Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 07:51 PM JST

PDB ID	:	4YRW
Title	:	rat xanthine oxidoreductase, C-terminal deletion protein variant
Authors	:	Okamoto, K.
Deposited on	:	2015-03-16
Resolution	:	1.99 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:

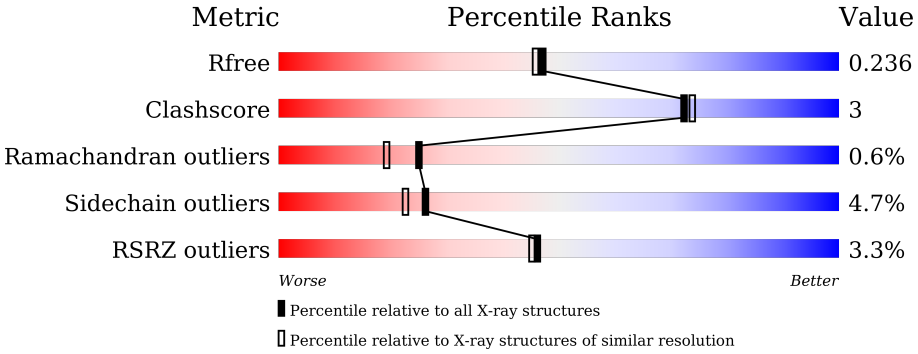
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	1315	4% 86% 10% • • •
1	B	1315	2% 87% 9% • •

2 Entry composition (i)

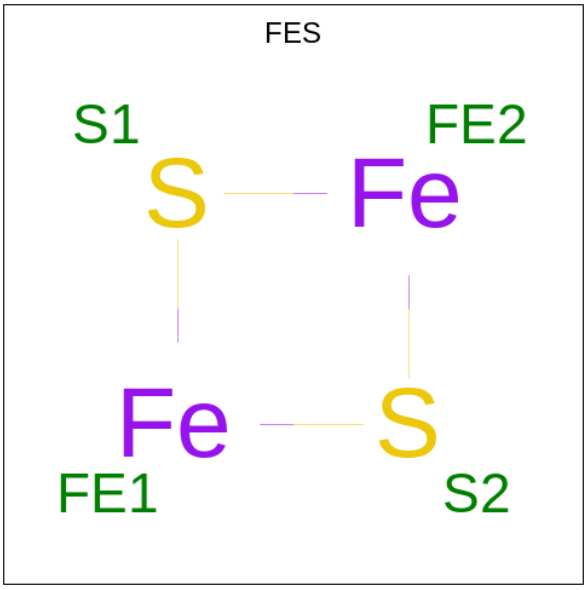
There are 8 unique types of molecules in this entry. The entry contains 20715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

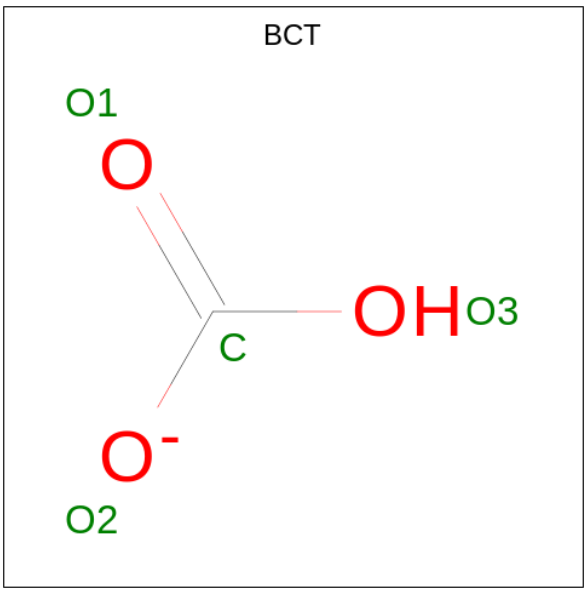
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1289	9964	6314	1714	1873	63	0	0	0
1	B	1286	9939	6298	1711	1867	63	0	0	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



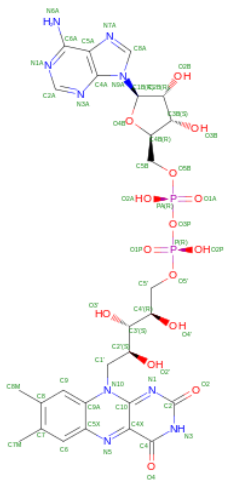
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	1	3	0	0
			Total	C	O		
3	B	1	4	1	3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

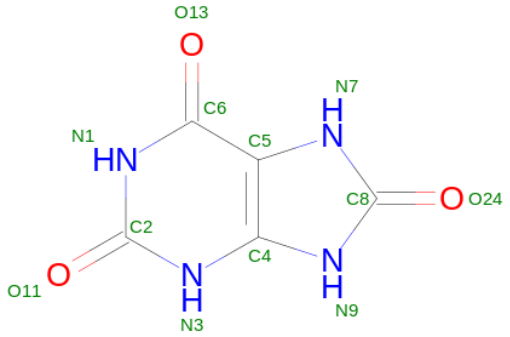
FAD



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

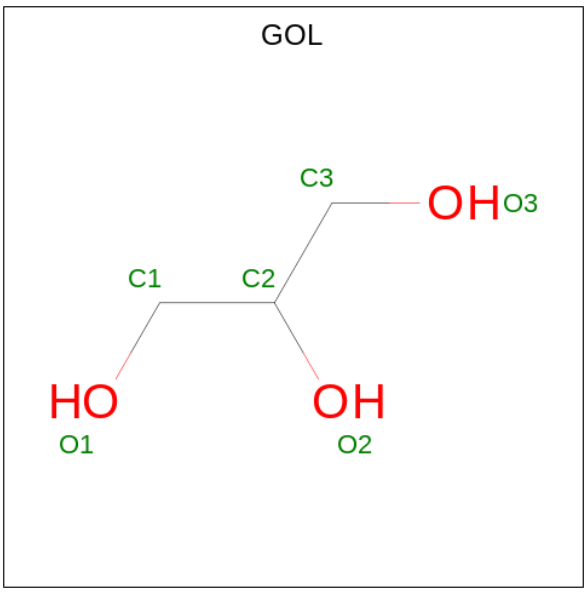
- Molecule 6 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).

URC



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

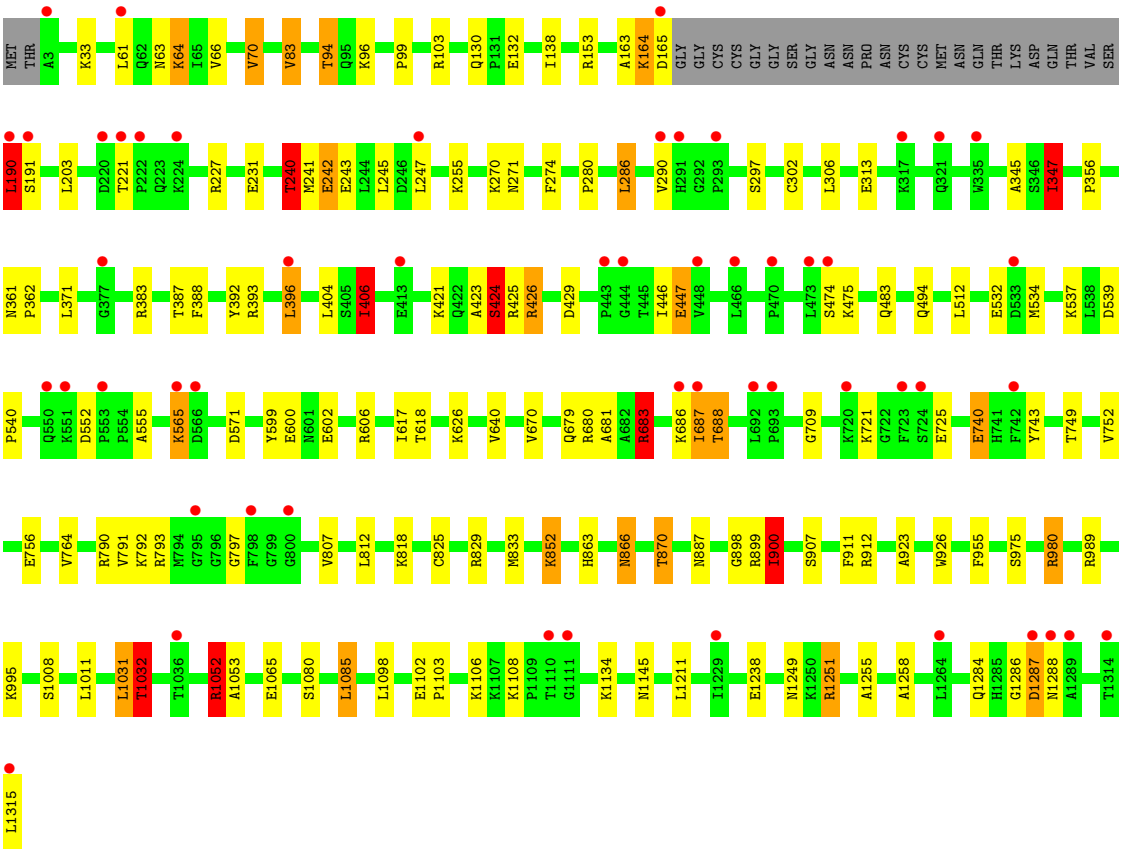
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	250	250	250	0	0
			Total	O		
8	B	388	388	388	0	0

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.

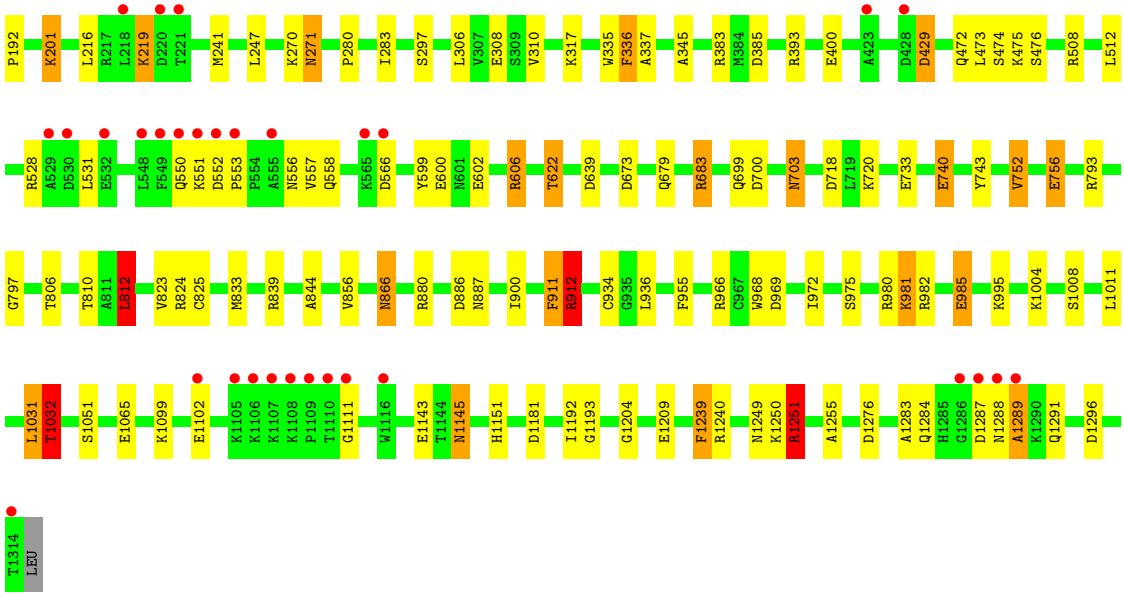
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:


P192 K201 L216 R217 L218 K219 D220 T221 M241 L247 K270 N271 P280 I283 S297 L306 V307 E308 S309 V310 K317 W335 F336 A337 A345 R383 M384 D385 R393 E400 A423 D428 D429 Q472 L473 S474 K475 S476 R508 L512
R528 A529 D530 L531 E532 L548 F549 Q550 K551 D552 P553 P554 A555 N556 V557 Q558 K565 D566 Y599 E600 N601 E602 R606 T622 D639 D673 Q679 R683 Q699 D700 N703 D718 L719 K720 E733 E740 Y743 V752 E756 R793
G797 T806 T810 A811 L812 V823 R824 C825 M833 R839 A844 V856 N866 R880 D886 N887 I900 F911 R912 C934 G935 L936 F955 R966 C967 W968 D969 I972 S975 R980 K981 R982 E985 K995 K1004 S1008 L1011
L1031 T1032 S1051 E1065 K1099 E1102 K1105 K1106 K1107 K1108 P1109 T1110 G1111 W1116 E1143 T1144 N1145 H1151 D1181 I1192 G1193 G1204 E1209 F1239 R1240 N1249 K1250 R1251 A1255 D1276 A1283 Q1284 H1285 G1286 D1287 N1288 A1289 K1290 Q1291 D1296
T1314 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.50Å 138.47Å 222.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.33 – 1.99 43.33 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.33-1.99) 99.6 (43.33-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.79 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.229 0.194 , 0.236	Depositor DCC
R_{free} test set	10396 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20715	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 3.00% 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: FAD, BCT, FES, URC, GOL, CA

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	0.94	4/10174 (0.0%)	1.00	28/13767 (0.2%)
1	B	1.06	12/10149 (0.1%)	1.04	44/13734 (0.3%)
All	All	1.00	16/20323 (0.1%)	1.02	72/27501 (0.3%)

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	B	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	740	GLU	CD-OE1	9.56	1.36	1.25
1	B	740	GLU	CD-OE2	8.97	1.35	1.25
1	B	308	GLU	CD-OE2	-7.06	1.17	1.25
1	A	600	GLU	CD-OE2	5.94	1.32	1.25
1	B	756	GLU	CB-CG	-5.89	1.41	1.52
1	B	602	GLU	CD-OE1	5.84	1.32	1.25
1	B	1193	GLY	N-CA	5.53	1.54	1.46
1	A	602	GLU	CD-OE1	5.50	1.31	1.25
1	B	600	GLU	CD-OE2	5.47	1.31	1.25
1	B	793	ARG	CZ-NH1	5.34	1.40	1.33
1	B	1239	PHE	CG-CD2	5.28	1.46	1.38
1	A	240	THR	CB-CG2	-5.28	1.34	1.52
1	B	102	GLU	CD-OE2	-5.24	1.19	1.25
1	B	756	GLU	CD-OE1	5.19	1.31	1.25
1	A	740	GLU	CD-OE1	5.12	1.31	1.25
1	B	429	ASP	CB-CG	-5.11	1.41	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1052	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	B	812	LEU	CA-CB-CG	-13.46	84.34	115.30
1	A	1052	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	B	793	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	989	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	793	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	793	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	70	VAL	CG1-CB-CG2	7.80	123.38	110.90
1	B	1031	LEU	CB-CG-CD2	7.55	123.83	111.00
1	B	1251	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	70	VAL	CG1-CB-CG2	7.06	122.19	110.90
1	A	790	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	683	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	856	VAL	CG1-CB-CG2	6.72	121.66	110.90
1	B	385	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	703	ASN	N-CA-CB	-6.61	98.70	110.60
1	A	406	ILE	CB-CA-C	-6.47	98.66	111.60
1	B	508	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	839	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	1251	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	1111	GLY	N-CA-C	-6.28	97.39	113.10
1	A	227	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	201	LYS	CA-CB-CG	6.25	127.16	113.40
1	A	900	ILE	CB-CA-C	6.23	124.05	111.60
1	B	1296	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	829	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	1032	THR	CB-CA-C	-6.15	94.99	111.60
1	B	740	GLU	OE1-CD-OE2	6.13	130.65	123.30
1	B	103	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	980	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	880	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	812	LEU	CD1-CG-CD2	6.07	128.70	110.50
1	B	912	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	83	VAL	CG1-CB-CG2	6.03	120.55	110.90
1	B	297	SER	CB-CA-C	6.00	121.50	110.10
1	B	793	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	1032	THR	N-CA-CB	5.93	121.57	110.30
1	B	1032	THR	CB-CA-C	-5.93	95.60	111.60
1	A	606	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	106	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	227	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	752	VAL	CG1-CB-CG2	5.85	120.25	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	LEU	CB-CG-CD1	5.83	120.91	111.00
1	B	639	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	880	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	1004	LYS	CD-CE-NZ	5.77	124.97	111.70
1	B	756	GLU	CB-CA-C	-5.73	98.93	110.40
1	B	718	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	385	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	393	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	824	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	673	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	1085	LEU	CB-CG-CD1	5.50	120.35	111.00
1	B	528	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	347	ILE	CB-CA-C	-5.43	100.74	111.60
1	A	203	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	429	ASP	N-CA-CB	-5.42	100.84	110.60
1	A	683	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	966	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	606	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	622	THR	N-CA-CB	-5.30	100.23	110.30
1	A	1031	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	989	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	1032	THR	OG1-CB-CG2	5.22	122.02	110.00
1	A	94	THR	N-CA-CB	-5.18	100.45	110.30
1	B	508	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	1296	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	1251	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	756	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	B	1276	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	1181	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	700	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	886	ASP	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	9964	0	9967	78	0
1	B	9939	0	9942	59	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	2	0
6	A	12	0	4	0	0
6	B	12	0	4	0	0
7	A	6	0	8	0	0
7	B	12	0	16	0	0
8	A	250	0	0	1	0
8	B	388	0	0	5	0
All	All	20715	0	20003	135	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 3.

All (135) 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:982:ARG:NH1	8:B:4101:HOH:O	1.56	1.21
1:B:192:PRO:HD2	8:B:4376:HOH:O	1.55	1.04
1:B:740:GLU:HG2	1:B:833:MET:SD	1.99	1.02
1:A:423:ALA:O	1:A:424:SER:HB3	1.69	0.92
1:A:618:THR:OG1	1:A:688:THR:HG22	1.71	0.89
1:B:982:ARG:CZ	8:B:4101:HOH:O	2.06	0.87
1:A:565:LYS:H	1:A:565:LYS:HD3	1.45	0.81
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.45	0.81
1:A:231:GLU:OE2	1:A:680:ARG:NH2	2.13	0.81
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.46	0.78
1:A:565:LYS:HD3	1:A:565:LYS:N	1.98	0.78
1:B:982:ARG:NH2	8:B:4101:HOH:O	2.13	0.78
1:A:426:ARG:HH11	1:A:426:ARG:HB3	1.51	0.75
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.68	0.75
1:A:709:GLY:O	1:A:899:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLN:HE21	1:B:132:GLU:H	1.34	0.74
1:B:472:GLN:HA	1:B:475:LYS:HD3	1.70	0.73
1:A:130:GLN:HE21	1:A:132:GLU:H	1.33	0.73
1:A:446:ILE:HD12	1:A:534:MET:HB2	1.70	0.72
1:A:423:ALA:O	1:A:424:SER:CB	2.37	0.72
1:A:446:ILE:HD12	1:A:534:MET:CB	2.21	0.70
1:B:271:ASN:HB2	1:B:683:ARG:NH1	2.05	0.70
1:A:388:PHE:HA	1:A:396:LEU:HG	1.75	0.69
1:B:981:LYS:O	1:B:985:GLU:HG2	1.93	0.69
1:A:812:LEU:HD11	1:A:825:CYS:CB	2.24	0.68
1:B:699:GLN:O	1:B:703:ASN:HB2	1.94	0.68
1:A:618:THR:OG1	1:A:688:THR:CG2	2.42	0.67
1:B:1283:ALA:HA	1:B:1288:ASN:HD21	1.59	0.67
1:A:371:LEU:CD2	1:A:406:ILE:HG23	2.26	0.66
1:A:421:LYS:HD2	8:A:3146:HOH:O	1.97	0.64
1:B:191:SER:OG	1:B:192:PRO:HD3	1.98	0.64
1:A:565:LYS:N	1:A:565:LYS:CD	2.61	0.63
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.81	0.62
1:A:240:THR:HG22	1:A:243:GLU:H	1.64	0.62
1:B:552:ASP:HB3	1:B:553:PRO:HD2	1.83	0.61
1:B:58:TYR:CE2	1:B:219:LYS:HD3	2.36	0.60
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.82	0.60
1:A:371:LEU:HD23	1:A:406:ILE:HG23	1.84	0.59
1:B:1250:LYS:HG3	1:B:1251:ARG:H	1.67	0.59
1:A:138:ILE:HD12	1:A:163:ALA:HB2	1.83	0.58
1:A:812:LEU:HD11	1:A:825:CYS:HB2	1.87	0.57
1:B:336:PHE:O	1:B:336:PHE:HD1	1.88	0.56
1:A:63:ASN:O	1:A:64:LYS:HB3	2.05	0.56
1:A:1286:GLY:O	1:A:1287:ASP:HB3	2.05	0.56
1:B:157:GLN:HE22	1:B:558:GLN:HE22	1.53	0.56
1:A:539:ASP:OD1	1:A:540:PRO:HD2	2.05	0.56
1:B:1032:THR:HG21	8:B:4364:HOH:O	2.06	0.55
1:B:1032:THR:CG2	1:B:1065:GLU:O	2.55	0.55
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.04	0.55
1:B:1288:ASN:O	1:B:1289:ALA:CB	2.55	0.55
1:A:532:GLU:OE1	1:A:537:LYS:HG2	2.07	0.54
1:A:812:LEU:HD21	1:A:825:CYS:N	2.22	0.54
1:B:271:ASN:HB2	1:B:683:ARG:CZ	2.37	0.54
1:A:446:ILE:O	1:A:446:ILE:CG2	2.55	0.54
1:B:1288:ASN:O	1:B:1289:ALA:HB3	2.07	0.54
1:B:271:ASN:O	1:B:271:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:THR:HG22	1:A:907:SER:OG	2.08	0.53
1:A:1032:THR:CG2	1:A:1065:GLU:O	2.58	0.52
1:A:280:PRO:HB2	1:A:286:LEU:HD23	1.91	0.51
1:A:852:LYS:CE	1:A:852:LYS:HA	2.41	0.51
1:A:1032:THR:HG23	1:A:1065:GLU:O	2.11	0.51
1:A:392:TYR:OH	1:A:429:ASP:OD2	2.25	0.50
1:B:472:GLN:HE22	1:B:475:LYS:NZ	2.09	0.50
1:A:240:THR:CG2	1:A:242:GLU:HB2	2.41	0.50
1:B:552:ASP:HB3	1:B:553:PRO:CD	2.41	0.50
1:B:969:ASP:HA	1:B:972:ILE:CG1	2.42	0.49
1:A:426:ARG:HH11	1:A:426:ARG:CB	2.24	0.49
1:A:555:ALA:O	1:A:1238:GLU:HA	2.13	0.48
1:A:255:LYS:HE2	1:A:274:PHE:CE1	2.48	0.48
1:A:721:LYS:O	1:A:725:GLU:HG3	2.13	0.48
1:A:866:ASN:C	1:A:866:ASN:HD22	2.16	0.48
1:A:1080:SER:O	1:A:1258:ALA:HB1	2.14	0.47
1:B:1032:THR:HG23	1:B:1065:GLU:O	2.14	0.47
1:A:764:VAL:O	1:A:791:VAL:HG22	2.14	0.47
1:A:64:LYS:HE3	1:A:66:VAL:HG12	1.96	0.47
1:A:792:LYS:HE3	1:B:756:GLU:OE1	2.15	0.47
1:A:565:LYS:H	1:A:565:LYS:CD	2.13	0.47
1:B:975:SER:O	1:B:980:ARG:HD3	2.14	0.47
1:B:306:LEU:O	1:B:310:VAL:HG13	2.15	0.46
1:A:361:ASN:N	1:A:362:PRO:CD	2.79	0.46
1:A:190:LEU:HD13	1:A:191:SER:H	1.80	0.46
1:A:571:ASP:OD1	1:A:1052:ARG:HD3	2.15	0.46
1:B:900:ILE:HD12	1:B:900:ILE:N	2.31	0.46
1:A:446:ILE:HD12	1:A:534:MET:HB3	1.94	0.46
1:B:337:ALA:HB2	5:B:4004:FAD:C6	2.46	0.46
1:B:557:VAL:HG13	1:B:1240:ARG:HG2	1.97	0.46
1:B:335:TRP:CE3	1:B:335:TRP:HA	2.50	0.46
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.46
1:A:863:HIS:O	1:A:898:GLY:HA2	2.16	0.45
1:B:1151:HIS:NE2	1:B:1251:ARG:HG3	2.31	0.45
1:A:749:THR:O	1:A:812:LEU:HD22	2.15	0.45
1:A:740:GLU:HG3	1:A:833:MET:CE	2.47	0.45
1:B:336:PHE:O	1:B:336:PHE:CD1	2.67	0.45
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.17	0.45
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	1.99	0.45
1:A:387:THR:O	1:A:396:LEU:HD21	2.16	0.45
1:A:740:GLU:HG2	1:A:1211:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.17	0.44
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.17	0.44
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.33	0.43
1:A:164:LYS:C	1:A:165:ASP:OD1	2.56	0.43
1:A:345:ALA:HB1	5:A:3005:FAD:H4'	2.00	0.43
1:A:302:CYS:HB2	1:A:347:ILE:HD11	2.01	0.43
1:B:812:LEU:HD21	1:B:823:VAL:O	2.19	0.43
1:A:900:ILE:HD12	1:A:900:ILE:C	2.39	0.43
1:A:99:PRO:O	1:A:103:ARG:HG3	2.19	0.43
1:A:679:GLN:HE21	1:A:683:ARG:NH2	2.17	0.43
1:A:356:PRO:HD2	1:A:429:ASP:OD1	2.19	0.42
1:A:617:ILE:HG23	1:A:687:ILE:CD1	2.49	0.42
1:B:812:LEU:HD11	1:B:825:CYS:CB	2.50	0.42
1:A:749:THR:O	1:A:812:LEU:CD2	2.68	0.42
1:A:571:ASP:CG	1:A:1052:ARG:HD3	2.41	0.42
1:B:473:LEU:O	1:B:474:SER:HB2	2.20	0.42
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.68	0.41
1:B:393:ARG:NH2	1:B:429:ASP:OD1	2.45	0.41
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.18	0.41
1:B:968:TRP:O	1:B:972:ILE:HG12	2.21	0.41
1:B:934:CYS:HB3	1:B:936:LEU:HD12	2.02	0.41
1:B:1151:HIS:O	1:B:1251:ARG:HD3	2.21	0.41
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	2.02	0.41
1:B:969:ASP:HA	1:B:972:ILE:HG12	2.02	0.41
1:B:1204:GLY:HA3	1:B:1209:GLU:OE2	2.21	0.41
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.41
1:A:446:ILE:O	1:A:446:ILE:HG22	2.19	0.41
1:A:599:TYR:HA	1:B:599:TYR:HA	2.03	0.41
1:A:975:SER:O	1:A:980:ARG:HD3	2.21	0.41
1:B:806:THR:O	1:B:810:THR:HG23	2.21	0.41
1:B:866:ASN:C	1:B:866:ASN:HD22	2.24	0.40
1:A:153:ARG:HD2	1:A:153:ARG:C	2.42	0.40
1:B:99:PRO:O	1:B:103:ARG:HG3	2.22	0.40
1:B:134:THR:OG1	1:B:137:GLU:HG3	2.22	0.40
1:A:241:MET:CE	1:A:245:LEU:HD11	2.51	0.40
1:A:447:GLU:HA	1:A:475:LYS:O	2.21	0.40
1:B:345:ALA:HB1	5:B:4004:FAD:H4'	2.04	0.40
1:B:733:GLU:HA	1:B:844:ALA:O	2.22	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	1285/1315 (98%)	1239 (96%)	38 (3%)	8 (1%)	25 19
1	B	1282/1315 (98%)	1242 (97%)	32 (2%)	8 (1%)	25 19
All	All	2567/2630 (98%)	2481 (97%)	70 (3%)	16 (1%)	25 19

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	B	1251	ARG
1	B	1287	ASP
1	B	1289	ALA
1	A	424	SER
1	B	912	ARG
1	A	797	GLY
1	A	912	ARG
1	A	1287	ASP
1	B	797	GLY
1	B	887	ASN
1	A	474	SER
1	A	552	ASP
1	A	887	ASN
1	B	556	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	1088/1109 (98%)	1029 (95%)	59 (5%)	22	18
1	B	1085/1109 (98%)	1042 (96%)	43 (4%)	31	29
All	All	2173/2218 (98%)	2071 (95%)	102 (5%)	26	22

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	61	LEU
1	A	64	LYS
1	A	70	VAL
1	A	83	VAL
1	A	94	THR
1	A	96	LYS
1	A	164	LYS
1	A	190	LEU
1	A	221	THR
1	A	240	THR
1	A	242	GLU
1	A	247	LEU
1	A	270	LYS
1	A	271	ASN
1	A	286	LEU
1	A	290	VAL
1	A	297	SER
1	A	306	LEU
1	A	313	GLU
1	A	347	ILE
1	A	383	ARG
1	A	396	LEU
1	A	404	LEU
1	A	406	ILE
1	A	424	SER
1	A	425	ARG
1	A	426	ARG
1	A	447	GLU
1	A	483	GLN
1	A	494	GLN
1	A	512	LEU
1	A	565	LYS
1	A	626	LYS
1	A	640	VAL

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Mol	Chain	Res	Type
1	A	683	ARG
1	A	686	LYS
1	A	687	ILE
1	A	688	THR
1	A	743	TYR
1	A	752	VAL
1	A	807	VAL
1	A	818	LYS
1	A	852	LYS
1	A	866	ASN
1	A	870	THR
1	A	900	ILE
1	A	911	PHE
1	A	1011	LEU
1	A	1031	LEU
1	A	1032	THR
1	A	1052	ARG
1	A	1085	LEU
1	A	1106	LYS
1	A	1108	LYS
1	A	1134	LYS
1	A	1251	ARG
1	A	1288	ASN
1	A	1315	LEU
1	B	28	VAL
1	B	61	LEU
1	B	62	GLN
1	B	64	LYS
1	B	70	VAL
1	B	164	LYS
1	B	201	LYS
1	B	216	LEU
1	B	219	LYS
1	B	247	LEU
1	B	270	LYS
1	B	271	ASN
1	B	280	PRO
1	B	317	LYS
1	B	336	PHE
1	B	383	ARG
1	B	400	GLU
1	B	476	SER

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Mol	Chain	Res	Type
1	B	512	LEU
1	B	531	LEU
1	B	550	GLN
1	B	551	LYS
1	B	566	ASP
1	B	622	THR
1	B	683	ARG
1	B	720	LYS
1	B	743	TYR
1	B	752	VAL
1	B	812	LEU
1	B	866	ASN
1	B	911	PHE
1	B	981	LYS
1	B	985	GLU
1	B	1011	LEU
1	B	1031	LEU
1	B	1032	THR
1	B	1051	SER
1	B	1099	LYS
1	B	1102	GLU
1	B	1143	GLU
1	B	1145	ASN
1	B	1239	PHE
1	B	1291	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	271	ASN
1	A	321	GLN
1	A	350	ASN
1	A	472	GLN
1	A	583	ASN
1	A	585	GLN
1	A	728	ASN
1	A	866	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1284	GLN
1	A	1285	HIS

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Mol	Chain	Res	Type
1	A	1288	ASN
1	B	62	GLN
1	B	130	GLN
1	B	157	GLN
1	B	223	GLN
1	B	271	ASN
1	B	291	HIS
1	B	350	ASN
1	B	472	GLN
1	B	583	ASN
1	B	642	ASN
1	B	703	ASN
1	B	866	ASN
1	B	1088	GLN
1	B	1145	ASN
1	B	1284	GLN
1	B	1288	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	GOL	B	4007	-	5,5,5	0.59	0	5,5,5	0.38	0
2	FES	A	3001	1	0,4,4	-	-	-		
5	FAD	B	4004	-	53,58,58	1.72	14 (26%)	68,89,89	1.46	11 (16%)
6	URC	B	4006	-	8,13,13	2.35	2 (25%)	5,19,19	6.23	4 (80%)
2	FES	B	4001	1	0,4,4	-	-	-		
2	FES	B	4002	1	0,4,4	-	-	-		
5	FAD	A	3005	-	53,58,58	1.59	13 (24%)	68,89,89	1.53	13 (19%)
3	BCT	B	4005	-	2,3,3	0.63	0	2,3,3	1.35	0
7	GOL	B	4008	-	5,5,5	0.51	0	5,5,5	0.36	0
7	GOL	A	3007	-	5,5,5	0.68	0	5,5,5	0.69	0
2	FES	A	3002	1	0,4,4	-	-	-		
3	BCT	A	3003	-	2,3,3	0.74	0	2,3,3	1.40	0
6	URC	A	3006	-	8,13,13	2.27	4 (50%)	5,19,19	7.08	4 (80%)

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	GOL	B	4007	-	-	0/4/4/4	-
5	FAD	B	4004	-	-	0/30/50/50	0/6/6/6
2	FES	A	3001	1	-	-	0/1/1/1
6	URC	B	4006	-	-	-	0/2/2/2
2	FES	B	4001	1	-	-	0/1/1/1
2	FES	B	4002	1	-	-	0/1/1/1
5	FAD	A	3005	-	-	0/30/50/50	0/6/6/6
7	GOL	B	4008	-	-	0/4/4/4	-
7	GOL	A	3007	-	-	0/4/4/4	-
2	FES	A	3002	1	-	-	0/1/1/1
6	URC	A	3006	-	-	-	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	FAD	C9A-C5X	4.63	1.48	1.41
6	B	4006	URC	C5-C6	4.54	1.49	1.41
6	B	4006	URC	C5-C4	4.04	1.51	1.40
5	B	4004	FAD	C9A-C5X	4.00	1.47	1.41
6	A	3006	URC	C5-C6	3.99	1.48	1.41
5	B	4004	FAD	C5X-N5	-3.84	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4004	FAD	PA-O2A	-3.25	1.40	1.55
5	B	4004	FAD	C4-N3	-3.18	1.32	1.38
5	B	4004	FAD	P-O1P	-2.92	1.40	1.50
6	A	3006	URC	C2-N3	-2.92	1.32	1.38
6	A	3006	URC	C5-C4	2.90	1.48	1.40
5	B	4004	FAD	C2B-C1B	-2.87	1.49	1.53
5	B	4004	FAD	C1'-N10	-2.71	1.41	1.48
5	A	3005	FAD	C8-C7	2.62	1.47	1.40
5	A	3005	FAD	O2-C2	2.57	1.29	1.24
5	B	4004	FAD	PA-O1A	-2.56	1.41	1.50
5	B	4004	FAD	C2-N3	-2.55	1.33	1.39
5	A	3005	FAD	C2A-N3A	2.52	1.36	1.32
5	B	4004	FAD	C8-C7	2.52	1.47	1.40
5	B	4004	FAD	P-O2P	-2.49	1.43	1.55
5	A	3005	FAD	C4X-N5	2.43	1.35	1.30
5	B	4004	FAD	C5A-N7A	-2.43	1.30	1.39
5	A	3005	FAD	O4B-C1B	2.43	1.44	1.41
5	A	3005	FAD	C2B-C1B	-2.40	1.50	1.53
5	A	3005	FAD	C2'-C3'	-2.36	1.49	1.53
5	A	3005	FAD	C4-N3	-2.34	1.34	1.38
6	A	3006	URC	O13-C6	2.31	1.30	1.24
5	A	3005	FAD	C9-C8	2.30	1.42	1.39
5	A	3005	FAD	C2B-C3B	-2.29	1.47	1.53
5	B	4004	FAD	C2'-C3'	-2.24	1.49	1.53
5	A	3005	FAD	O2'-C2'	2.21	1.48	1.43
5	A	3005	FAD	C5X-N5	-2.19	1.35	1.39
5	B	4004	FAD	O4B-C4B	-2.11	1.40	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3006	URC	C2-N1-C6	10.27	123.81	115.14
6	A	3006	URC	C4-N9-C8	9.84	107.09	101.12
6	B	4006	URC	C2-N1-C6	9.72	123.34	115.14
6	B	4006	URC	C4-N9-C8	7.66	105.77	101.12
6	A	3006	URC	C5-C6-N1	-5.70	115.64	123.43
6	B	4006	URC	C4-C5-C6	-4.78	116.23	120.80
6	B	4006	URC	C5-C6-N1	-4.25	117.62	123.43
5	A	3005	FAD	O3'-C3'-C2'	-3.97	99.22	108.81
6	A	3006	URC	C4-C5-C6	-3.88	117.09	120.80
5	B	4004	FAD	O3'-C3'-C2'	-3.84	99.53	108.81
5	B	4004	FAD	C4-C4X-N5	3.44	123.13	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	4004	FAD	C9A-C5X-N5	-3.15	119.01	122.43
5	B	4004	FAD	C5X-N5-C4X	3.00	123.07	118.07
5	A	3005	FAD	C5'-C4'-C3'	-2.97	106.46	112.20
5	A	3005	FAD	O4-C4-C4X	-2.94	118.81	126.60
5	A	3005	FAD	O4'-C4'-C3'	2.93	116.22	109.10
5	A	3005	FAD	C9A-C5X-N5	-2.87	119.31	122.43
5	B	4004	FAD	O4-C4-C4X	-2.79	119.20	126.60
5	A	3005	FAD	C1B-N9A-C4A	-2.78	121.75	126.64
5	B	4004	FAD	C4A-C5A-N7A	-2.77	106.51	109.40
5	A	3005	FAD	C4-C4X-N5	2.70	122.07	118.23
5	B	4004	FAD	C10-N1-C2	2.63	122.16	116.90
5	A	3005	FAD	N6A-C6A-N1A	2.35	123.46	118.57
5	B	4004	FAD	N3A-C2A-N1A	-2.34	125.02	128.68
5	B	4004	FAD	O5B-C5B-C4B	2.22	116.62	108.99
5	A	3005	FAD	N3A-C2A-N1A	-2.21	125.22	128.68
5	B	4004	FAD	C4X-C10-N1	-2.18	119.66	124.73
5	A	3005	FAD	C4A-C5A-N7A	-2.16	107.15	109.40
5	A	3005	FAD	C2B-C3B-C4B	2.12	106.77	102.64
5	A	3005	FAD	O2'-C2'-C1'	2.10	114.89	109.80
5	B	4004	FAD	O2'-C2'-C1'	2.08	114.83	109.80
5	A	3005	FAD	O2-C2-N1	-2.06	118.41	121.83

There are no chirality outliers.

There are no torsion outliers.

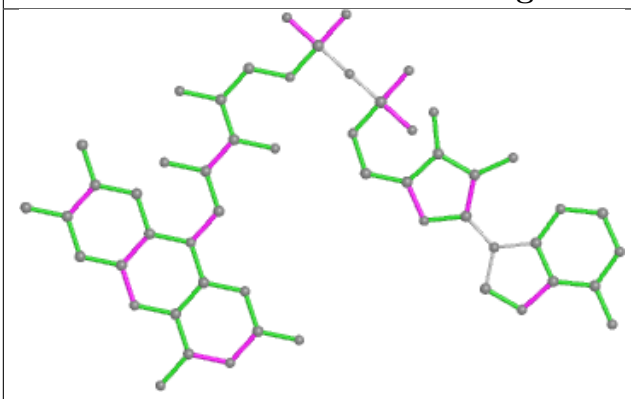
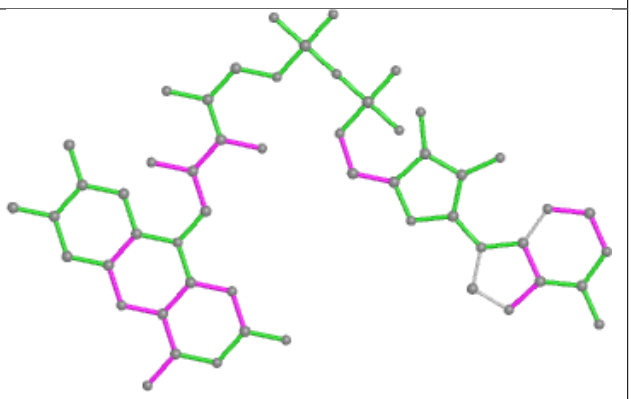
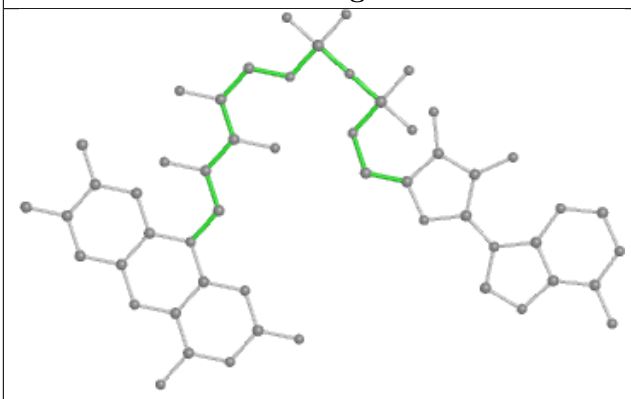
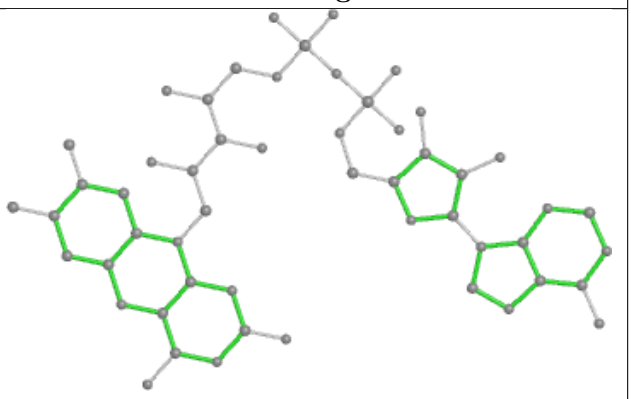
There are no ring outliers.

2 monomers are involved in 3 short contacts:

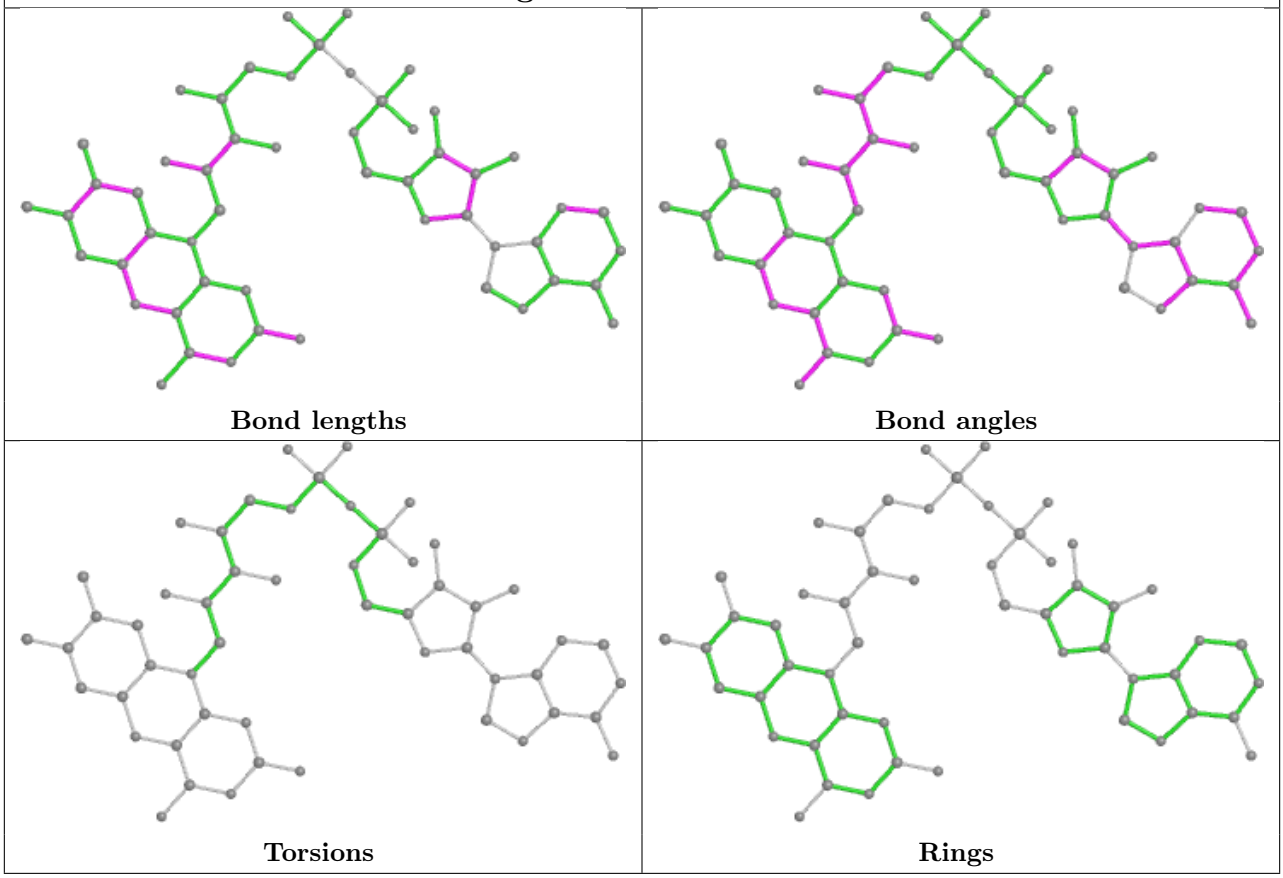
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	4004	FAD	2	0
5	A	3005	FAD	1	0

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 B 4004	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand FAD A 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	1289/1315 (98%)	0.29	53 (4%)	37	36	17, 30, 51, 86	0
1	B	1286/1315 (97%)	0.06	32 (2%)	57	56	15, 24, 46, 85	0
All	All	2575/2630 (97%)	0.17	85 (3%)	46	45	15, 27, 49, 86	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	SER	6.4
1	A	1287	ASP	6.2
1	A	3	ALA	5.9
1	B	1289	ALA	5.7
1	A	1315	LEU	5.5
1	B	1286	GLY	5.2
1	B	423	ALA	5.2
1	A	165	ASP	5.0
1	B	1287	ASP	4.5
1	A	1111	GLY	4.3
1	A	550	GLN	4.1
1	A	290	VAL	4.0
1	B	1314	THR	3.8
1	B	1106	LYS	3.8
1	A	396	LEU	3.7
1	B	551	LYS	3.7
1	A	473	LEU	3.6
1	B	555	ALA	3.6
1	B	553	PRO	3.6
1	B	1288	ASN	3.4
1	B	1111	GLY	3.2
1	A	1288	ASN	3.2
1	B	530	ASP	3.1
1	B	549	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	190	LEU	3.1
1	A	377	GLY	3.1
1	B	428	ASP	3.0
1	B	552	ASP	3.0
1	A	1110	THR	2.9
1	B	218	LEU	2.9
1	B	550	GLN	2.9
1	A	687	ILE	2.9
1	A	474	SER	2.8
1	A	222	PRO	2.8
1	A	61	LEU	2.7
1	A	693	PRO	2.7
1	B	1108	LYS	2.7
1	A	448	VAL	2.7
1	B	566	ASP	2.7
1	A	566	ASP	2.6
1	B	565	LYS	2.6
1	A	800	GLY	2.6
1	B	532	GLU	2.6
1	A	191	SER	2.6
1	A	335	TRP	2.6
1	A	321	GLN	2.6
1	B	1110	THR	2.6
1	A	551	LYS	2.5
1	A	220	ASP	2.5
1	A	553	PRO	2.5
1	A	798	PHE	2.5
1	B	220	ASP	2.4
1	B	221	THR	2.4
1	A	470	PRO	2.4
1	B	529	ALA	2.4
1	A	742	PHE	2.4
1	A	686	LYS	2.4
1	B	1107	LYS	2.4
1	B	1109	PRO	2.4
1	A	247	LEU	2.3
1	A	221	THR	2.3
1	B	1105	LYS	2.3
1	A	466	LEU	2.3
1	A	1289	ALA	2.3
1	A	565	LYS	2.3
1	A	724	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1314	THR	2.3
1	A	317	LYS	2.3
1	A	443	PRO	2.2
1	A	1264	LEU	2.2
1	A	444	GLY	2.2
1	A	723	PHE	2.2
1	A	224	LYS	2.2
1	A	413	GLU	2.1
1	B	548	LEU	2.1
1	B	1116	TRP	2.1
1	A	692	LEU	2.1
1	A	795	GLY	2.1
1	B	1102	GLU	2.1
1	A	293	PRO	2.1
1	A	720	LYS	2.1
1	A	1036	THR	2.0
1	A	1229	ILE	2.0
1	A	533	ASP	2.0
1	A	291	HIS	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 monosaccharides 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
7	GOL	A	3007	6/6	0.94	0.16	25,27,28,29	0
7	GOL	B	4008	6/6	0.94	0.11	23,27,28,28	0
7	GOL	B	4007	6/6	0.95	0.10	26,30,31,31	0
6	URC	A	3006	12/12	0.96	0.11	24,27,31,31	0

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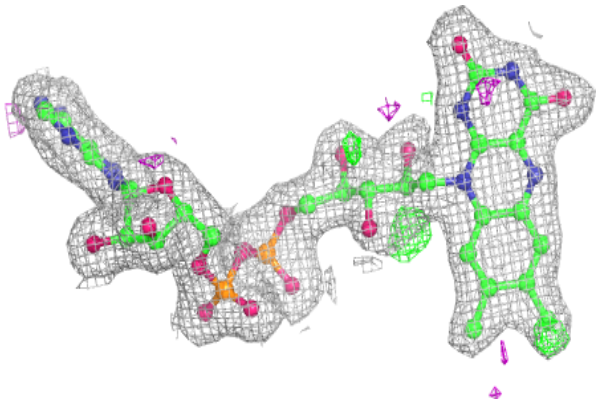
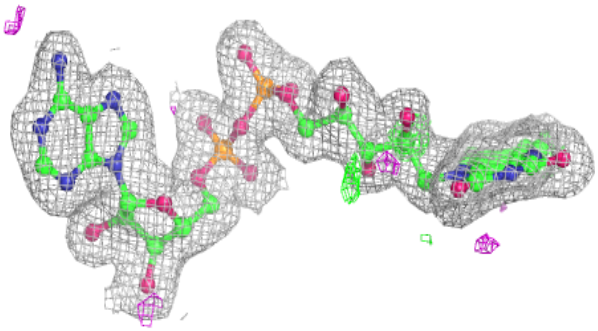
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FAD	B	4004	53/53	0.97	0.10	16,21,25,27	0
5	FAD	A	3005	53/53	0.97	0.10	23,30,34,36	0
6	URC	B	4006	12/12	0.97	0.10	22,24,28,29	0
2	FES	A	3001	4/4	0.99	0.05	23,23,25,29	0
2	FES	A	3002	4/4	0.99	0.08	19,21,24,25	0
2	FES	B	4001	4/4	0.99	0.04	20,22,25,25	0
2	FES	B	4002	4/4	0.99	0.08	15,15,18,18	0
3	BCT	A	3003	4/4	0.99	0.12	26,28,28,29	0
3	BCT	B	4005	4/4	0.99	0.14	19,20,21,23	0
4	CA	A	3004	1/1	0.99	0.05	34,34,34,34	0
4	CA	B	4003	1/1	1.00	0.04	24,24,24,24	0

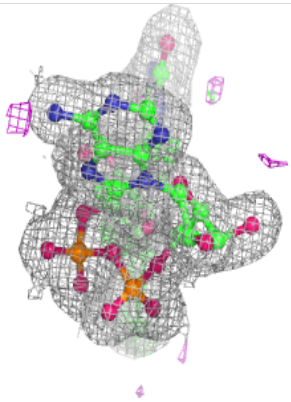
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

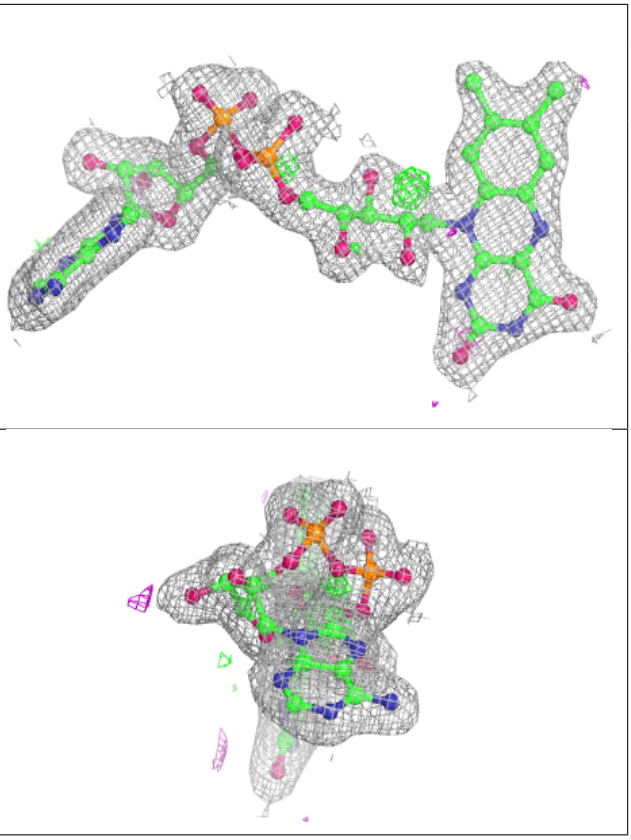






Electron density around FAD A 3005:

$2mF_o$-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.