Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 07:32 AM UTC

PDB ID	:	4YTY / pdb_00004yty
Title	:	Structure of rat xanthine oxidoreductase, C535A/C992R/C1324S, NADH bound form
Authors	:	Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Matsumura, T.; Eger, B.T.; Pai, E.F.
Deposited on	:	2015-03-18
Resolution	:	2.20 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:

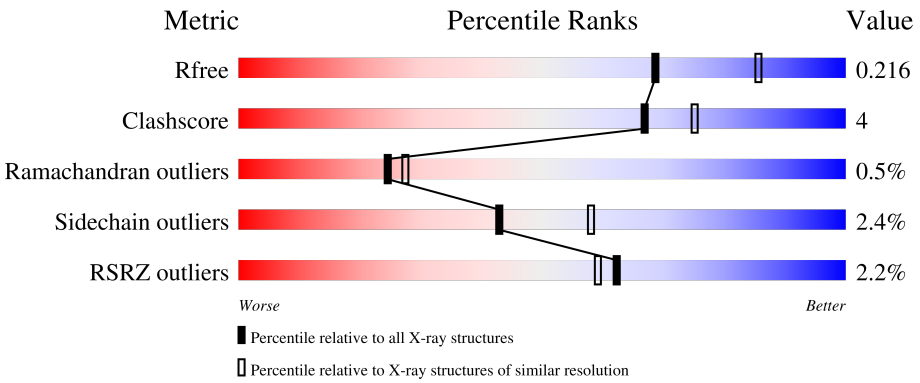
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	2% 89% 8% • •
1	B	1331	2% 88% 9% • •

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21734 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.

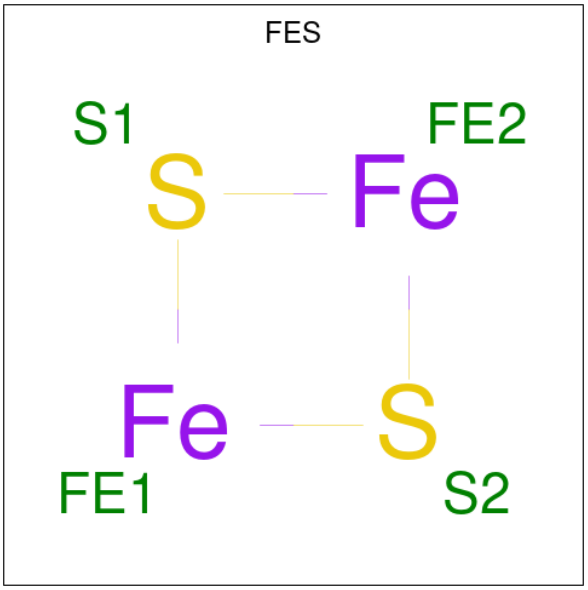
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1304	10080	6386	1738	1894	62	0	0	0
1	B	1293	9991	6333	1721	1875	62	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	ALA	CYS	engineered mutation	UNP P22985
A	992	ARG	CYS	engineered mutation	UNP P22985
A	1324	SER	CYS	engineered mutation	UNP P22985
B	535	ALA	CYS	engineered mutation	UNP P22985
B	992	ARG	CYS	engineered mutation	UNP P22985
B	1324	SER	CYS	engineered mutation	UNP P22985

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

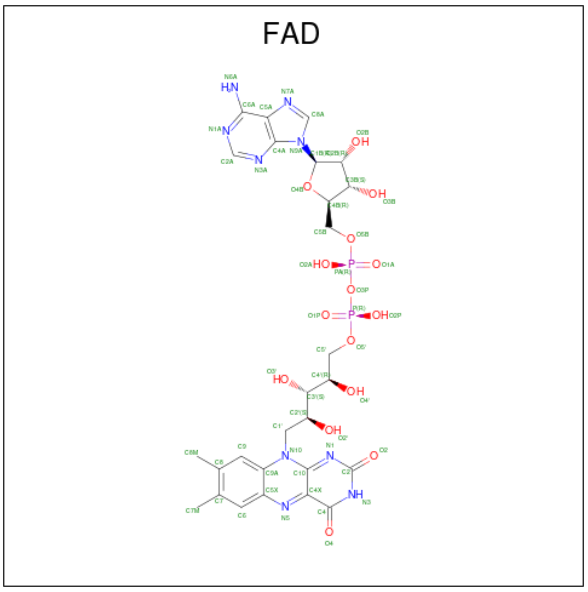


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Fe	S		0	0
			4	2	2			
2	A	1	Total	Fe	S		0	0
			4	2	2			
2	B	1	Total	Fe	S		0	0
			4	2	2			
2	B	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

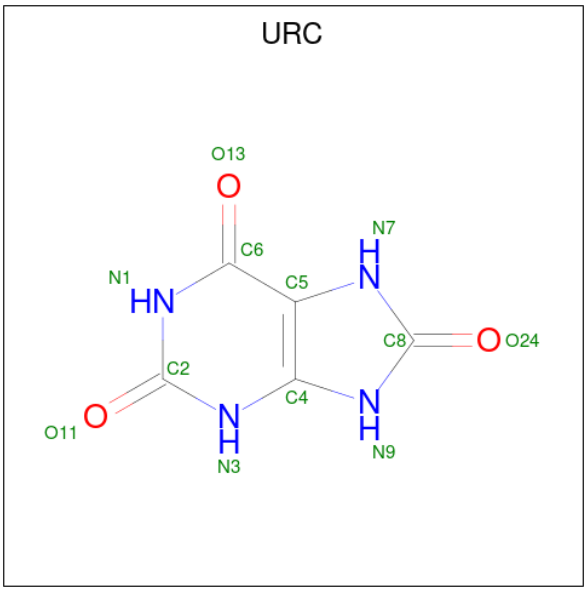
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



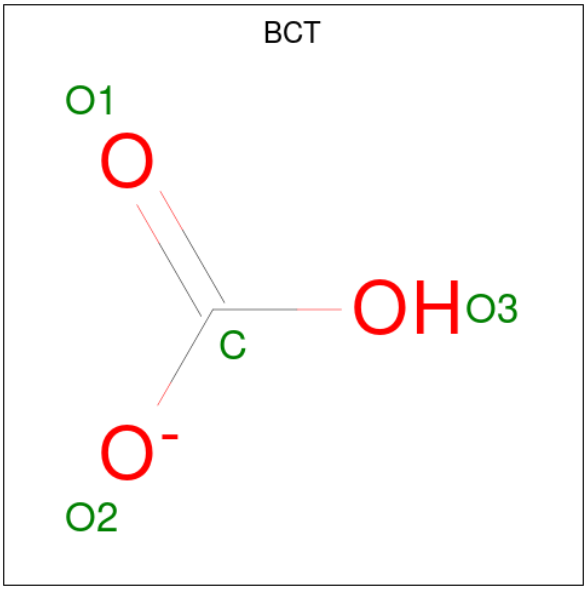
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



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

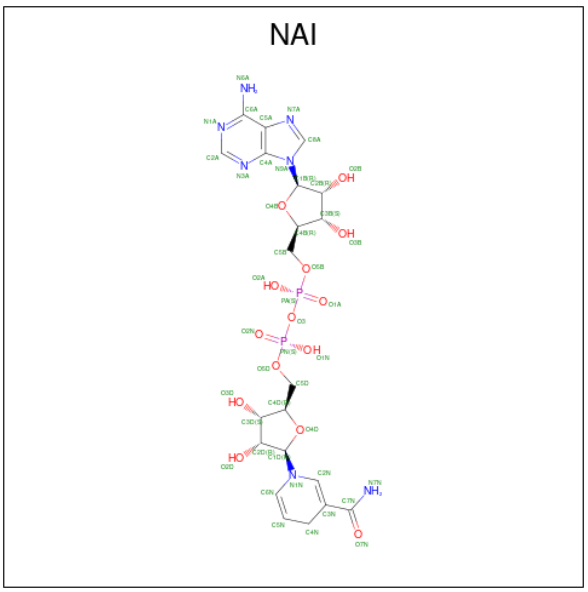
- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

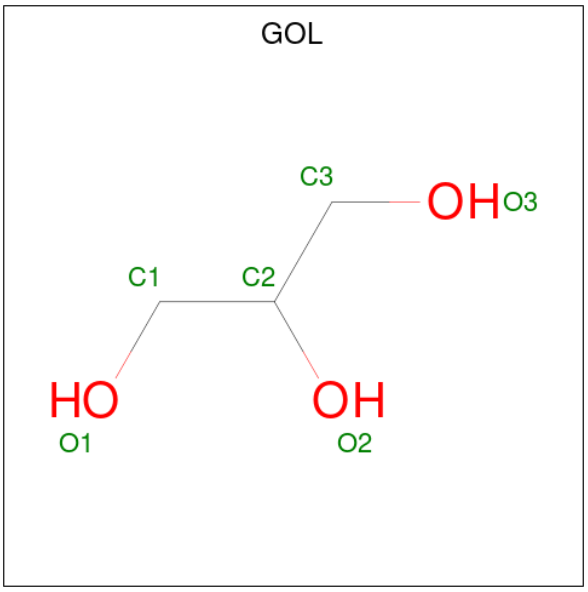
- Molecule 7 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID:

NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0
			Total	C	O		
8	B	1	6	3	3	0	0
			Total	C	O		
8	B	1	6	3	3	0	0

- Molecule 9 is water.

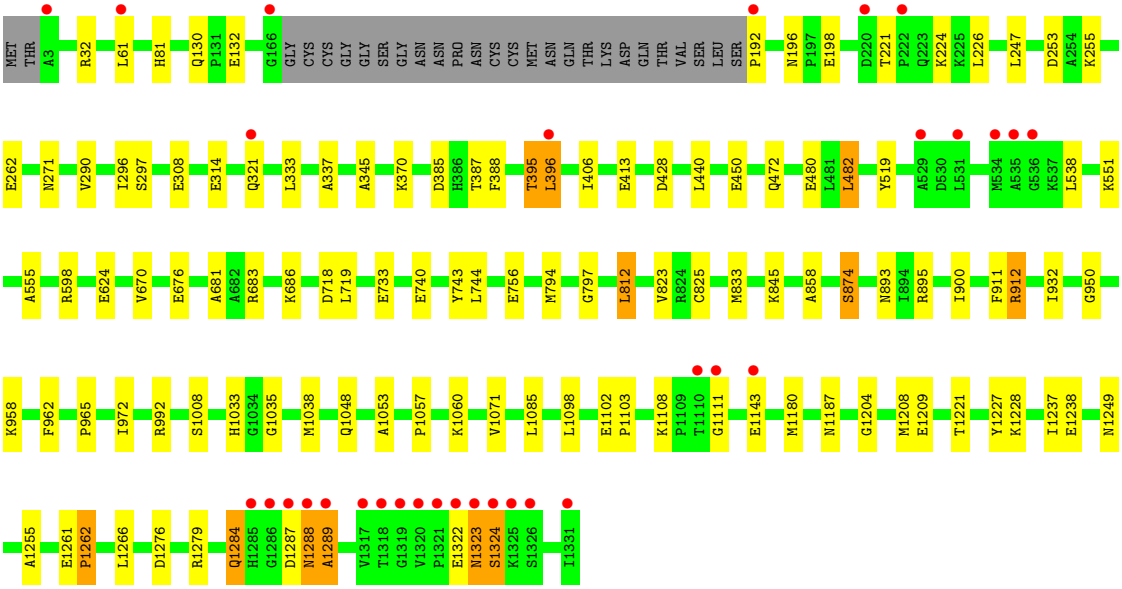
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	646	646	646	0	0
			Total	O		
9	B	761	761	761	0	0

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.

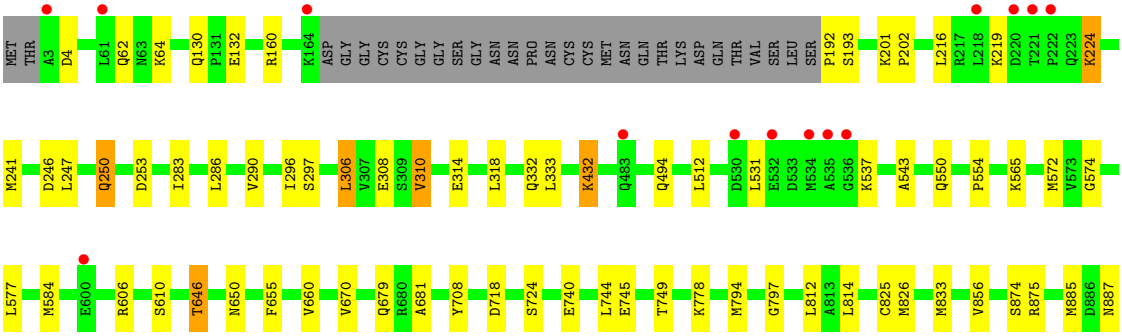
• Molecule 1: Xanthine dehydrogenase/oxidase

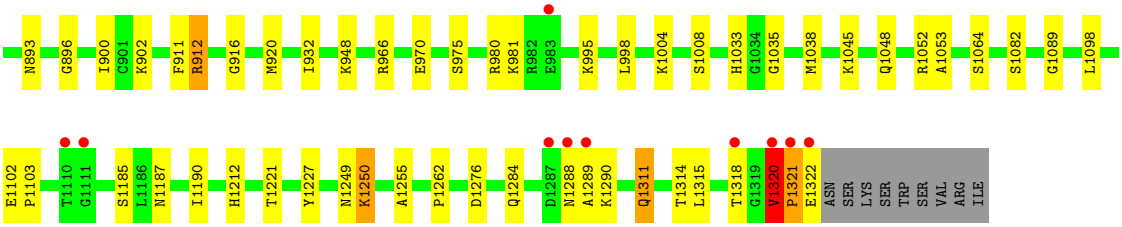
Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:




N893
G896
I900
G901
K902
F911
R912
G916
M920
I932
K948
R966
E970
S975
R980
K981
R982
E983
K995
L998
K1004
S1008
H1033
G1034
G1035
M1038
K1045
Q1048
R1052
A1053
S1064
S1082
G1089
L1098
E1102
P1103
T1110
G1111
S1185
L1186
N1187
I1190
H1212
T1221
Y1227
N1249
K1250
A1255
P1262
D1276
Q1284
D1287
N1288
A1289
K1290
Q1311
T1314
L1315
T1318
G1319
V1320
P1321
E1322
ASN
SER
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	98.99Å 137.40Å 222.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.20 49.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.50-2.20) 99.6 (49.50-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.88 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.221 0.174 , 0.216	Depositor DCC
R_{free} test set	7678 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21734	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: URC, NAI, FES, CA, GOL, BCT, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.62	1/10293 (0.0%)	0.83	5/13928 (0.0%)
1	B	0.65	0/10202	0.84	6/13806 (0.0%)
All	All	0.63	1/20495 (0.0%)	0.83	11/27734 (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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1071	VAL	CA-CB	5.35	1.58	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1262	PRO	N-CA-C	7.30	119.61	110.70
1	B	1320	VAL	CA-C-N	7.22	128.86	119.84
1	B	1320	VAL	C-N-CA	7.22	128.86	119.84
1	A	395	THR	N-CA-C	-7.02	98.77	109.85
1	B	1262	PRO	N-CA-C	6.32	118.41	110.70
1	A	395	THR	CA-C-N	6.27	133.52	121.54
1	A	395	THR	C-N-CA	6.27	133.52	121.54
1	B	1320	VAL	N-CA-C	6.12	122.11	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1082	SER	N-CA-C	5.69	117.48	111.28
1	A	874	SER	N-CA-C	5.13	117.26	111.11
1	B	543	ALA	N-CA-C	5.03	116.77	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	395	THR	Peptide
1	B	1320	VAL	Peptide

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	10080	0	10086	71	0
1	B	9991	0	10001	80	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	3	0
4	B	53	0	31	0	0
5	A	12	0	4	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	44	0	27	0	0
7	B	44	0	27	0	0
8	A	12	0	16	0	0
8	B	12	0	16	0	0
9	A	646	0	0	4	0
9	B	761	0	0	12	0
All	All	21734	0	20239	151	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 (151) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:GLY:HA3	9:B:4446:HOH:O	0.94	1.09
1:A:1323:ASN:HA	1:A:1324:SER:HB2	1.28	1.07
1:A:1323:ASN:HA	1:A:1324:SER:CB	1.88	1.03
1:B:718:ASP:H	1:B:893:ASN:HD22	1.15	0.91
1:B:1311:GLN:HE21	1:B:1311:GLN:H	1.20	0.89
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.56	0.87
1:B:749:THR:HB	1:B:812:LEU:HD12	1.56	0.85
1:A:1288:ASN:HA	1:A:1289:ALA:HB2	1.59	0.84
1:B:646:THR:CG2	9:B:4257:HOH:O	2.28	0.81
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.63	0.80
1:A:290:VAL:HG23	1:A:297:SER:HB2	1.62	0.79
1:B:812:LEU:HD11	1:B:825:CYS:HB3	1.65	0.77
1:B:826:MET:CE	9:B:4745:HOH:O	2.33	0.76
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.16	0.74
1:B:646:THR:HG23	9:B:4257:HOH:O	1.86	0.74
1:A:812:LEU:CD1	1:A:825:CYS:HB3	2.16	0.74
1:B:130:GLN:HE21	1:B:132:GLU:H	1.35	0.74
1:A:130:GLN:HE21	1:A:132:GLU:H	1.36	0.73
1:A:1323:ASN:CA	1:A:1324:SER:HB2	2.14	0.72
1:B:1314:THR:HG22	1:B:1321:PRO:HD3	1.71	0.72
1:A:812:LEU:HD11	1:A:825:CYS:CB	2.20	0.71
1:A:555:ALA:HB3	1:A:1238:GLU:HG2	1.73	0.71
1:A:718:ASP:H	1:A:893:ASN:HD22	1.40	0.69
1:B:290:VAL:HG22	1:B:297:SER:HB2	1.73	0.69
1:B:749:THR:HB	1:B:812:LEU:CD1	2.22	0.69
1:A:321:GLN:HG2	1:A:413:GLU:OE1	1.94	0.68
1:B:812:LEU:HD21	1:B:825:CYS:CB	2.23	0.68
1:A:388:PHE:HA	1:A:396:LEU:HD13	1.74	0.68
1:A:192:PRO:HD2	9:A:3486:HOH:O	1.93	0.67
1:B:826:MET:HE3	9:B:4745:HOH:O	1.94	0.66
1:B:826:MET:HE1	9:B:4745:HOH:O	1.94	0.66
1:B:812:LEU:HD21	1:B:825:CYS:HB2	1.78	0.66
1:B:718:ASP:H	1:B:893:ASN:ND2	1.90	0.65
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.78	0.65
1:B:565:LYS:HD3	1:B:565:LYS:H	1.62	0.65
1:B:565:LYS:HD3	1:B:565:LYS:N	2.13	0.64
1:B:565:LYS:H	1:B:565:LYS:CD	2.10	0.64
1:B:246:ASP:O	1:B:250:GLN:HG2	1.98	0.64
1:A:385:ASP:OD1	1:A:387:THR:HG22	1.99	0.63
1:B:1033:HIS:HD2	1:B:1035:GLY:H	1.46	0.63
1:A:1288:ASN:CA	1:A:1289:ALA:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:ARG:O	1:B:970:GLU:HG3	2.00	0.61
1:A:1102:GLU:HG2	1:A:1103:PRO:HD3	1.83	0.61
1:A:718:ASP:H	1:A:893:ASN:ND2	1.99	0.60
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.49	0.60
1:A:345:ALA:HB1	4:A:3004:FAD:H4'	1.83	0.60
1:A:932:ILE:HD11	9:A:3590:HOH:O	2.02	0.60
1:B:432:LYS:HA	1:B:432:LYS:HE3	1.85	0.59
1:B:224:LYS:H	1:B:224:LYS:HD2	1.67	0.58
1:B:62:GLN:HB2	1:B:64:LYS:HG2	1.84	0.58
1:A:551:LYS:HD2	1:A:1237:ILE:HD11	1.85	0.57
1:A:1323:ASN:CA	1:A:1324:SER:CB	2.72	0.57
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.34	0.57
1:B:1315:LEU:HA	1:B:1321:PRO:HD2	1.85	0.56
1:A:296:ILE:HD11	1:A:314:GLU:HG3	1.86	0.56
1:A:271:ASN:HB3	1:A:683:ARG:CZ	2.35	0.56
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.88	0.55
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.25	0.55
1:B:794:MET:HE3	1:B:1038:MET:HB3	1.89	0.55
1:B:296:ILE:HD11	1:B:314:GLU:HG3	1.89	0.54
1:A:1180:MET:HE1	1:A:1266:LEU:CD1	2.36	0.53
1:B:874:SER:HB3	1:B:900:ILE:HG21	1.90	0.53
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.91	0.53
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.91	0.53
1:B:216:LEU:O	1:B:219:LYS:HG3	2.09	0.53
1:B:745:GLU:HA	9:B:4745:HOH:O	2.09	0.52
1:B:1048:GLN:HE22	1:B:1187:ASN:HD22	1.55	0.52
1:A:308:GLU:HG3	1:A:333:LEU:HD13	1.91	0.52
1:B:812:LEU:HD21	1:B:825:CYS:HB3	1.89	0.52
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.40	0.52
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.10	0.51
1:A:740:GLU:HG2	1:A:833:MET:HE3	1.92	0.51
1:B:1314:THR:HB	1:B:1321:PRO:HG3	1.92	0.51
1:A:440:LEU:HB3	1:A:450:GLU:HB2	1.92	0.51
1:A:794:MET:HE3	1:A:1038:MET:HB3	1.93	0.51
1:B:708:TYR:CZ	1:B:902:LYS:HG3	2.46	0.50
1:B:290:VAL:CG2	1:B:297:SER:HB2	2.40	0.50
1:B:565:LYS:CD	1:B:565:LYS:N	2.74	0.50
1:A:196:ASN:ND2	1:A:198:GLU:HG2	2.26	0.50
1:B:572:MET:HE2	1:B:577:LEU:HD13	1.94	0.50
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.37	0.49
1:B:646:THR:HG22	9:B:4257:HOH:O	2.04	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1250:LYS:HG3	9:B:4701:HOH:O	2.12	0.49
1:B:1289:ALA:O	1:B:1290:LYS:HB2	2.13	0.49
1:A:812:LEU:HD21	1:A:823:VAL:O	2.13	0.48
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.48	0.48
1:A:1288:ASN:HA	1:A:1289:ALA:CB	2.36	0.48
1:B:308:GLU:HG3	1:B:333:LEU:HD13	1.95	0.48
1:B:911:PHE:O	1:B:912:ARG:C	2.56	0.48
1:A:950:GLY:HA2	1:A:958:LYS:HE2	1.95	0.48
1:B:1033:HIS:CD2	1:B:1035:GLY:H	2.30	0.47
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.61	0.47
1:B:192:PRO:HD2	9:B:4638:HOH:O	2.14	0.47
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.22	0.47
1:A:337:ALA:HA	1:A:428:ASP:OD1	2.15	0.47
1:A:992:ARG:CD	1:A:1284:GLN:HG2	2.46	0.46
1:B:332:GLN:NE2	9:B:4117:HOH:O	2.48	0.46
1:A:900:ILE:HD12	1:A:900:ILE:N	2.30	0.46
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.13	0.46
1:B:1048:GLN:NE2	1:B:1187:ASN:HD22	2.13	0.46
1:A:196:ASN:HD21	1:A:198:GLU:HG2	1.78	0.46
1:B:932:ILE:CG2	1:B:1290:LYS:HA	2.45	0.46
1:A:756:GLU:HB3	1:B:584:MET:SD	2.55	0.46
1:A:1323:ASN:HA	1:A:1324:SER:HB3	1.88	0.46
1:A:1288:ASN:CA	1:A:1289:ALA:CB	2.94	0.46
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	1.97	0.46
1:A:911:PHE:O	1:A:912:ARG:C	2.59	0.45
1:A:932:ILE:HD13	1:A:1279:ARG:NH2	2.32	0.45
1:B:1315:LEU:HB2	1:B:1321:PRO:HG2	1.98	0.45
1:B:740:GLU:HG3	1:B:833:MET:HE3	1.97	0.45
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.99	0.45
1:B:241:MET:HE1	1:B:286:LEU:HG	1.98	0.44
1:B:201:LYS:HA	1:B:202:PRO:HD3	1.88	0.44
1:B:885:MET:SD	1:B:896:GLY:HA3	2.57	0.44
1:B:610:SER:HB2	1:B:660:VAL:HG11	1.99	0.44
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.17	0.44
1:A:1208:MET:HG3	1:A:1228:LYS:O	2.18	0.44
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.18	0.44
1:B:670:VAL:HG11	1:B:681:ALA:HB3	2.00	0.44
1:A:1204:GLY:HA3	1:A:1209:GLU:OE1	2.18	0.44
1:B:565:LYS:H	1:B:565:LYS:CE	2.31	0.44
1:A:598:ARG:NH1	9:A:3124:HOH:O	2.51	0.43
1:A:858:ALA:HA	1:A:893:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:GLU:HG2	1:B:1103:PRO:HD3	1.99	0.43
1:B:160:ARG:NH2	1:B:554:PRO:CG	2.82	0.43
1:B:1212:HIS:HD2	9:B:4828:HOH:O	2.01	0.43
1:A:555:ALA:O	1:A:1238:GLU:HA	2.19	0.43
1:B:1318:THR:HG23	1:B:1320:VAL:HG12	2.00	0.43
1:A:1108:LYS:HG2	1:A:1111:GLY:HA3	2.01	0.43
1:B:250:GLN:HG2	1:B:250:GLN:H	1.66	0.42
1:A:733:GLU:HG2	1:A:845:LYS:HG2	2.01	0.42
1:A:81:HIS:CD2	1:A:226:LEU:HD11	2.54	0.42
1:B:981:LYS:HG2	1:B:998:LEU:HD23	2.01	0.42
1:A:482:LEU:HG	1:A:519:TYR:CD2	2.54	0.42
1:A:1102:GLU:CG	1:A:1103:PRO:HD3	2.49	0.42
1:B:574:GLY:HA2	1:B:1185:SER:O	2.20	0.42
1:B:975:SER:HB2	1:B:980:ARG:HH21	1.84	0.42
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.20	0.42
1:B:916:GLY:C	1:B:920:MET:HE2	2.45	0.42
1:A:1180:MET:HE2	1:A:1180:MET:HB2	1.89	0.41
1:B:1045:LYS:HE3	1:B:1190:ILE:HG21	2.02	0.41
1:A:262:GLU:HB2	4:A:3004:FAD:H52A	2.02	0.41
1:B:160:ARG:NH2	1:B:554:PRO:HG2	2.34	0.41
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.84	0.41
1:B:606:ARG:HD3	1:B:679:GLN:HA	2.02	0.41
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.84	0.41
1:B:875:ARG:HG2	1:B:900:ILE:HD13	2.01	0.41
1:B:306:LEU:O	1:B:310:VAL:HG13	2.21	0.40
1:B:650:ASN:OD1	1:B:778:LYS:NZ	2.52	0.40
4:A:3004:FAD:HM73	9:A:3401:HOH:O	2.20	0.40
1:A:1057:PRO:HD2	1:A:1060:LYS:HD2	2.03	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	1300/1331 (98%)	1258 (97%)	37 (3%)	5 (0%)	30	34
1	B	1289/1331 (97%)	1249 (97%)	32 (2%)	8 (1%)	21	23
All	All	2589/2662 (97%)	2507 (97%)	69 (3%)	13 (0%)	24	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	A	1289	ALA
1	A	1324	SER
1	B	1008	SER
1	B	1288	ASN
1	B	1321	PRO
1	B	912	ARG
1	A	797	GLY
1	A	912	ARG
1	B	797	GLY
1	B	4	ASP
1	B	1320	VAL
1	B	887	ASN

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	1100/1123 (98%)	1073 (98%)	27 (2%)	42	56
1	B	1090/1123 (97%)	1064 (98%)	26 (2%)	43	58
All	All	2190/2246 (98%)	2137 (98%)	53 (2%)	43	58

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	221	THR
1	A	224	LYS

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Mol	Chain	Res	Type
1	A	247	LEU
1	A	253	ASP
1	A	255	LYS
1	A	370	LYS
1	A	396	LEU
1	A	406	ILE
1	A	472	GLN
1	A	480	GLU
1	A	482	LEU
1	A	538	LEU
1	A	624	GLU
1	A	686	LYS
1	A	743	TYR
1	A	744	LEU
1	A	812	LEU
1	A	972	ILE
1	A	1085	LEU
1	A	1143	GLU
1	A	1276	ASP
1	A	1284	GLN
1	A	1287	ASP
1	A	1288	ASN
1	A	1322	GLU
1	A	1323	ASN
1	B	193	SER
1	B	224	LYS
1	B	247	LEU
1	B	250	GLN
1	B	253	ASP
1	B	306	LEU
1	B	310	VAL
1	B	318	LEU
1	B	432	LYS
1	B	494	GLN
1	B	512	LEU
1	B	531	LEU
1	B	537	LYS
1	B	550	GLN
1	B	646	THR
1	B	724	SER
1	B	744	LEU
1	B	856	VAL

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Mol	Chain	Res	Type
1	B	948	LYS
1	B	1004	LYS
1	B	1052	ARG
1	B	1064	SER
1	B	1250	LYS
1	B	1276	ASP
1	B	1311	GLN
1	B	1322	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	145	ASN
1	A	157	GLN
1	A	291	HIS
1	A	332	GLN
1	A	386	HIS
1	A	472	GLN
1	A	483	GLN
1	A	556	ASN
1	A	558	GLN
1	A	585	GLN
1	A	650	ASN
1	A	679	GLN
1	A	705	ASN
1	A	893	ASN
1	A	1033	HIS
1	A	1048	GLN
1	A	1173	ASN
1	A	1284	GLN
1	A	1294	GLN
1	A	1323	ASN
1	B	130	GLN
1	B	143	GLN
1	B	145	ASN
1	B	250	GLN
1	B	332	GLN
1	B	472	GLN
1	B	483	GLN
1	B	524	GLN
1	B	556	ASN

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Mol	Chain	Res	Type
1	B	585	GLN
1	B	705	ASN
1	B	869	ASN
1	B	893	ASN
1	B	1033	HIS
1	B	1048	GLN
1	B	1088	GLN
1	B	1173	ASN
1	B	1194	GLN
1	B	1220	HIS
1	B	1284	GLN
1	B	1288	ASN
1	B	1311	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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	$\#\|Z\| > 2$
7	NAI	B	4006	-	47,48,48	1.30	6 (12%)	64,73,73	1.67	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	URC	A	3005	-	13,13,13	3.52	2 (15%)	17,19,19	2.51	7 (41%)
8	GOL	B	4007	-	5,5,5	0.11	0	5,5,5	0.76	0
4	FAD	B	4004	-	58,58,58	1.11	6 (10%)	85,89,89	1.61	17 (20%)
8	GOL	B	4008	-	5,5,5	0.34	0	5,5,5	0.49	0
2	FES	B	4002	1	0,4,4	-	-	-		
2	FES	B	4001	1	0,4,4	-	-	-		
6	BCT	B	4005	-	3,3,3	1.23	0	2,3,3	0.35	0
7	NAI	A	3007	-	47,48,48	1.36	6 (12%)	64,73,73	1.73	12 (18%)
6	BCT	A	3006	-	3,3,3	1.18	0	2,3,3	0.02	0
2	FES	A	3002	1	0,4,4	-	-	-		
8	GOL	A	3009	-	5,5,5	0.39	0	5,5,5	0.55	0
4	FAD	A	3004	-	58,58,58	1.06	4 (6%)	85,89,89	1.56	15 (17%)
8	GOL	A	3008	-	5,5,5	0.16	0	5,5,5	0.70	0
2	FES	A	3001	1	0,4,4	-	-	-		

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
7	NAI	B	4006	-	-	2/29/72/72	0/5/5/5
8	GOL	B	4007	-	-	0/4/4/4	-
5	URC	A	3005	-	-	-	0/2/2/2
4	FAD	B	4004	-	-	4/34/50/50	0/6/6/6
8	GOL	B	4008	-	-	0/4/4/4	-
2	FES	B	4002	1	-	-	0/1/1/1
2	FES	B	4001	1	-	-	0/1/1/1
7	NAI	A	3007	-	-	3/29/72/72	0/5/5/5
2	FES	A	3002	1	-	-	0/1/1/1
8	GOL	A	3009	-	-	2/4/4/4	-
4	FAD	A	3004	-	-	2/34/50/50	0/6/6/6
8	GOL	A	3008	-	-	2/4/4/4	-
2	FES	A	3001	1	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	URC	O24-C8	12.00	1.48	1.23
7	A	3007	NAI	C4N-C3N	-5.19	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4006	NAI	C4N-C3N	-4.97	1.40	1.50
7	A	3007	NAI	C4N-C5N	-3.70	1.39	1.49
4	B	4004	FAD	C4X-N5	3.60	1.38	1.30
4	A	3004	FAD	C4X-N5	3.53	1.38	1.30
7	B	4006	NAI	C4N-C5N	-3.52	1.39	1.49
4	A	3004	FAD	C10-N1	2.82	1.38	1.33
4	B	4004	FAD	C10-N1	2.76	1.38	1.33
4	B	4004	FAD	PA-O3P	2.69	1.62	1.59
7	A	3007	NAI	PA-O3	2.48	1.62	1.59
4	A	3004	FAD	C2A-N3A	2.39	1.38	1.33
4	A	3004	FAD	C2A-N1A	2.36	1.38	1.33
4	B	4004	FAD	C2A-N1A	2.35	1.38	1.33
7	A	3007	NAI	C6N-C5N	2.28	1.40	1.33
5	A	3005	URC	C5-C6	2.26	1.48	1.41
4	B	4004	FAD	C8A-N7A	2.17	1.35	1.31
7	A	3007	NAI	C6N-N1N	2.17	1.42	1.37
7	B	4006	NAI	C6N-N1N	2.16	1.42	1.37
7	A	3007	NAI	C5A-N7A	-2.14	1.35	1.39
7	B	4006	NAI	C6N-C5N	2.11	1.39	1.33
7	B	4006	NAI	PA-O3	2.11	1.61	1.59
7	B	4006	NAI	C8A-N7A	2.04	1.35	1.31
4	B	4004	FAD	C2A-N3A	2.01	1.37	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	4004	FAD	N3A-C2A-N1A	-6.03	119.45	128.58
4	A	3004	FAD	N3A-C2A-N1A	-5.74	119.89	128.58
5	A	3005	URC	N7-C8-N9	5.62	115.18	107.22
7	B	4006	NAI	C5A-C4A-N3A	-5.53	119.10	126.72
7	A	3007	NAI	N3A-C2A-N1A	-5.33	120.52	128.58
7	A	3007	NAI	C5A-C4A-N3A	-5.30	119.42	126.72
7	B	4006	NAI	N3A-C2A-N1A	-5.14	120.80	128.58
4	A	3004	FAD	N9A-C8A-N7A	-4.20	107.97	113.94
4	B	4004	FAD	N9A-C8A-N7A	-4.06	108.18	113.94
4	A	3004	FAD	C5A-C4A-N3A	-3.99	121.22	126.72
7	A	3007	NAI	O4D-C1D-N1N	3.98	115.67	108.08
5	A	3005	URC	N3-C2-N1	3.97	121.98	115.74
7	B	4006	NAI	C2A-N3A-C4A	3.88	121.30	111.83
5	A	3005	URC	C5-N7-C8	-3.82	103.89	108.82
4	A	3004	FAD	C5A-N7A-C8A	3.76	109.36	103.45
7	A	3007	NAI	N3A-C4A-N9A	3.75	133.54	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	3007	NAI	C2A-N3A-C4A	3.68	120.82	111.83
5	A	3005	URC	C6-N1-C2	-3.59	121.42	126.37
7	B	4006	NAI	N3A-C4A-N9A	3.54	133.18	127.17
4	B	4004	FAD	C5A-C4A-N3A	-3.47	121.94	126.72
7	A	3007	NAI	C6N-N1N-C2N	-3.42	115.66	119.32
4	A	3004	FAD	C2A-N3A-C4A	3.31	119.91	111.83
7	B	4006	NAI	N9A-C8A-N7A	-3.24	109.34	113.94
7	A	3007	NAI	C1D-N1N-C6N	-3.18	114.04	120.77
4	B	4004	FAD	C5A-N7A-C8A	3.18	108.45	103.45
7	A	3007	NAI	N9A-C8A-N7A	-3.15	109.47	113.94
4	B	4004	FAD	C4-N3-C2	-3.09	120.15	125.64
4	A	3004	FAD	O2A-PA-O3P	3.08	115.59	107.27
5	A	3005	URC	O13-C6-C5	-3.05	119.91	127.26
4	B	4004	FAD	C2A-N3A-C4A	2.93	118.98	111.83
4	B	4004	FAD	C4X-C10-N10	2.92	120.66	116.48
7	B	4006	NAI	C4A-C5A-N7A	-2.83	107.35	110.58
4	A	3004	FAD	C4X-C10-N10	2.80	120.49	116.48
7	B	4006	NAI	C5A-N7A-C8A	2.75	107.77	103.45
4	A	3004	FAD	C4A-C5A-N7A	-2.74	107.45	110.58
4	B	4004	FAD	C10-C4X-N5	-2.68	119.34	124.81
4	B	4004	FAD	O2A-PA-O3P	2.66	114.47	107.27
4	A	3004	FAD	N3A-C4A-N9A	2.57	131.55	127.17
4	B	4004	FAD	C4X-C4-N3	2.56	119.78	113.25
4	A	3004	FAD	C4-N3-C2	-2.56	121.09	125.64
4	A	3004	FAD	C10-C4X-N5	-2.54	119.61	124.81
7	A	3007	NAI	C1D-N1N-C2N	-2.54	116.96	121.14
7	B	4006	NAI	C1D-N1N-C6N	-2.53	115.41	120.77
7	A	3007	NAI	C5A-N7A-C8A	2.47	107.33	103.45
7	A	3007	NAI	C4A-N9A-C8A	2.46	108.32	105.74
4	B	4004	FAD	O2P-P-O3P	2.46	113.91	107.27
4	B	4004	FAD	N3A-C4A-N9A	2.42	131.28	127.17
7	A	3007	NAI	C4A-C5A-N7A	-2.40	107.84	110.58
7	B	4006	NAI	O2B-C2B-C1B	-2.32	102.13	110.10
4	B	4004	FAD	C9A-C5X-N5	-2.31	120.00	122.45
5	A	3005	URC	O24-C8-N7	-2.31	121.36	125.56
4	A	3004	FAD	C4X-C4-N3	2.31	119.13	113.25
4	B	4004	FAD	C4'-C3'-C2'	-2.30	109.73	113.57
4	B	4004	FAD	C4A-N9A-C8A	2.26	108.12	105.74
4	B	4004	FAD	C4X-C10-N1	-2.25	119.07	124.59
7	B	4006	NAI	O4D-C1D-N1N	2.23	112.33	108.08
4	B	4004	FAD	C2A-N1A-C6A	2.21	122.37	118.73
4	A	3004	FAD	O2P-P-O3P	2.13	113.04	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3004	FAD	C4A-N9A-C8A	2.13	107.97	105.74
5	A	3005	URC	C5-C6-N1	2.07	117.81	112.13
4	A	3004	FAD	C4X-C10-N1	-2.06	119.53	124.59

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3004	FAD	N10-C1'-C2'-O2'
4	A	3004	FAD	N10-C1'-C2'-C3'
4	B	4004	FAD	N10-C1'-C2'-O2'
4	B	4004	FAD	N10-C1'-C2'-C3'
7	B	4006	NAI	C2D-C1D-N1N-C6N
8	A	3008	GOL	O1-C1-C2-C3
8	A	3009	GOL	C1-C2-C3-O3
7	A	3007	NAI	C2D-C1D-N1N-C6N
8	A	3009	GOL	O2-C2-C3-O3
8	A	3008	GOL	O1-C1-C2-O2
7	B	4006	NAI	O4D-C1D-N1N-C6N
7	A	3007	NAI	O4D-C1D-N1N-C6N
7	A	3007	NAI	C2N-C3N-C7N-N7N
4	B	4004	FAD	C2'-C3'-C4'-O4'
4	B	4004	FAD	O3'-C3'-C4'-O4'

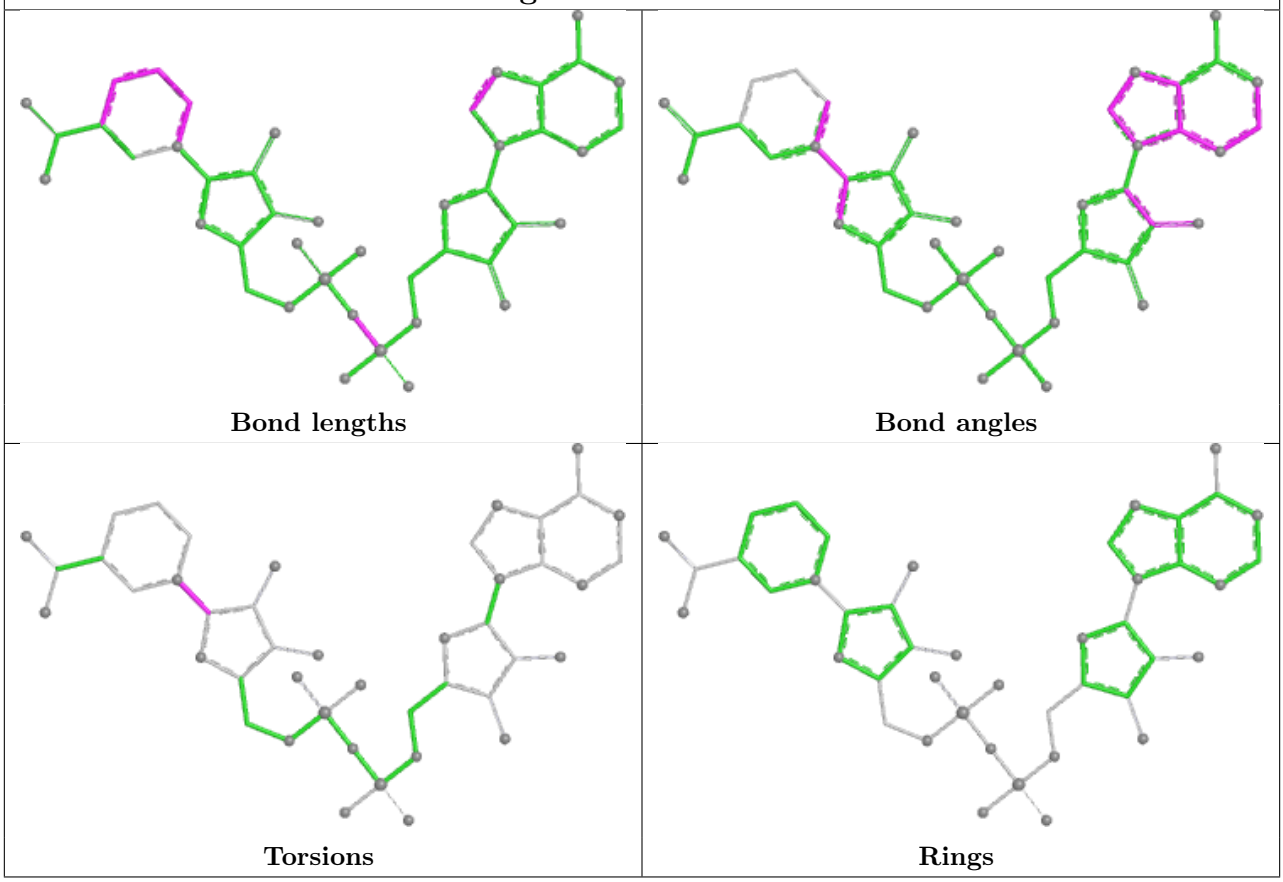
There are no ring outliers.

1 monomer is involved in 3 short contacts:

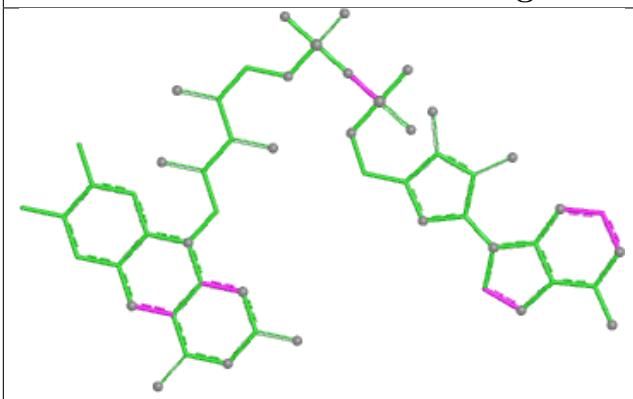
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3004	FAD	3	0

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.

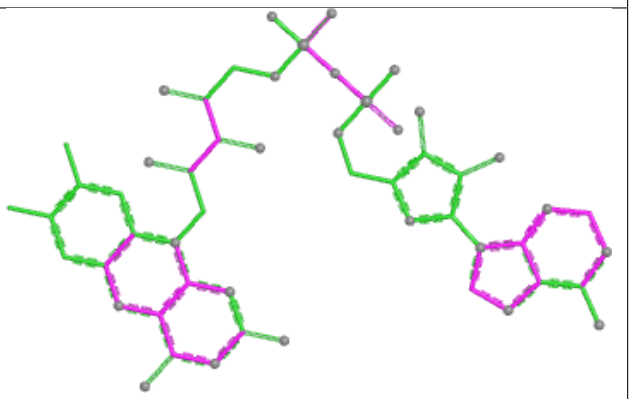
Ligand NAI B 4006



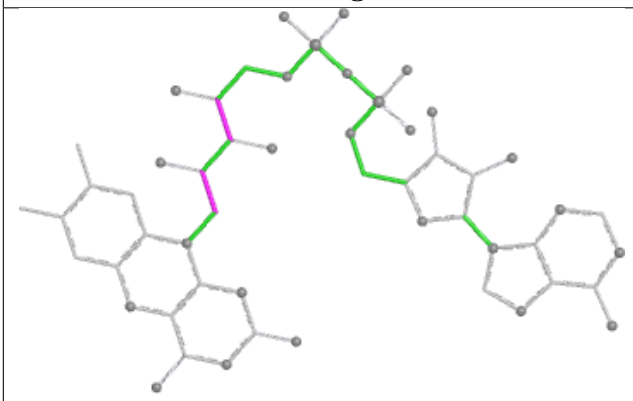
Ligand FAD B 4004



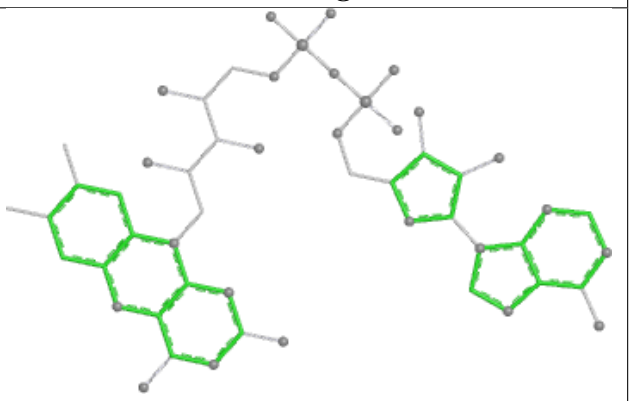
Bond lengths



Bond angles

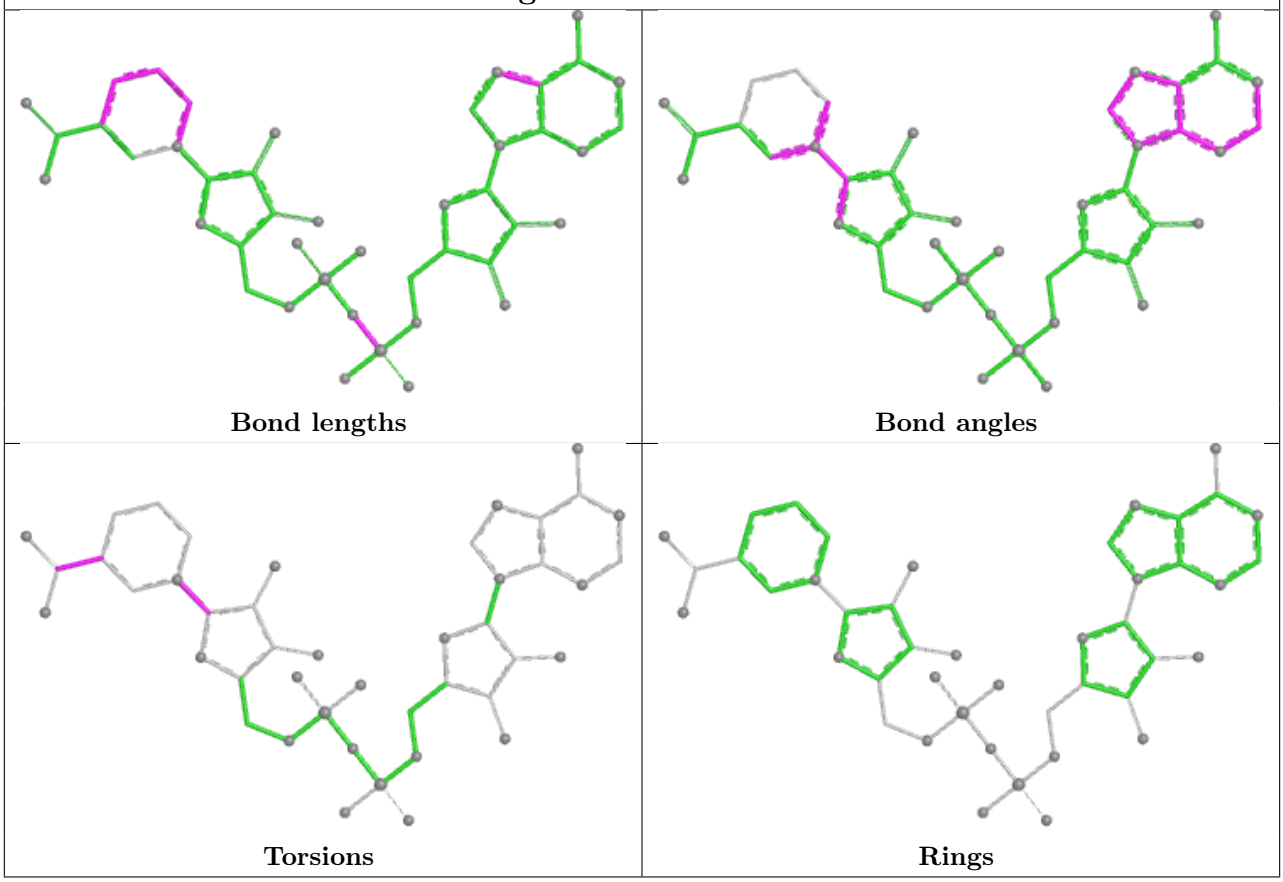


Torsions

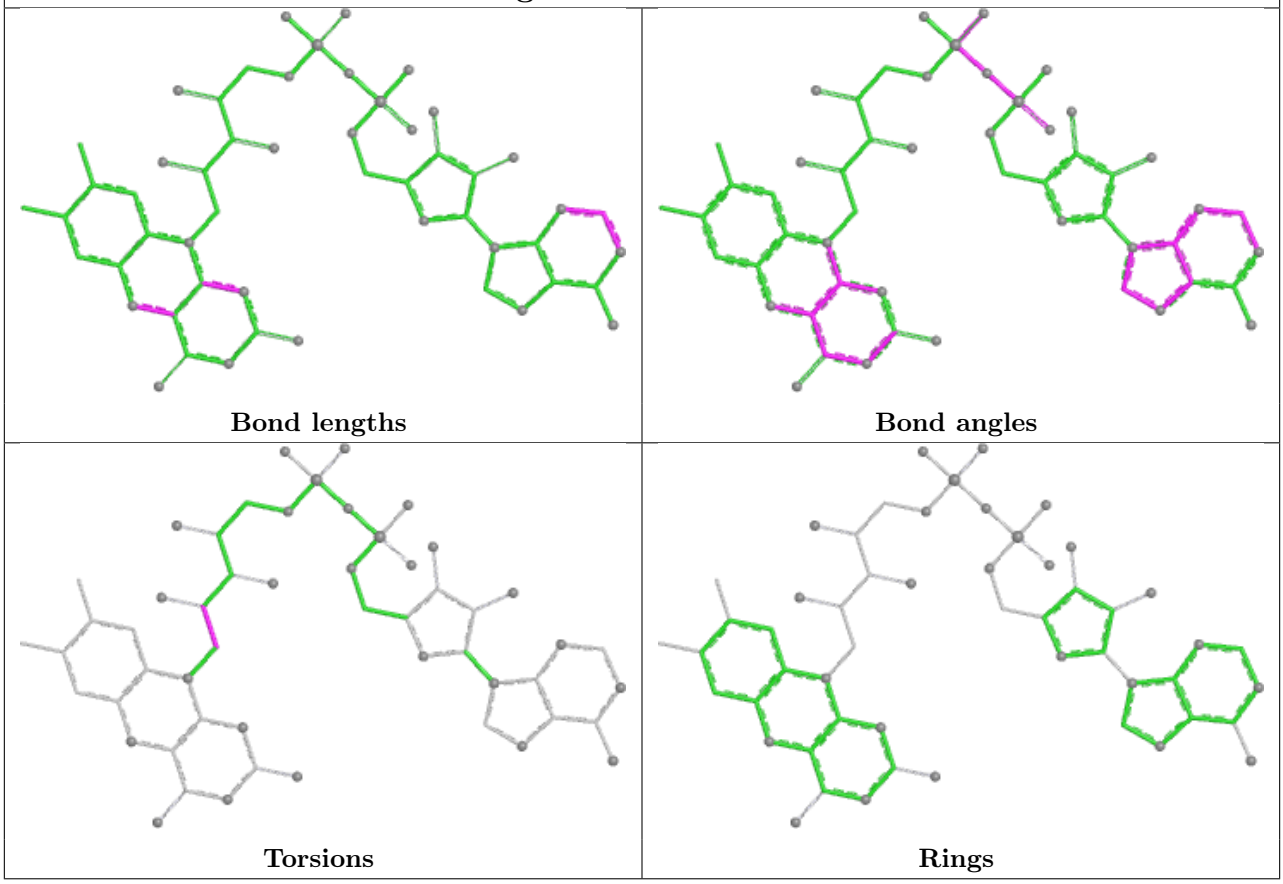


Rings

Ligand NAI A 3007



Ligand FAD A 3004



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%)	-0.17	32 (2%)	58	55	10, 21, 38, 63	0
1	B	1293/1331 (97%)	-0.33	24 (1%)	66	63	9, 17, 32, 56	0
All	All	2597/2662 (97%)	-0.25	56 (2%)	62	59	9, 19, 37, 63	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1320	VAL	6.3
1	B	1287	ASP	6.0
1	A	1318	THR	6.0
1	A	3	ALA	4.8
1	B	1321	PRO	4.7
1	A	1287	ASP	4.6
1	A	1321	PRO	4.6
1	A	1111	GLY	4.2
1	A	1288	ASN	4.1
1	A	1319	GLY	4.1
1	B	535	ALA	4.0
1	B	61	LEU	3.9
1	A	1322	GLU	3.9
1	A	61	LEU	3.9
1	B	1289	ALA	3.9
1	A	1331	ILE	3.7
1	B	1111	GLY	3.7
1	A	1317	VAL	3.5
1	A	1285	HIS	3.5
1	A	1289	ALA	3.4
1	B	1322	GLU	3.4
1	A	1110	THR	3.3
1	B	1320	VAL	3.1
1	A	166	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	534	MET	3.1
1	B	1318	THR	3.1
1	A	1286	GLY	3.0
1	A	396	LEU	3.0
1	A	321	GLN	2.7
1	B	532	GLU	2.7
1	A	220	ASP	2.7
1	B	536	GLY	2.6
1	B	530	ASP	2.6
1	B	1110	THR	2.6
1	B	220	ASP	2.5
1	B	983	GLU	2.5
1	B	3	ALA	2.5
1	A	192	PRO	2.4
1	B	221	THR	2.4
1	A	1326	SER	2.3
1	A	222	PRO	2.3
1	B	600	GLU	2.3
1	A	1323	ASN	2.3
1	A	1324	SER	2.3
1	A	536	GLY	2.2
1	A	535	ALA	2.2
1	B	164	LYS	2.2
1	A	1325	LYS	2.2
1	A	534	MET	2.1
1	B	218	LEU	2.1
1	A	1143	GLU	2.1
1	A	529	ALA	2.0
1	B	483	GLN	2.0
1	A	531	LEU	2.0
1	B	1288	ASN	2.0
1	B	222	PRO	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)

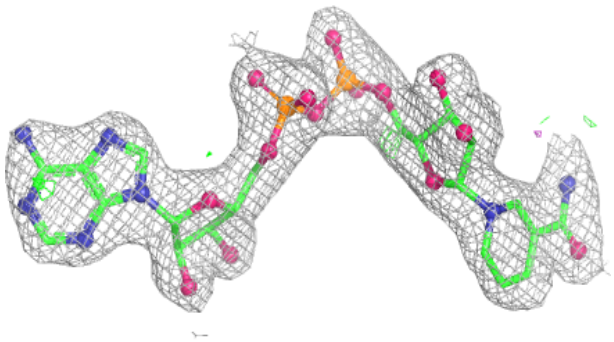
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

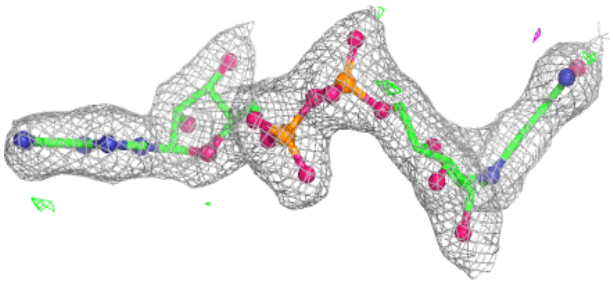
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	B	4007	6/6	0.85	0.15	29,30,32,35	0
8	GOL	A	3008	6/6	0.90	0.11	27,28,29,32	0
8	GOL	A	3009	6/6	0.92	0.10	21,24,26,26	0
8	GOL	B	4008	6/6	0.92	0.09	20,21,23,23	0
5	URC	A	3005	12/12	0.95	0.08	23,23,24,24	0
7	NAI	A	3007	44/44	0.95	0.07	19,29,33,33	0
4	FAD	A	3004	53/53	0.96	0.07	16,19,21,22	0
7	NAI	B	4006	44/44	0.97	0.05	13,16,20,20	0
4	FAD	B	4004	53/53	0.98	0.05	9,11,13,14	0
2	FES	B	4001	4/4	0.98	0.07	20,20,22,23	0
6	BCT	A	3006	4/4	0.98	0.07	17,18,18,18	0
6	BCT	B	4005	4/4	0.98	0.04	12,13,13,13	0
2	FES	A	3001	4/4	0.98	0.08	20,20,21,23	0
3	CA	A	3003	1/1	0.99	0.02	21,21,21,21	0
3	CA	B	4003	1/1	1.00	0.02	14,14,14,14	0
2	FES	B	4002	4/4	1.00	0.02	9,10,10,10	0
2	FES	A	3002	4/4	1.00	0.02	10,10,11,11	0

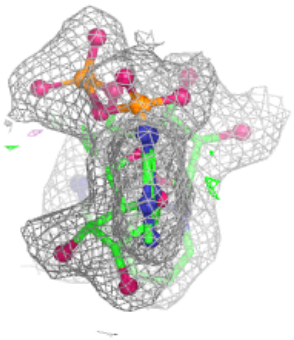
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI A 3007:

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

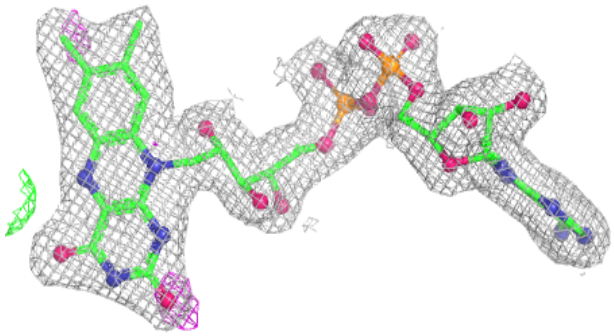


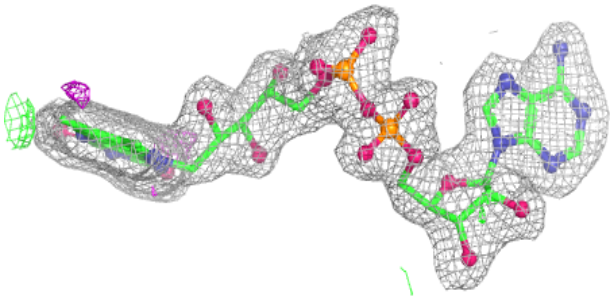


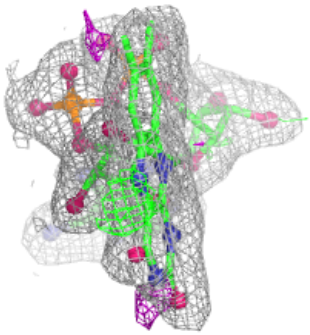


Electron density around FAD A 3004:

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

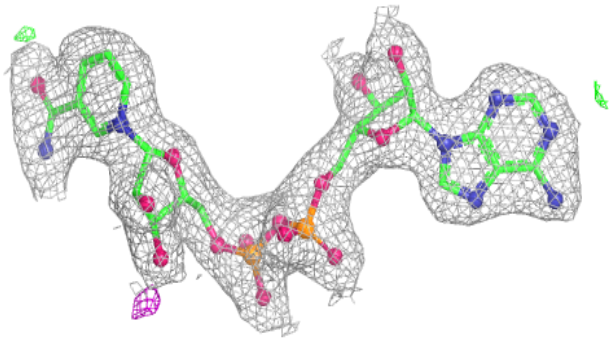


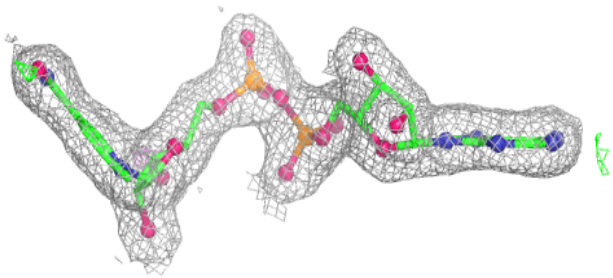




Electron density around NAI B 4006:

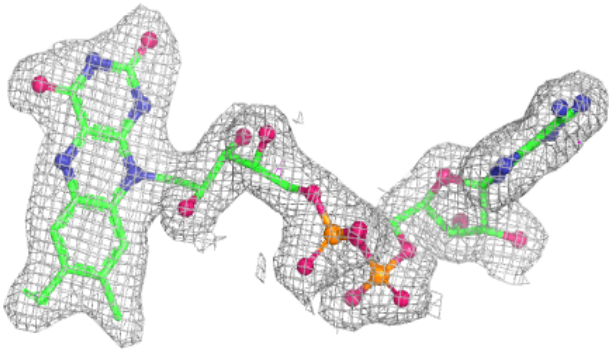
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

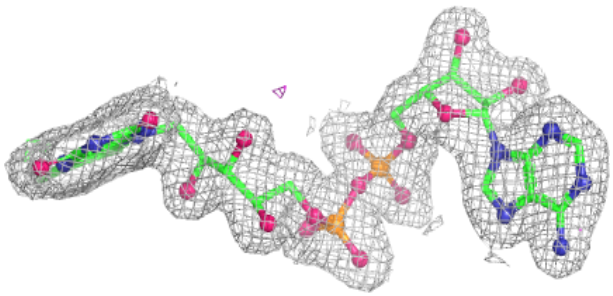


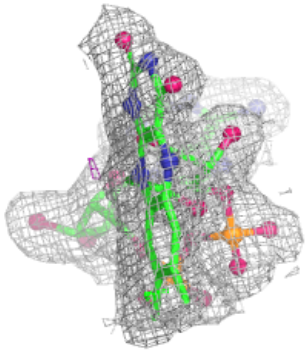


Electron density around FAD B 4004:

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







6.5 Other polymers (i)

There are no such residues in this entry.