FAD	C2A-N3A-C4A	3.64	120.35	111.75
5	A	1505	FAD	N3A-C4A-N9A	3.47	132.80	127.08
2	B	3003	URC	N3-C2-N1	3.45	121.34	115.80
2	A	1501	URC	N3-C2-N1	3.41	121.29	115.80
5	B	3005	FAD	N9A-C8A-N7A	-3.31	109.38	113.91
5	A	1505	FAD	C4-C4X-N5	3.22	122.81	118.23
6	A	1506	NAI	C5A-C6A-N6A	-3.10	116.68	123.43
5	A	1505	FAD	O4B-C1B-N9A	-3.06	102.03	108.06
5	B	3005	FAD	O4B-C1B-N9A	-3.05	102.05	108.06
6	B	3006	NAI	C4A-N9A-C8A	3.04	109.02	105.73
2	A	1501	URC	N9-C4-N3	2.97	134.92	122.78
6	B	3006	NAI	C5A-N7A-C8A	2.96	107.71	103.51
6	B	3006	NAI	N9A-C8A-N7A	-2.94	109.89	113.91
5	A	1505	FAD	C5A-C4A-N3A	-2.92	122.94	126.75
5	A	1505	FAD	N6A-C6A-N1A	2.92	124.75	118.35
5	B	3005	FAD	C9A-C5X-N5	-2.92	119.26	122.43
5	A	1505	FAD	C2A-N1A-C6A	2.87	123.69	118.77
5	A	1505	FAD	N9A-C8A-N7A	-2.86	110.01	113.91
6	B	3006	NAI	C4A-C5A-N7A	-2.78	107.23	110.62
5	A	1505	FAD	C5'-C4'-C3'	2.77	117.56	112.20
5	A	1505	FAD	O4-C4-C4X	-2.74	119.32	126.60
5	B	3005	FAD	C5A-C6A-N6A	-2.67	117.63	123.43
5	A	1505	FAD	C5A-N7A-C8A	2.64	107.26	103.51
6	A	1506	NAI	N9A-C8A-N7A	-2.62	110.34	113.91
6	B	3006	NAI	C6A-C5A-N7A	2.57	136.81	132.02
3	B	3004	BCT	O2-C-O1	2.50	126.02	119.55
2	B	3003	URC	N9-C4-N3	2.46	132.85	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1506	NAI	C5A-N7A-C8A	2.45	106.98	103.51
2	A	1501	URC	C6-N1-C2	-2.43	122.84	126.34
5	A	1505	FAD	O2'-C2'-C1'	2.36	115.51	109.80
6	A	1506	NAI	C6A-C5A-N7A	2.34	136.39	132.02
2	A	1501	URC	O13-C6-C5	-2.31	121.95	127.24
5	B	3005	FAD	C2B-C1B-N9A	2.25	118.99	113.30
6	A	1506	NAI	N6A-C6A-N1A	2.19	123.15	118.35
6	A	1506	NAI	O4D-C4D-C3D	-2.15	100.86	105.11
5	B	3005	FAD	C5A-N7A-C8A	2.13	106.53	103.51
2	B	3003	URC	O11-C2-N3	-2.12	117.82	121.82
5	B	3005	FAD	C5X-N5-C4X	2.12	121.59	118.07
6	A	1506	NAI	C3N-C7N-N7N	2.12	121.43	117.67
5	A	1505	FAD	O4'-C4'-C3'	-2.11	103.97	109.10
6	A	1506	NAI	O2B-C2B-C1B	-2.06	103.14	110.02
5	B	3005	FAD	C4-C4X-N5	2.06	121.16	118.23
2	B	3003	URC	C6-C5-N7	2.03	136.31	131.96
5	A	1505	FAD	C2B-C3B-C4B	2.03	106.58	102.64
5	A	1505	FAD	C4X-C4-N3	2.01	118.28	113.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1505	FAD	N10-C1'-C2'-O2'
5	A	1505	FAD	N10-C1'-C2'-C3'
5	B	3005	FAD	N10-C1'-C2'-O2'
5	B	3005	FAD	N10-C1'-C2'-C3'
5	A	1505	FAD	C2'-C3'-C4'-O4'
6	A	1506	NAI	C2D-C1D-N1N-C6N
5	A	1505	FAD	C2'-C3'-C4'-C5'
6	B	3006	NAI	C2D-C1D-N1N-C6N
6	A	1506	NAI	O4D-C1D-N1N-C6N
6	B	3006	NAI	O4D-C1D-N1N-C6N
5	A	1505	FAD	O3'-C3'-C4'-O4'
5	A	1505	FAD	O3'-C3'-C4'-C5'
6	A	1506	NAI	O4D-C4D-C5D-O5D
6	B	3006	NAI	O4D-C4D-C5D-O5D
6	A	1506	NAI	C2N-C3N-C7N-N7N
6	B	3006	NAI	C2N-C3N-C7N-N7N
5	B	3005	FAD	C2'-C3'-C4'-C5'
5	A	1505	FAD	C2'-C1'-N10-C10

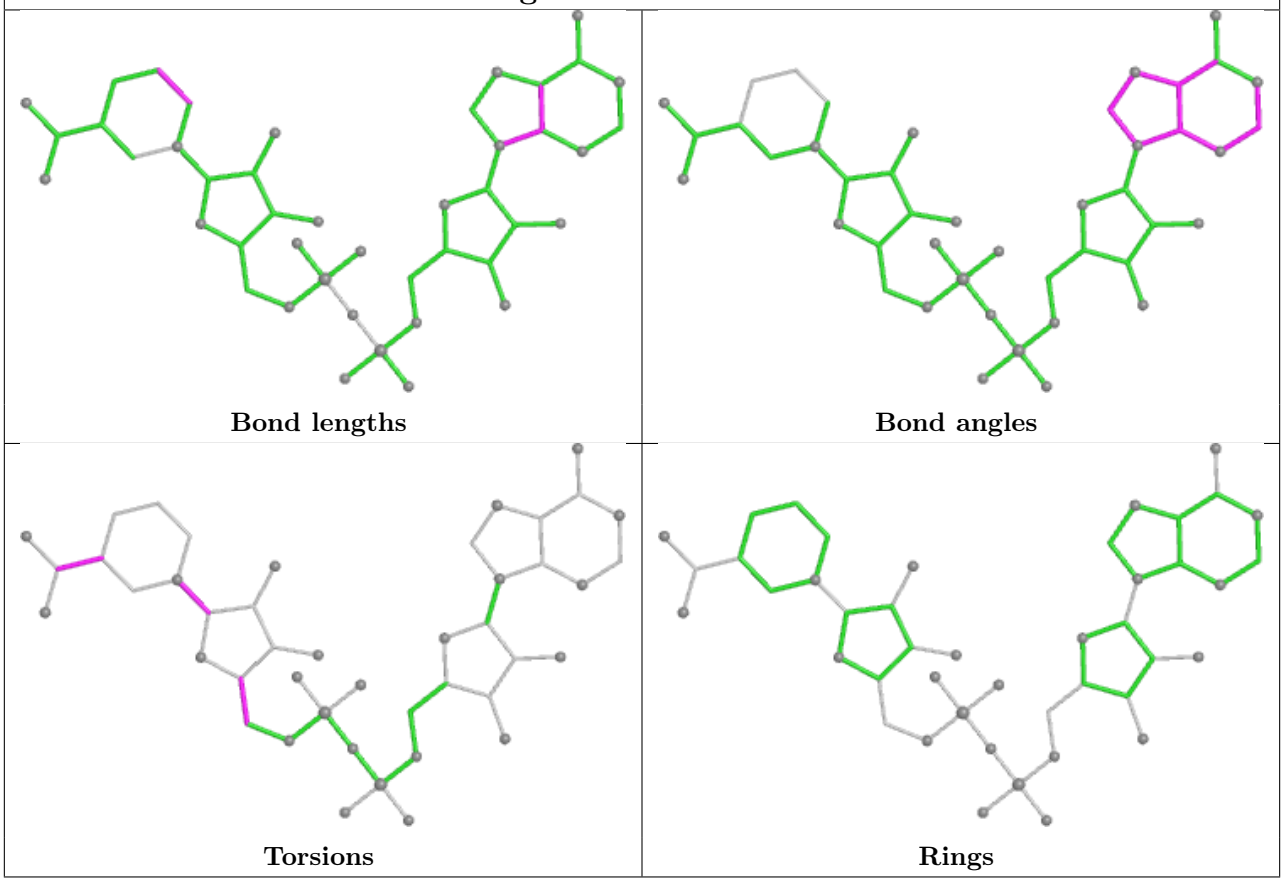
There are no ring outliers.

6 monomers are involved in 8 short contacts:

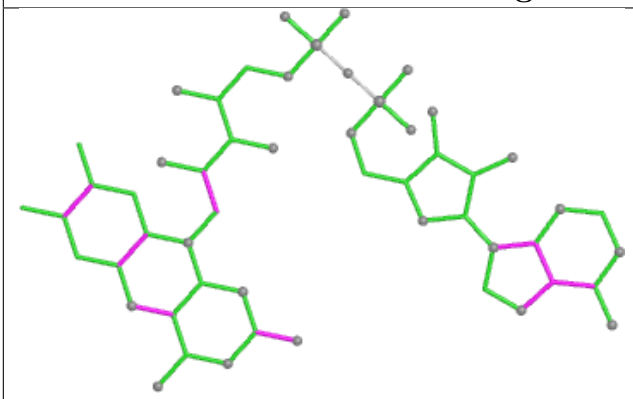
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	3006	NAI	1	0
5	A	1505	FAD	3	0
6	A	1506	NAI	2	0
5	B	3005	FAD	2	0
4	A	1504	FES	1	0
4	B	3001	FES	2	0

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 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.

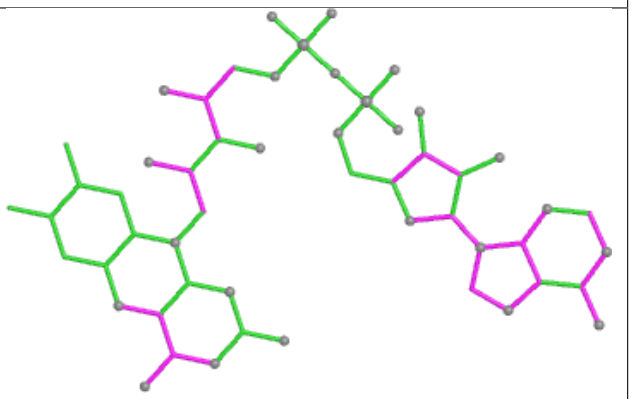
Ligand NAI B 3006



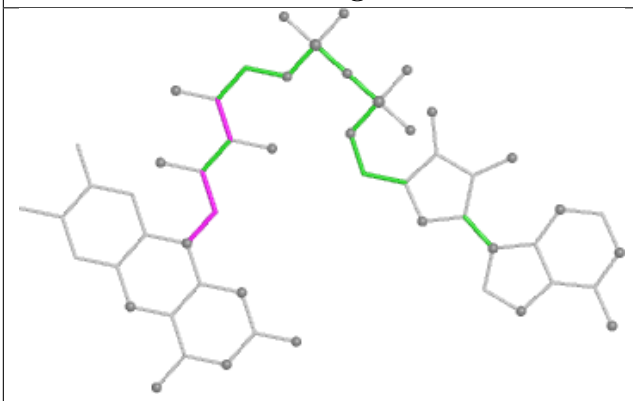
Ligand FAD A 1505



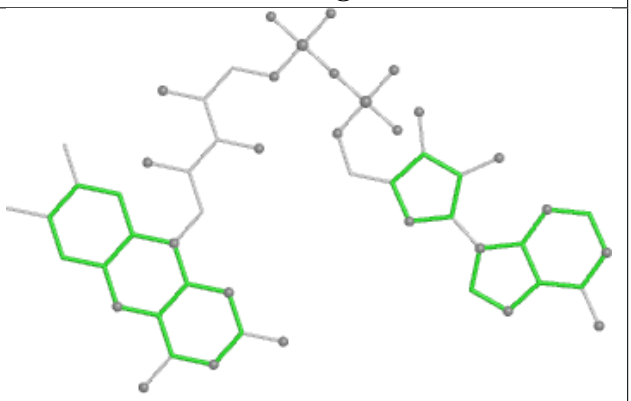
Bond lengths



Bond angles

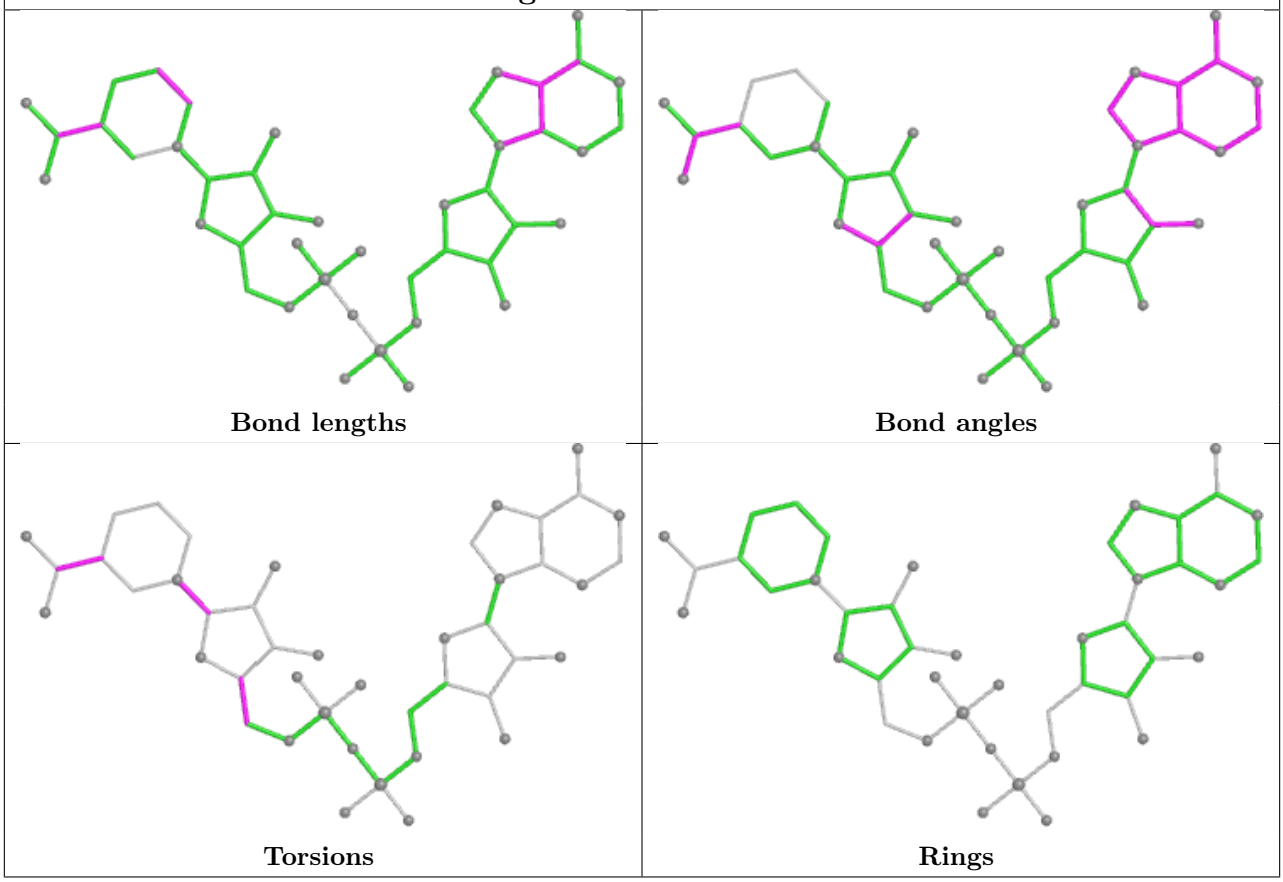


Torsions

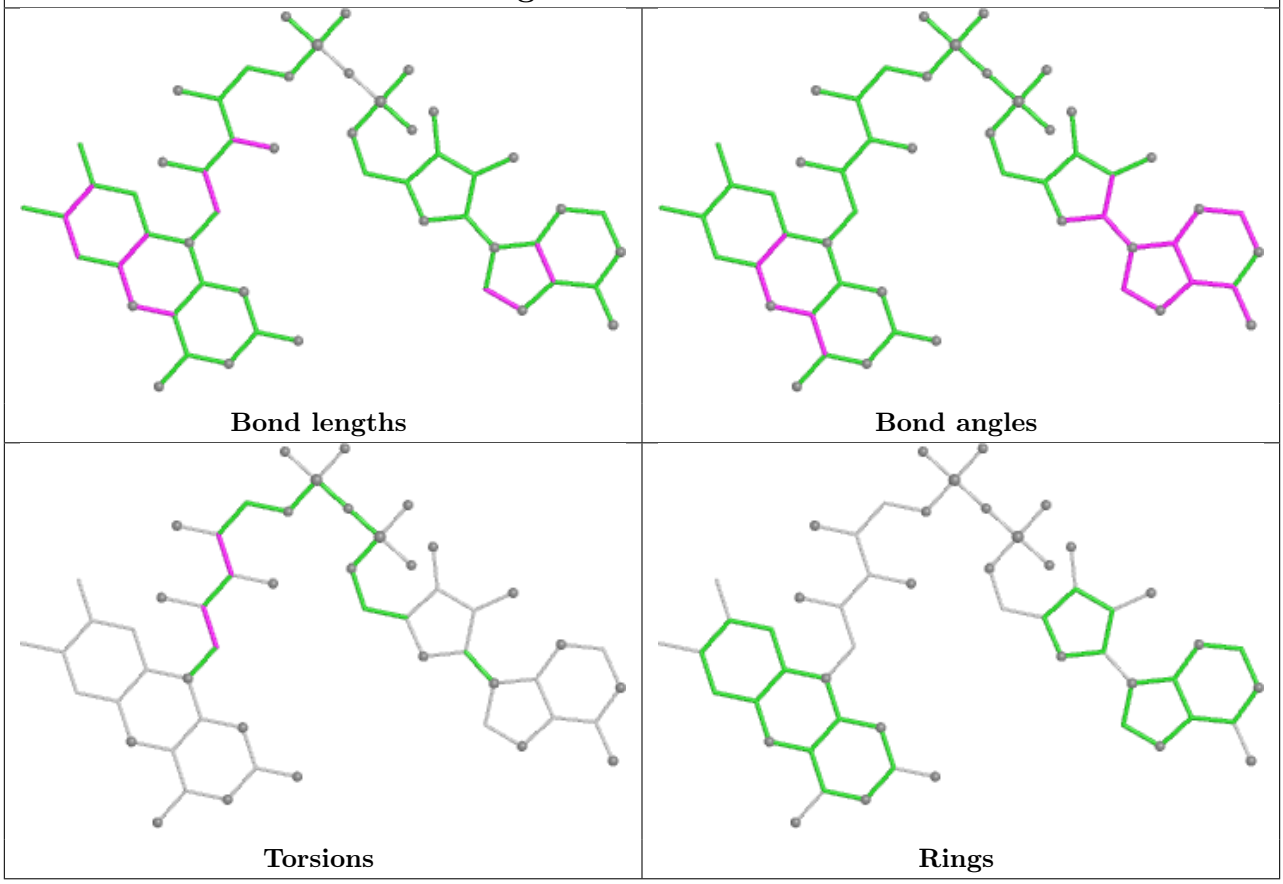


Rings

Ligand NAI A 1506



Ligand FAD B 3005



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	1297/1331 (97%)	0.15	47 (3%)	46	52	15, 25, 49, 88	0
1	B	1291/1331 (96%)	-0.10	25 (1%)	66	74	14, 21, 40, 73	0
All	All	2588/2662 (97%)	0.03	72 (2%)	55	62	14, 23, 46, 88	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1321	PRO	7.4
1	B	1289	ALA	6.8
1	A	1317	VAL	6.1
1	A	192	PRO	5.5
1	A	3	ALA	4.9
1	A	1111	GLY	4.5
1	B	3	ALA	4.2
1	A	1331	ILE	4.0
1	B	1111	GLY	4.0
1	B	1320	VAL	3.9
1	A	466	LEU	3.8
1	A	1322	GLU	3.8
1	A	1329	VAL	3.8
1	A	1324	CYS	3.7
1	B	164	LYS	3.5
1	B	221	THR	3.5
1	A	1325	LYS	3.5
1	A	1323	ASN	3.4
1	A	396	LEU	3.2
1	B	218	LEU	3.2
1	B	1288	ASN	3.1
1	B	1287	ASP	3.1
1	B	535	CYS	3.1
1	A	61	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1110	THR	3.0
1	A	1327	TRP	2.9
1	B	1110	THR	2.9
1	B	1318	THR	2.8
1	A	1315	LEU	2.8
1	B	271	ASN	2.8
1	A	290	VAL	2.8
1	B	61	LEU	2.8
1	A	272	MET	2.8
1	A	386	HIS	2.8
1	A	222	PRO	2.8
1	A	166	GLY	2.7
1	A	1107	LYS	2.7
1	B	192	PRO	2.6
1	A	249	ALA	2.6
1	B	1286	GLY	2.6
1	A	531	LEU	2.6
1	A	1250	LYS	2.6
1	A	496	ALA	2.6
1	A	566	ASP	2.5
1	B	812	LEU	2.5
1	B	222	PRO	2.5
1	B	1106	LYS	2.5
1	A	534	MET	2.5
1	A	719	LEU	2.5
1	A	221	THR	2.5
1	A	218	LEU	2.4
1	A	537	LYS	2.4
1	B	494	GLN	2.4
1	A	812	LEU	2.3
1	A	224	LYS	2.3
1	A	321	GLN	2.3
1	A	529	ALA	2.3
1	B	1250	LYS	2.3
1	A	720	LYS	2.3
1	A	536	GLY	2.2
1	A	1326	SER	2.2
1	B	530	ASP	2.2
1	A	390	PRO	2.2
1	A	247	LEU	2.1
1	A	1105	LYS	2.1
1	B	683	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	565	LYS	2.1
1	A	1290	LYS	2.1
1	B	377	GLY	2.1
1	A	553	PRO	2.1
1	A	377	GLY	2.0
1	B	536	GLY	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)

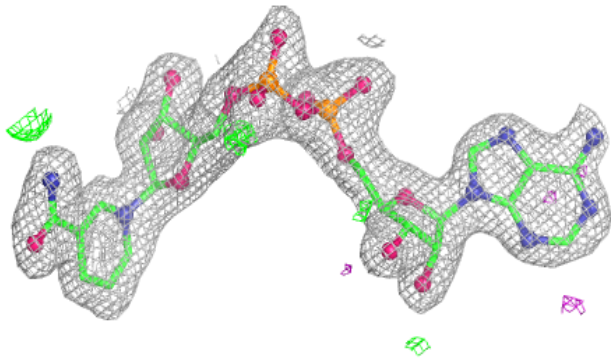
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

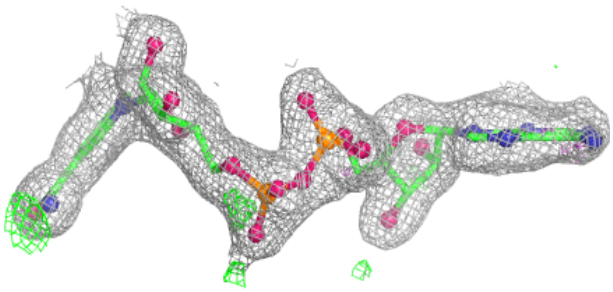
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAI	A	1506	44/44	0.95	0.07	26,33,41,47	0
5	FAD	A	1505	53/53	0.97	0.06	21,24,29,32	0
2	URC	A	1501	12/12	0.97	0.05	18,20,22,23	0
6	NAI	B	3006	44/44	0.97	0.06	19,23,26,32	0
4	FES	A	1504	4/4	0.98	0.09	26,29,32,32	0
4	FES	B	3001	4/4	0.98	0.11	25,28,31,33	0
2	URC	B	3003	12/12	0.98	0.03	17,19,21,21	0
5	FAD	B	3005	53/53	0.98	0.05	16,18,20,21	0
3	BCT	A	1502	4/4	0.98	0.06	22,24,25,27	0
3	BCT	B	3004	4/4	0.98	0.04	18,19,21,22	0
4	FES	A	1503	4/4	1.00	0.02	18,18,18,18	0
4	FES	B	3002	4/4	1.00	0.03	16,16,16,17	0

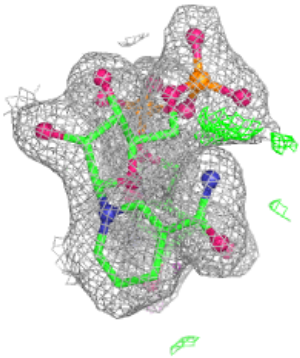
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI A 1506:

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

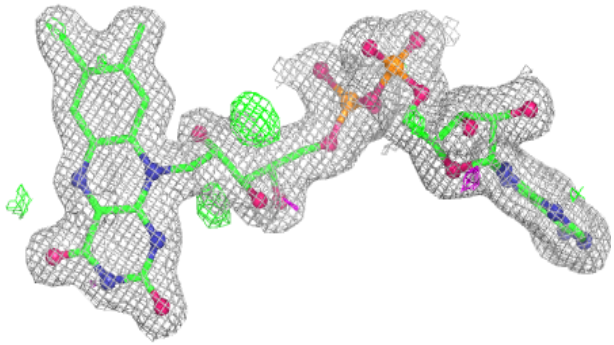


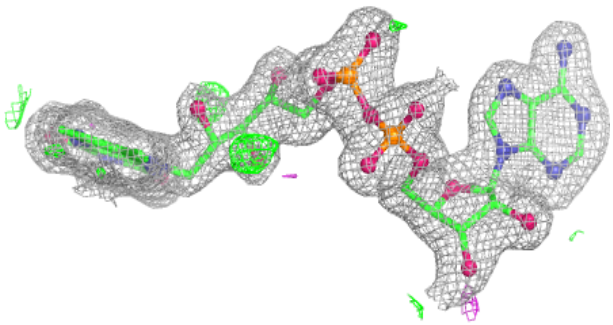


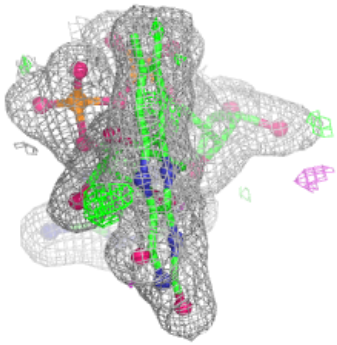


Electron density around FAD A 1505:

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

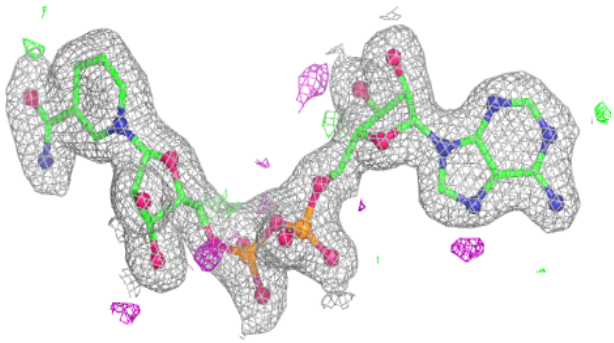


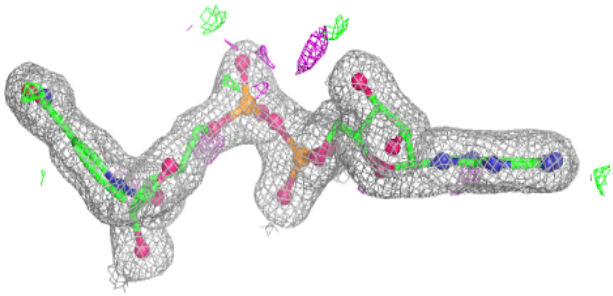


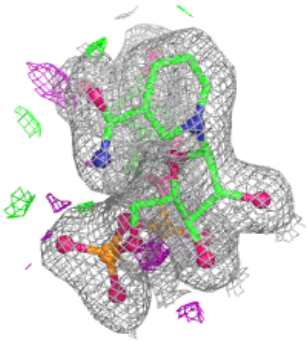


Electron density around NAI B 3006:

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







Electron density around FAD B 3005:

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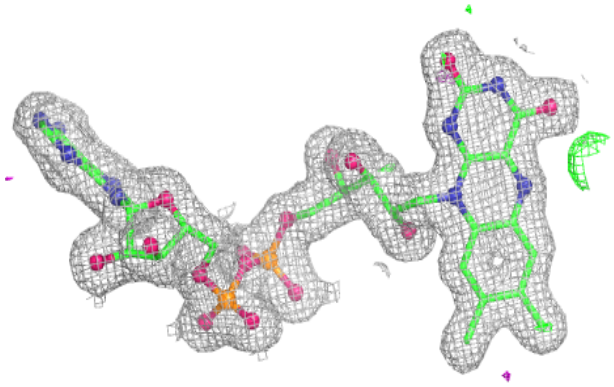
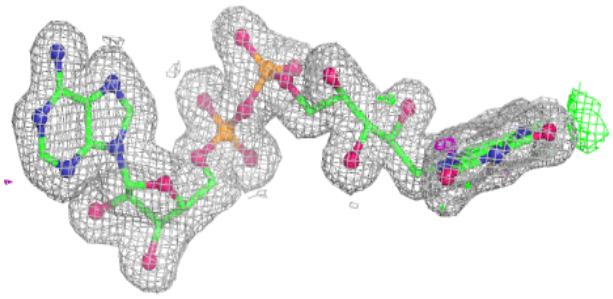
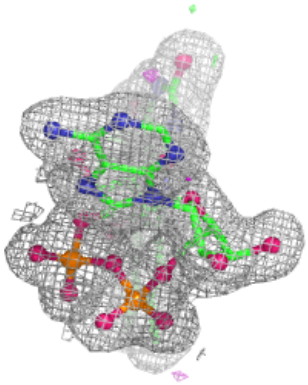
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.