Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 05:01 AM EDT

PDB ID	:	3BDJ / pdb_00003bdj
Title	:	Crystal Structure of Bovine Milk Xanthine Dehydrogenase with a Covalently Bound Oxipurinol Inhibitor
Authors	:	Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.; Nishino, T.
Deposited on	:	2007-11-14
Resolution	:	2.00 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:

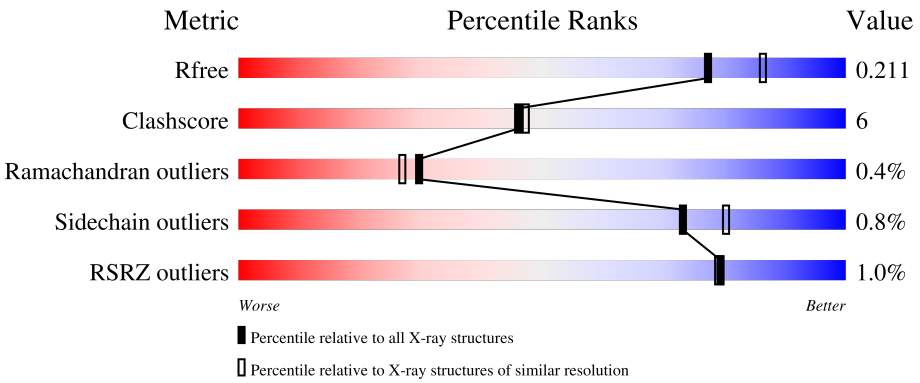
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	1332	% 82% 13% • •
1	B	1332	% 81% 15% • •

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
3	FES	B	4002	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21626 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	1286	9991	6354	1712	1865	60	0	0	0
1	B	1286	9991	6354	1712	1865	60	0	0	0

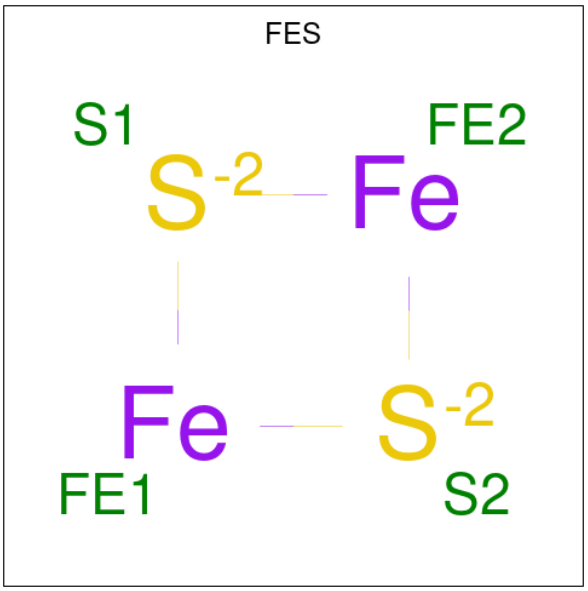
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	HIS	ASP	SEE REMARK 999	UNP P80457
B	552	HIS	ASP	SEE REMARK 999	UNP P80457

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

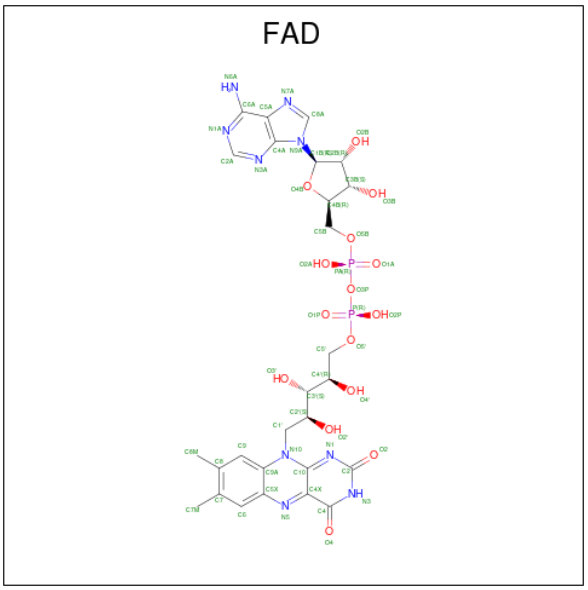
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



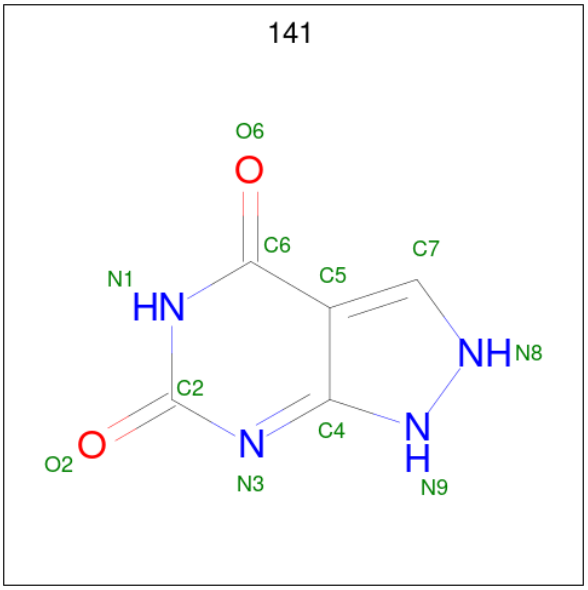
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0
			Total	Fe	S		
3	A	1	4	2	2	0	0
			Total	Fe	S		
3	B	1	4	2	2	0	0
			Total	Fe	S		
3	B	1	4	2	2	0	0

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



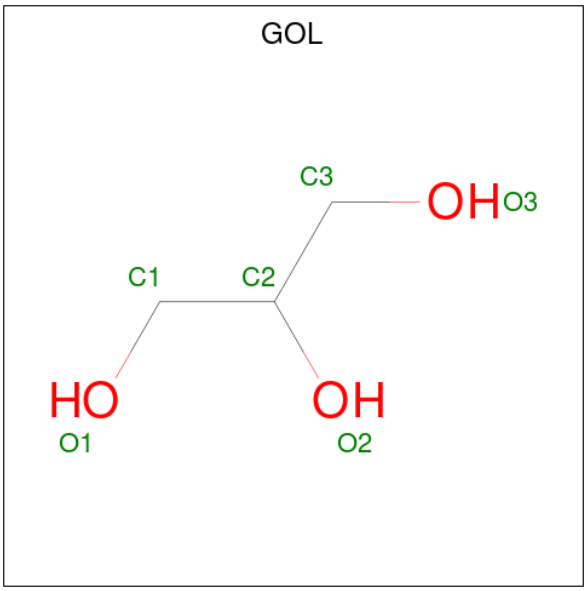
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is Oxypurinol (CCD ID: 141) (formula: $C_5H_4N_4O_2$).



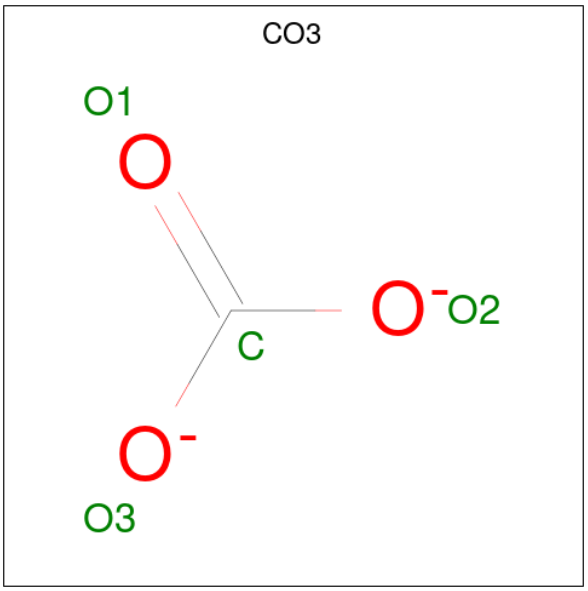
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	5	4	2		
5	B	1	Total	C	N	O	0	0
			11	5	4	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



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

- Molecule 8 is Molybdopterin oxo thio molybdenum (CCD ID: HOH) (formula: H_2O).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Mo	N	O	P	S		
8	A	1	27	10	1	5	7	1	3	0	0
8	B	1	27	10	1	5	7	1	3	0	0

- Molecule 9 is water.

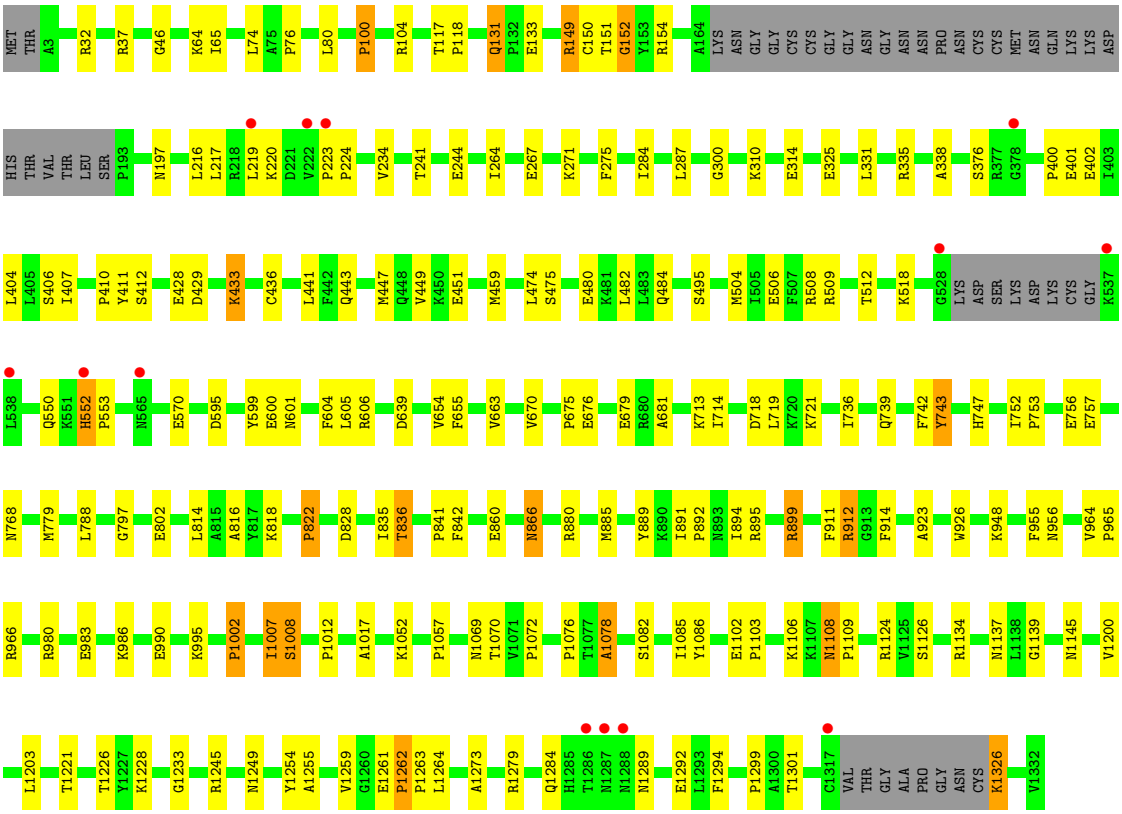
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	706	706	706	0	0
9	B	688	688	688	0	0

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.

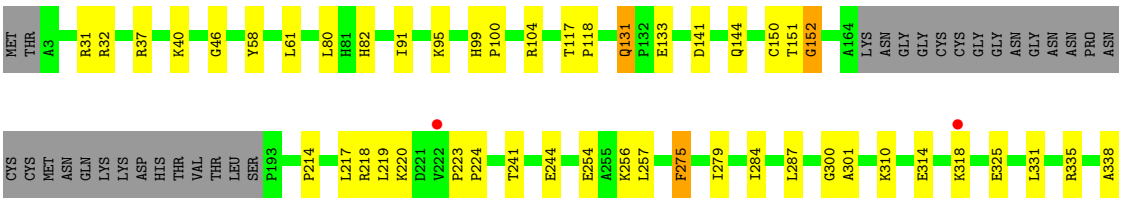
• Molecule 1: Xanthine dehydrogenase/oxidase

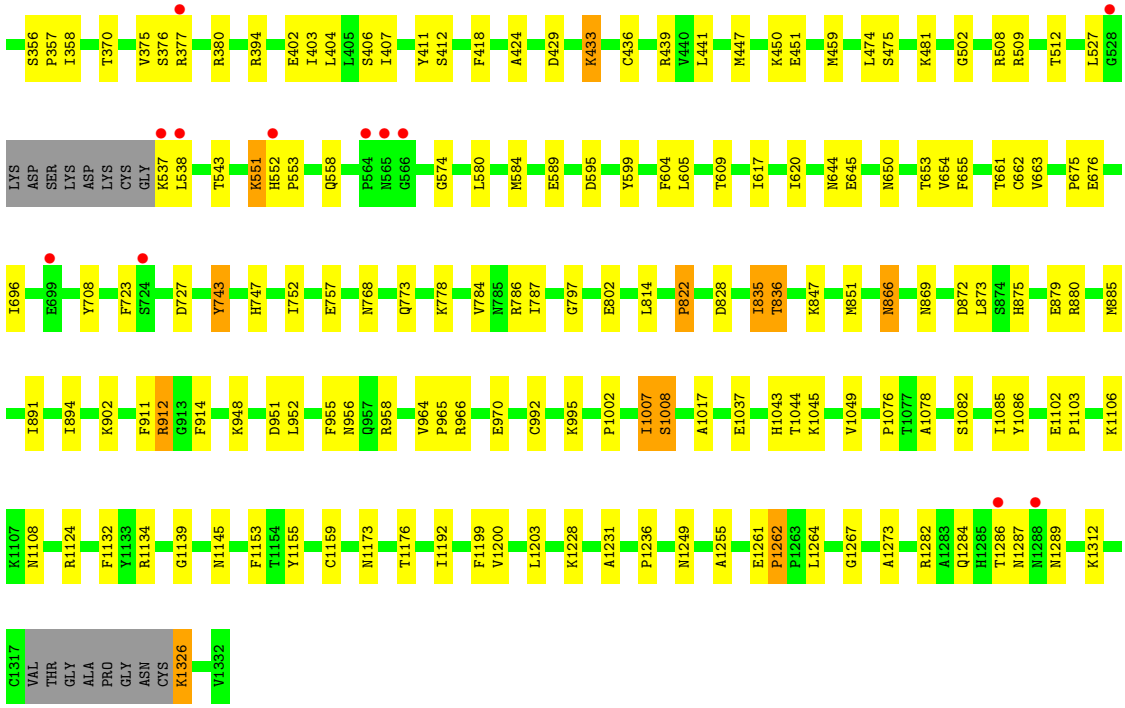
Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:




S356 P357 I358 T370 V375 S376 R377 R380 R394 E402 I403 L404 L405 S406 I407 Y411 S412 F418 A424 D429 K433 C436 R439 V440 L441 M447 K450 E451 M459 L474 S475 K481 G502 R508 R509 T512 L527 G528
LYS ASP SER LYS ASP LYS CYS GLY K537 L538 T543 K551 H552 P553 Q558 P564 N565 G566 G574 L580 M584 E589 D595 Y599 F604 L605 T609 I617 I620 N644 E645 N650 T653 V654 F655 T661 C662 V663 P675 E676
I696 E699 Y708 F723 S724 D727 Y743 H747 I752 E757 N768 Q773 K778 V784 N785 R786 I787 G797 E802 L814 P822 D828 I835 T836 K847 M851 N866 N869 D872 L873 S874 H875 E879 R880 M885
I891 I894 K902 F911 R912 G913 F914 K948 D951 L952 F955 N956 Q957 R958 V964 P965 R966 E970 C992 K995 P1002 I1007 S1008 A1017 E1037 H1043 T1044 K1045 V1049 P1076 T1077 A1078 S1082 I1085 Y1086 E1102 P1103 K1106
K1107 N1108 R1124 F1132 Y1133 R1134 G1139 N1145 F1153 T1154 Y1155 C1159 N1173 T1176 I1192 F1199 V1200 L1203 K1228 A1231 P1236 N1249 A1255 E1261 P1262 P1263 L1264 G1267 A1273 R1282 A1283 Q1284 H1285 T1286 N1287 N1288 N1289 K1312
C1317 VAL THR GLY ALA PRO GLY ASN CYS K1326 V1332

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.52Å 124.07Å 148.80Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	19.96 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (19.96-2.00) 89.5 (19.96-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.191 , 0.224 0.180 , 0.211	Depositor DCC
R_{free} test set	2424 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21626	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 3.11% 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: GOL, EAK, FES, 141, CO3, FAD, 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	0.37	0/10210	0.91	39/13818 (0.3%)
1	B	0.36	0/10210	0.92	37/13818 (0.3%)
All	All	0.37	0/20420	0.92	76/27636 (0.3%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	835	ILE	N-CA-C	12.36	122.94	111.45
1	A	835	ILE	N-CA-C	11.78	122.40	111.45
1	A	151	THR	N-CA-C	10.16	123.61	111.82
1	B	151	THR	N-CA-C	9.65	124.39	112.23
1	B	836	THR	N-CA-C	8.65	123.49	113.19
1	B	433	LYS	N-CA-C	-8.47	99.85	112.04
1	B	1262	PRO	N-CA-C	7.72	120.12	110.70
1	A	836	THR	N-CA-C	7.65	122.29	113.19
1	B	1085	ILE	N-CA-C	7.48	118.08	110.82
1	A	956	ASN	N-CA-C	7.47	121.70	111.54
1	A	433	LYS	N-CA-C	-7.31	101.51	112.04
1	A	1262	PRO	N-CA-C	7.22	119.50	110.70
1	B	828	ASP	N-CA-C	-7.11	101.15	110.53
1	A	743	TYR	N-CA-C	-7.10	99.78	110.28
1	A	654	VAL	N-CA-C	-7.06	103.30	111.00
1	B	654	VAL	N-CA-C	-6.89	103.49	111.00
1	B	956	ASN	N-CA-C	6.85	121.00	112.24
1	B	743	TYR	N-CA-C	-6.78	100.25	110.28
1	A	1273	ALA	N-CA-C	-6.76	103.99	111.36
1	A	411	TYR	N-CA-C	-6.70	100.56	110.48
1	B	131	GLN	CA-C-N	6.60	127.13	119.47
1	B	131	GLN	C-N-CA	6.60	127.13	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1108	ASN	CA-C-N	6.58	126.83	119.32
1	B	1108	ASN	C-N-CA	6.58	126.83	119.32
1	B	1273	ALA	N-CA-C	-6.53	104.24	111.36
1	A	828	ASP	N-CA-C	-6.51	101.76	110.55
1	B	436	CYS	N-CA-C	6.31	117.81	108.60
1	B	869	ASN	N-CA-C	6.14	120.28	113.21
1	A	152	GLY	N-CA-C	-6.14	106.77	115.43
1	A	663	VAL	N-CA-C	-6.09	101.68	109.30
1	A	197	ASN	CA-C-N	6.03	126.47	119.47
1	A	197	ASN	C-N-CA	6.03	126.47	119.47
1	B	152	GLY	N-CA-C	-5.93	107.05	115.30
1	B	663	VAL	N-CA-C	-5.93	101.89	109.30
1	B	696	ILE	N-CA-C	5.83	117.21	111.67
1	A	443	GLN	N-CA-C	-5.80	102.08	110.08
1	A	436	CYS	N-CA-C	5.79	117.58	108.96
1	A	1085	ILE	N-CA-C	5.71	117.23	111.00
1	A	1108	ASN	CA-C-N	5.71	126.09	119.47
1	A	1108	ASN	C-N-CA	5.71	126.09	119.47
1	B	891	ILE	CA-C-N	5.69	125.16	119.24
1	B	891	ILE	C-N-CA	5.69	125.16	119.24
1	A	822	PRO	N-CA-C	-5.68	102.36	111.38
1	A	447	MET	N-CA-C	-5.61	105.12	112.41
1	B	1007	ILE	N-CA-C	5.56	116.10	107.99
1	A	1137	ASN	N-CA-C	5.55	118.85	111.30
1	B	822	PRO	N-CA-C	-5.54	102.57	111.38
1	B	275	PHE	CA-C-N	5.40	125.05	119.05
1	B	275	PHE	C-N-CA	5.40	125.05	119.05
1	B	450	LYS	N-CA-C	-5.38	106.40	113.12
1	A	1070	THR	N-CA-C	-5.37	106.78	113.55
1	B	411	TYR	N-CA-C	-5.37	102.53	110.48
1	A	841	PRO	N-CA-C	-5.35	102.87	111.38
1	B	787	ILE	N-CA-C	5.34	115.64	108.17
1	B	80	LEU	N-CA-C	5.28	119.35	113.02
1	B	1228	LYS	N-CA-C	5.27	117.56	107.75
1	A	131	GLN	CA-C-N	5.26	125.58	119.47
1	A	131	GLN	C-N-CA	5.26	125.58	119.47
1	A	449	VAL	N-CA-C	5.24	116.45	109.37
1	B	31	ARG	N-CA-C	5.24	117.07	111.36
1	A	1007	ILE	N-CA-C	5.23	115.63	107.99
1	B	150	CYS	N-CA-C	5.23	119.57	112.04
1	A	80	LEU	N-CA-C	5.19	119.30	112.92
1	A	275	PHE	CA-C-N	5.16	124.96	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	275	PHE	C-N-CA	5.16	124.96	119.28
1	A	1228	LYS	N-CA-C	5.16	117.35	107.75
1	A	1078	ALA	N-CA-C	5.15	115.04	108.24
1	A	410	PRO	N-CA-C	5.13	119.54	111.38
1	B	543	THR	N-CA-C	5.13	117.27	111.11
1	B	300	GLY	N-CA-C	-5.10	106.07	111.93
1	A	234	VAL	N-CA-C	5.09	117.16	108.86
1	A	300	GLY	N-CA-C	-5.08	105.58	112.14
1	B	40	LYS	N-CA-C	5.07	117.59	110.14
1	B	104	ARG	N-CA-C	5.07	116.89	111.36
1	A	150	CYS	N-CA-C	5.04	119.29	112.04
1	A	889	TYR	N-CA-C	5.03	117.69	109.59

There are no chirality outliers.

There are no planarity outliers.

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	9991	0	9991	115	0
1	B	9991	0	9991	125	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	2	0
4	A	53	0	31	1	0
4	B	53	0	31	0	0
5	A	11	0	3	2	0
5	B	11	0	3	2	0
6	A	18	0	24	0	0
6	B	24	0	32	1	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	A	27	0	0	0	0
8	B	27	0	0	0	0
9	A	706	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	688	0	0	6	0
All	All	21626	0	20106	232	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 6.

All (232) 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:A:757:GLU:H	1:B:584:MET:HE1	1.28	0.98
1:B:551:LYS:H	1:B:551:LYS:HD2	1.33	0.92
1:B:1326:LYS:HZ2	1:B:1326:LYS:N	1.68	0.91
1:B:131:GLN:HE21	1:B:133:GLU:H	1.18	0.90
1:B:404:LEU:HD21	1:B:407:ILE:HD11	1.53	0.88
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.39	0.86
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.39	0.84
1:A:757:GLU:N	1:B:584:MET:HE1	1.95	0.80
1:A:756:GLU:HA	1:B:584:MET:HE1	1.66	0.77
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.85	0.76
1:A:131:GLN:HE21	1:A:133:GLU:H	1.31	0.76
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.51	0.75
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.18	0.74
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.71	0.71
1:B:314:GLU:O	1:B:318:LYS:HG2	1.92	0.70
1:B:1287:ASN:ND2	1:B:1289:ASN:HB3	2.06	0.70
1:B:406:SER:C	1:B:407:ILE:HD12	2.20	0.67
1:B:404:LEU:CD2	1:B:407:ILE:HD11	2.24	0.66
1:A:406:SER:C	1:A:407:ILE:HD12	2.22	0.65
1:A:757:GLU:H	1:B:584:MET:CE	2.07	0.65
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.77	0.65
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	1.98	0.64
9:A:5302:EAK:O1	9:A:5302:EAK:MO1	1.68	0.64
9:B:5303:EAK:O1	9:B:5303:EAK:MO1	1.67	0.64
1:B:1078:ALA:HB1	5:B:5102:141:C7	2.30	0.62
1:B:885:MET:HE2	1:B:894:ILE:HD11	1.81	0.62
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.01	0.61
1:A:217:LEU:O	1:A:220:LYS:HG2	2.00	0.60
1:A:639:ASP:HB3	1:A:818:LYS:HD2	1.84	0.60
1:B:474:LEU:O	1:B:475:SER:HB2	2.01	0.60
1:B:37:ARG:HD3	1:B:595:ASP:O	2.01	0.60
1:B:551:LYS:H	1:B:551:LYS:CD	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.83	0.59
1:A:1078:ALA:HB1	5:A:5101:141:C7	2.32	0.59
1:B:375:VAL:HG12	1:B:380:ARG:HG3	1.85	0.59
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.68	0.58
1:B:459:MET:HE2	1:B:512:THR:HG21	1.85	0.58
1:B:131:GLN:NE2	1:B:133:GLU:H	1.96	0.58
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.10	0.58
1:A:756:GLU:CA	1:B:584:MET:HE1	2.34	0.58
1:B:552:HIS:CG	1:B:553:PRO:HD2	2.39	0.58
1:A:1221:THR:HG22	1:A:1226:THR:HB	1.86	0.57
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.85	0.57
1:A:37:ARG:HD3	1:A:595:ASP:O	2.04	0.57
1:A:756:GLU:HA	1:B:584:MET:CE	2.36	0.56
1:A:64:LYS:HG2	1:A:65:ILE:N	2.20	0.56
1:A:216:LEU:HD23	1:A:219:LEU:HD12	1.87	0.56
1:A:911:PHE:O	1:A:912:ARG:C	2.50	0.55
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.42	0.55
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.88	0.55
1:B:310:LYS:O	1:B:314:GLU:HG3	2.07	0.55
1:B:46:GLY:HA2	3:B:4002:FES:S1	2.47	0.54
1:A:428:GLU:OE2	1:A:1233:GLY:HA3	2.07	0.54
1:B:241:THR:OG1	1:B:244:GLU:HG3	2.06	0.54
1:B:131:GLN:HE21	1:B:133:GLU:N	1.96	0.54
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.08	0.54
1:B:1287:ASN:HD22	1:B:1289:ASN:HB3	1.72	0.53
1:A:459:MET:HE2	1:A:512:THR:HG21	1.90	0.53
1:A:433:LYS:HE2	1:A:504:MET:SD	2.48	0.53
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.74	0.52
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.90	0.52
1:A:100:PRO:O	1:A:104:ARG:HG3	2.10	0.52
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.52
1:A:264:ILE:HD11	4:A:3005:FAD:H3B	1.91	0.52
1:A:1326:LYS:N	1:A:1326:LYS:HD2	2.25	0.52
1:B:256:LYS:HE3	1:B:275:PHE:CE2	2.45	0.51
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.92	0.51
1:A:1082:SER:HB2	9:A:5302:EAK:O3P	2.10	0.51
1:B:605:LEU:C	1:B:605:LEU:HD23	2.36	0.51
1:A:948:LYS:NZ	1:A:948:LYS:HB2	2.25	0.51
1:B:727:ASP:HB2	1:B:851:MET:HA	1.92	0.51
1:B:377:ARG:HB3	1:B:377:ARG:NH1	2.25	0.51
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:HD13	1:A:860:GLU:HG2	1.92	0.51
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.75	0.50
1:A:713:LYS:HG2	1:A:714:ILE:N	2.26	0.50
1:B:370:THR:CG2	1:B:407:ILE:HG23	2.41	0.50
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.46	0.50
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.11	0.50
1:A:474:LEU:O	1:A:475:SER:HB2	2.11	0.50
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.47	0.50
1:B:217:LEU:O	1:B:220:LYS:HG2	2.12	0.50
1:B:376:SER:HB3	1:B:402:GLU:HG2	1.93	0.50
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.77	0.49
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.42	0.49
1:A:508:ARG:O	1:A:512:THR:HG23	2.11	0.49
1:B:551:LYS:HD2	1:B:551:LYS:N	2.14	0.49
1:B:257:LEU:HA	1:B:279:ILE:O	2.13	0.49
1:B:82:HIS:NE2	1:B:219:LEU:HD13	2.28	0.49
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.13	0.49
1:A:605:LEU:HD23	1:A:605:LEU:C	2.38	0.48
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.48	0.48
1:A:966:ARG:HG3	9:A:5839:HOH:O	2.13	0.48
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	1.94	0.48
1:B:1264:LEU:C	1:B:1264:LEU:HD23	2.37	0.48
1:B:644:ASN:O	1:B:653:THR:HA	2.13	0.48
1:A:284:ILE:CG2	1:A:287:LEU:HD23	2.43	0.48
1:B:1326:LYS:N	1:B:1326:LYS:NZ	2.51	0.48
1:A:752:ILE:HD13	1:A:822:PRO:HB3	1.95	0.48
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.49	0.48
1:B:1282:ARG:O	1:B:1286:THR:HB	2.14	0.48
1:A:407:ILE:HD12	1:A:407:ILE:N	2.28	0.48
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.96	0.48
1:A:599:TYR:HA	1:B:599:TYR:HA	1.96	0.48
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.49	0.48
1:B:537:LYS:O	1:B:537:LYS:HG2	2.15	0.47
1:A:149:ARG:HG3	1:A:742:PHE:O	2.13	0.47
1:A:400:PRO:HG2	1:A:401:GLU:OE1	2.15	0.47
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	1.97	0.47
1:A:154:ARG:C	1:A:154:ARG:HD2	2.40	0.47
1:B:1007:ILE:O	1:B:1008:SER:CB	2.61	0.47
1:B:1102:GLU:OE2	1:B:1106:LYS:HE3	2.14	0.47
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.97	0.47
1:A:495:SER:HA	1:A:509:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:ASN:N	1:A:1109:PRO:HD3	2.30	0.46
1:A:506:GLU:CD	1:A:506:GLU:H	2.23	0.46
1:A:46:GLY:HA2	3:A:3002:FES:S1	2.56	0.46
1:A:866:ASN:C	1:A:866:ASN:HD22	2.23	0.46
1:A:310:LYS:O	1:A:314:GLU:HG3	2.16	0.46
1:A:899:ARG:HA	1:A:899:ARG:HD2	1.78	0.46
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	1.97	0.46
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.50	0.46
1:A:1245:ARG:HG2	9:A:5542:HOH:O	2.16	0.46
1:B:424:ALA:HA	1:B:433:LYS:HG2	1.97	0.46
1:B:574:GLY:CA	6:B:5003:GOL:H12	2.46	0.46
1:A:1102:GLU:OE2	1:A:1106:LYS:HE3	2.16	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.79	0.45
1:B:61:LEU:HD12	1:B:61:LEU:N	2.31	0.45
1:A:325:GLU:HB2	1:A:412:SER:CB	2.46	0.45
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.17	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.80	0.45
1:A:284:ILE:HG21	1:A:287:LEU:HD23	1.98	0.45
1:A:518:LYS:HE3	9:A:5595:HOH:O	2.15	0.45
1:A:718:ASP:HB3	1:A:721:LYS:HE3	1.98	0.45
1:A:1052:LYS:HD3	1:A:1254:TYR:CE1	2.51	0.45
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.51	0.45
1:B:287:LEU:HD12	1:B:301:ALA:HB3	1.98	0.45
1:B:992:CYS:HA	1:B:1284:GLN:NE2	2.32	0.45
1:B:394:ARG:HD2	9:B:5750:HOH:O	2.16	0.45
1:B:768:ASN:ND2	1:B:1076:PRO:HB3	2.32	0.45
1:A:325:GLU:HB2	1:A:412:SER:HB3	1.99	0.45
1:A:1007:ILE:O	1:A:1008:SER:CB	2.64	0.45
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.52	0.44
1:A:482:LEU:C	1:A:482:LEU:HD23	2.43	0.44
1:B:1312:LYS:HG2	9:B:5915:HOH:O	2.18	0.44
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.42	0.44
1:B:325:GLU:HB2	1:B:412:SER:HB3	1.99	0.44
1:A:441:LEU:HD23	1:A:451:GLU:HG3	1.98	0.44
1:A:980:ARG:HA	1:A:983:GLU:OE1	2.18	0.44
1:B:802:GLU:OE2	5:B:5102:141:H1	2.18	0.44
1:B:46:GLY:CA	3:B:4002:FES:S1	3.06	0.44
1:B:95:LYS:HG3	1:B:589:GLU:OE2	2.17	0.44
1:B:708:TYR:CE2	1:B:902:LYS:HD3	2.53	0.44
1:B:966:ARG:O	1:B:970:GLU:HG3	2.18	0.44
1:B:331:LEU:O	1:B:335:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:C	1:B:358:ILE:HD12	2.43	0.43
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.53	0.43
1:A:1264:LEU:C	1:A:1264:LEU:HD23	2.43	0.43
1:B:661:THR:O	1:B:662:CYS:HB3	2.18	0.43
1:B:1082:SER:HB2	9:B:5303:EAK:O3P	2.18	0.43
1:B:403:ILE:C	1:B:403:ILE:HD12	2.44	0.43
1:A:1134:ARG:CD	1:B:1124:ARG:HB2	2.49	0.43
1:B:508:ARG:O	1:B:512:THR:HG23	2.18	0.43
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.93	0.43
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.18	0.43
1:A:376:SER:HB3	1:A:402:GLU:HG2	2.01	0.43
1:A:986:LYS:O	1:A:990:GLU:HG3	2.19	0.43
1:A:964:VAL:HB	1:A:965:PRO:HD3	2.00	0.42
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.44	0.42
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.54	0.42
1:A:1203:LEU:HD23	1:A:1203:LEU:C	2.45	0.42
1:B:433:LYS:HA	1:B:433:LYS:HE2	2.00	0.42
1:B:872:ASP:CG	1:B:873:LEU:H	2.26	0.42
1:A:480:GLU:HG3	1:A:484:GLN:HE21	1.84	0.42
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.55	0.42
1:B:141:ASP:O	1:B:144:GLN:HG3	2.20	0.42
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.54	0.42
1:A:117:THR:HB	1:A:118:PRO:HD3	2.01	0.42
1:B:875:HIS:O	1:B:879:GLU:HG3	2.20	0.42
1:B:1159:CYS:O	1:B:1176:THR:HA	2.19	0.42
1:A:1289:ASN:ND2	1:A:1292:GLU:HB2	2.34	0.42
1:B:214:PRO:O	1:B:218:ARG:HG3	2.20	0.42
1:B:609:THR:HG21	1:B:835:ILE:HD11	2.00	0.42
1:B:773:GLN:HG2	1:B:784:VAL:HG13	2.02	0.42
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.55	0.42
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.20	0.42
1:B:447:MET:HG2	1:B:527:LEU:HD13	2.02	0.42
1:A:676:GLU:CD	1:A:676:GLU:H	2.28	0.42
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	2.02	0.42
1:B:866:ASN:C	1:B:866:ASN:HD22	2.28	0.42
1:A:1124:ARG:CB	1:B:1134:ARG:HD3	2.50	0.41
1:B:58:TYR:CZ	1:B:220:LYS:HD2	2.55	0.41
1:B:418:PHE:CD1	1:B:439:ARG:HB2	2.55	0.41
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.93	0.41
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.50	0.41
1:A:802:GLU:OE2	5:A:5101:141:H1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.86	0.41
1:B:1231:ALA:HB1	9:B:5694:HOH:O	2.20	0.41
1:A:779:MET:SD	1:A:779:MET:C	3.04	0.41
1:A:788:LEU:HD13	1:A:1069:ASN:HB3	2.03	0.41
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.18	0.41
1:B:580:LEU:HG	1:B:1044:THR:HG23	2.01	0.41
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.18	0.41
1:B:1287:ASN:HD22	1:B:1289:ASN:H	1.67	0.41
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	2.02	0.41
1:B:502:GLY:HA3	9:B:5831:HOH:O	2.20	0.41
1:B:723:PHE:CE2	1:B:847:LYS:HG2	2.55	0.41
1:A:267:GLU:HA	1:A:271:LYS:HG2	2.02	0.41
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.50	0.41
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.21	0.41
1:A:32:ARG:NH1	1:A:676:GLU:OE2	2.42	0.41
1:A:331:LEU:O	1:A:335:ARG:HG3	2.21	0.41
1:A:1012:PRO:HB2	9:A:5821:HOH:O	2.21	0.41
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.03	0.41
1:B:952:LEU:HD23	1:B:958:ARG:HA	2.02	0.41
1:A:600:GLU:HG3	1:A:601:ASN:N	2.36	0.41
1:A:606:ARG:CZ	1:A:679:GLU:HG3	2.51	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD2	1.92	0.41
1:B:117:THR:HB	1:B:118:PRO:HD3	2.03	0.41
1:B:254:GLU:OE2	1:B:254:GLU:N	2.36	0.41
1:B:617:ILE:CG2	1:B:620:ILE:HD11	2.51	0.41
1:B:91:ILE:O	1:B:99:HIS:HB2	2.21	0.40
1:B:1045:LYS:O	1:B:1049:VAL:HG23	2.21	0.40
1:A:768:ASN:ND2	1:A:1076:PRO:HB3	2.36	0.40
1:A:74:LEU:O	1:A:76:PRO:HD3	2.22	0.40
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.37	0.40
1:B:284:ILE:CG2	1:B:287:LEU:HD23	2.52	0.40
1:B:325:GLU:HB2	1:B:412:SER:CB	2.52	0.40
1:B:356:SER:HA	1:B:357:PRO:HD3	1.95	0.40
1:A:433:LYS:HD3	1:A:433:LYS:HA	1.91	0.40
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.40
1:A:1262:PRO:HB2	1:A:1263:PRO:HD3	2.02	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	1278/1332 (96%)	1238 (97%)	35 (3%)	5 (0%)	30	27
1	B	1278/1332 (96%)	1232 (96%)	41 (3%)	5 (0%)	30	27
All	All	2556/2664 (96%)	2470 (97%)	76 (3%)	10 (0%)	30	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	1139	GLY
1	A	1139	GLY
1	B	912	ARG
1	A	797	GLY
1	B	797	GLY
1	B	538	LEU
1	A	1002	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1091/1128 (97%)	1081 (99%)	10 (1%)	70	78
1	B	1091/1128 (97%)	1084 (99%)	7 (1%)	78	85
All	All	2182/2256 (97%)	2165 (99%)	17 (1%)	73	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	A	149	ARG
1	A	550	GLN
1	A	552	HIS
1	A	743	TYR
1	A	866	ASN
1	A	899	ARG
1	A	1002	PRO
1	A	1072	PRO
1	A	1326	LYS
1	B	100	PRO
1	B	481	LYS
1	B	551	LYS
1	B	743	TYR
1	B	866	ASN
1	B	1002	PRO
1	B	1326	LYS

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

Mol	Chain	Res	Type
1	A	131	GLN
1	A	226	GLN
1	A	252	HIS
1	A	272	ASN
1	A	484	GLN
1	A	556	ASN
1	A	626	GLN
1	A	683	HIS
1	A	705	ASN
1	A	866	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1284	GLN
1	B	71	ASN
1	B	130	ASN
1	B	131	GLN
1	B	226	GLN
1	B	261	ASN
1	B	351	ASN
1	B	471	GLN

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Mol	Chain	Res	Type
1	B	473	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	866	ASN
1	B	869	ASN
1	B	875	HIS
1	B	1088	GLN
1	B	1122	GLN
1	B	1145	ASN
1	B	1220	HIS
1	B	1284	GLN
1	B	1289	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
6	GOL	B	5004	-	5,5,5	0.66	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	B	5002	-	5,5,5	0.63	0	5,5,5	0.50	0
3	FES	B	4002	1	0,4,4	-	-	-		
3	FES	A	3001	1	0,4,4	-	-	-		
9	EAK	B	5303	5	22,30,30	3.48	8 (36%)	22,48,48	2.96	10 (45%)
3	FES	B	4001	1	0,4,4	-	-	-		
5	141	B	5102	9	11,12,12	1.81	3 (27%)	11,17,17	1.77	2 (18%)
6	GOL	A	5006	-	5,5,5	0.65	0	5,5,5	0.38	0
6	GOL	B	5001	-	5,5,5	0.65	0	5,5,5	0.36	0
6	GOL	B	5003	-	5,5,5	0.62	0	5,5,5	0.41	0
4	FAD	B	4005	-	58,58,58	2.36	20 (34%)	85,89,89	2.05	21 (24%)
3	FES	A	3002	1	0,4,4	-	-	-		
4	FAD	A	3005	-	58,58,58	2.35	19 (32%)	85,89,89	2.05	20 (23%)
5	141	A	5101	9	11,12,12	1.82	3 (27%)	11,17,17	1.79	3 (27%)
6	GOL	A	5007	-	5,5,5	0.69	0	5,5,5	0.31	0
7	CO3	B	5202	-	3,3,3	0.25	0	2,3,3	0.10	0
6	GOL	A	5005	-	5,5,5	0.68	0	5,5,5	0.48	0
7	CO3	A	5201	-	3,3,3	0.27	0	2,3,3	0.11	0
9	EAK	A	5302	5	22,30,30	3.46	8 (36%)	22,48,48	3.00	9 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	5007	-	-	0/4/4/4	-
3	FES	B	4002	1	-	-	0/1/1/1
6	GOL	B	5001	-	-	0/4/4/4	-
6	GOL	B	5003	-	-	2/4/4/4	-
6	GOL	B	5004	-	-	1/4/4/4	-
5	141	A	5101	9	-	-	0/2/2/2
9	EAK	B	5303	5	-	1/6/44/44	0/4/4/4
3	FES	A	3001	1	-	-	0/1/1/1
3	FES	B	4001	1	-	-	0/1/1/1
4	FAD	B	4005	-	-	6/34/50/50	0/6/6/6
5	141	B	5102	9	-	-	0/2/2/2
6	GOL	A	5005	-	-	4/4/4/4	-
6	GOL	A	5006	-	-	0/4/4/4	-
3	FES	A	3002	1	-	-	0/1/1/1
4	FAD	A	3005	-	-	6/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EAK	A	5302	5	-	1/6/44/44	0/4/4/4
6	GOL	B	5002	-	-	4/4/4/4	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	5303	EAK	C10-N8	11.21	1.47	1.35
9	A	5302	EAK	C10-N8	10.85	1.46	1.35
9	A	5302	EAK	O4-C4	6.14	1.35	1.23
4	B	4005	FAD	C9A-C5X	6.05	1.50	1.41
4	A	3005	FAD	C9A-N10	5.97	1.51	1.41
4	B	4005	FAD	C9A-N10	5.79	1.51	1.41
4	A	3005	FAD	C9A-C5X	5.60	1.50	1.41
9	B	5303	EAK	O4-C4	5.59	1.34	1.23
9	A	5302	EAK	C9-C10	5.52	1.48	1.38
9	B	5303	EAK	C9-C10	5.24	1.47	1.38
4	A	3005	FAD	C9-C9A	5.22	1.48	1.39
9	A	5302	EAK	C9-N5	5.02	1.49	1.37
9	B	5303	EAK	C9-N5	4.85	1.49	1.37
4	B	4005	FAD	C9-C9A	4.80	1.47	1.39
4	A	3005	FAD	C2A-N1A	4.40	1.41	1.33
4	B	4005	FAD	C4A-N3A	4.37	1.42	1.34
4	A	3005	FAD	C4A-N3A	4.33	1.42	1.34
4	B	4005	FAD	C6-C5X	4.31	1.46	1.40
4	A	3005	FAD	C5A-C4A	4.30	1.46	1.39
4	A	3005	FAD	C6-C5X	4.26	1.46	1.40
4	B	4005	FAD	C5A-C4A	4.26	1.46	1.39
4	B	4005	FAD	O4B-C1B	4.23	1.51	1.42
4	A	3005	FAD	O4B-C1B	4.16	1.51	1.42
9	B	5303	EAK	O3'-C3'	4.13	1.51	1.43
4	B	4005	FAD	C8-C7	4.11	1.50	1.40
4	B	4005	FAD	C2A-N1A	4.08	1.41	1.33
4	A	3005	FAD	C8-C7	3.99	1.50	1.40
5	A	5101	141	C5-C4	-3.81	1.38	1.45
9	A	5302	EAK	O3'-C3'	3.81	1.50	1.43
4	A	3005	FAD	O4B-C4B	3.79	1.53	1.45
4	B	4005	FAD	O4B-C4B	3.74	1.53	1.45
5	B	5102	141	C5-C4	-3.74	1.38	1.45
9	B	5303	EAK	O3'-C7	3.71	1.49	1.43
9	A	5302	EAK	O3'-C7	3.67	1.49	1.43
4	A	3005	FAD	C10-N1	3.58	1.40	1.33
4	B	4005	FAD	C4X-N5	3.54	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4005	FAD	C5A-C6A	3.44	1.50	1.41
4	A	3005	FAD	C5A-C6A	3.39	1.50	1.41
4	A	3005	FAD	C2A-N3A	3.26	1.39	1.33
4	A	3005	FAD	C4X-N5	3.26	1.37	1.30
4	B	4005	FAD	C2-N3	3.24	1.46	1.39
4	B	4005	FAD	C2A-N3A	3.16	1.39	1.33
4	B	4005	FAD	C10-N1	3.14	1.39	1.33
4	A	3005	FAD	C2-N3	3.14	1.45	1.39
5	B	5102	141	C7-N8	-3.12	1.31	1.33
9	A	5302	EAK	C2-N1	2.94	1.40	1.33
5	A	5101	141	C7-N8	-2.87	1.31	1.33
9	B	5303	EAK	C7-C6	2.87	1.55	1.53
5	A	5101	141	C4-N3	2.80	1.37	1.32
5	B	5102	141	C4-N3	2.66	1.37	1.32
9	B	5303	EAK	C2-N1	2.63	1.39	1.33
9	A	5302	EAK	C7-C6	2.49	1.55	1.53
4	A	3005	FAD	C9-C8	2.48	1.43	1.39
4	B	4005	FAD	C4X-C10	2.36	1.51	1.44
4	A	3005	FAD	C6A-N1A	2.33	1.42	1.35
4	A	3005	FAD	C4X-C10	2.32	1.51	1.44
4	B	4005	FAD	C6-C7	2.27	1.42	1.39
4	B	4005	FAD	C9-C8	2.14	1.42	1.39
4	B	4005	FAD	C6A-N1A	2.12	1.41	1.35
4	B	4005	FAD	P-O3P	2.04	1.61	1.59
4	A	3005	FAD	C6-C7	2.00	1.42	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3005	FAD	C9-C9A-N10	7.08	131.38	121.85
4	B	4005	FAD	C5X-C9A-N10	-7.05	111.60	117.97
4	A	3005	FAD	C5X-C9A-N10	-7.04	111.61	117.97
4	B	4005	FAD	C9-C9A-N10	6.99	131.25	121.85
9	B	5303	EAK	C2-N1-C10	6.99	125.69	113.36
9	A	5302	EAK	C2-N1-C10	6.78	125.33	113.36
9	A	5302	EAK	O4-C4-C9	-5.09	114.99	127.26
9	A	5302	EAK	O3'-C7-C6	-5.06	105.59	108.96
9	B	5303	EAK	O4-C4-C9	-5.01	115.18	127.26
4	B	4005	FAD	C4-C4X-N5	4.98	125.09	118.21
9	B	5303	EAK	O3'-C7-C6	-4.78	105.78	108.96
4	A	3005	FAD	C4-C4X-N5	4.77	124.79	118.21
4	A	3005	FAD	N3A-C2A-N1A	-4.72	121.44	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	4005	FAD	N3A-C2A-N1A	-4.58	121.65	128.58
9	A	5302	EAK	C7-C6-N5	4.25	112.05	107.87
5	A	5101	141	C4-N9-N8	-4.23	105.09	109.99
5	B	5102	141	C4-N9-N8	-4.19	105.14	109.99
9	B	5303	EAK	C4-C9-N5	4.05	127.31	116.27
4	A	3005	FAD	O4B-C1B-N9A	-3.94	100.52	108.09
9	A	5302	EAK	C4-C9-N5	3.94	127.00	116.27
9	A	5302	EAK	N2-C2-N3	3.89	124.97	116.76
9	B	5303	EAK	C7-C6-N5	3.82	111.62	107.87
9	B	5303	EAK	N2-C2-N3	3.73	124.63	116.76
4	B	4005	FAD	C10-N1-C2	3.68	124.82	116.85
4	B	4005	FAD	C4'-C3'-C2'	-3.64	107.51	113.57
4	B	4005	FAD	O4B-C1B-N9A	-3.63	101.12	108.09
9	A	5302	EAK	N3-C2-N1	-3.63	116.68	123.32
4	A	3005	FAD	C10-N1-C2	3.60	124.64	116.85
9	B	5303	EAK	N3-C2-N1	-3.50	116.91	123.32
9	B	5303	EAK	C9-C4-N3	3.47	121.66	112.13
9	A	5302	EAK	C9-C4-N3	3.43	121.55	112.13
4	B	4005	FAD	C9A-N10-C10	3.42	125.96	120.75
4	B	4005	FAD	C8M-C8-C7	3.38	127.66	120.76
4	A	3005	FAD	C9A-N10-C10	3.36	125.87	120.75
4	A	3005	FAD	C8M-C8-C7	3.35	127.60	120.76
4	A	3005	FAD	C4'-C3'-C2'	-3.32	108.04	113.57
4	B	4005	FAD	C8M-C8-C9	-3.07	114.17	119.57
9	B	5303	EAK	O4'-C4'-C3'	3.03	116.06	108.58
4	A	3005	FAD	C8M-C8-C9	-3.01	114.27	119.57
9	A	5302	EAK	O4'-C4'-C3'	2.96	115.89	108.58
4	A	3005	FAD	C2A-N3A-C4A	2.76	118.57	111.83
4	A	3005	FAD	O3B-C3B-C4B	-2.71	103.29	111.08
4	B	4005	FAD	O3B-C3B-C4B	-2.69	103.35	111.08
4	B	4005	FAD	C2A-N3A-C4A	2.67	118.35	111.83
4	A	3005	FAD	O4-C4-C4X	-2.63	119.59	126.53
4	B	4005	FAD	O3'-C3'-C4'	2.55	114.73	108.93
4	A	3005	FAD	O3'-C3'-C4'	2.55	114.72	108.93
4	A	3005	FAD	C5X-N5-C4X	2.50	122.14	118.09
4	B	4005	FAD	O4-C4-C4X	-2.45	120.06	126.53
4	B	4005	FAD	C5X-N5-C4X	2.44	122.03	118.09
4	B	4005	FAD	C10-C4X-N5	-2.41	119.88	124.81
4	A	3005	FAD	N3A-C4A-N9A	2.36	131.19	127.17
4	A	3005	FAD	C10-C4X-N5	-2.32	120.06	124.81
4	B	4005	FAD	N3A-C4A-N9A	2.25	130.99	127.17
4	A	3005	FAD	C1'-N10-C9A	-2.22	116.32	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	5303	EAK	C2'-C1'-S1'	-2.21	118.90	120.15
5	A	5101	141	O6-C6-N1	2.18	124.21	120.11
5	B	5102	141	O6-C6-N1	2.15	124.15	120.11
4	B	4005	FAD	C1'-N10-C9A	-2.12	116.50	120.63
4	A	3005	FAD	C4X-C4-N3	2.10	118.59	113.25
4	B	4005	FAD	O3P-PA-O1A	-2.06	104.52	110.70
4	B	4005	FAD	C6A-C5A-C4A	-2.05	114.37	117.18
4	B	4005	FAD	C4X-C4-N3	2.04	118.45	113.25
4	A	3005	FAD	O2'-C2'-C3'	2.01	113.95	109.25
5	A	5101	141	C7-N8-N9	2.01	113.98	109.42

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
4	B	4005	FAD	N10-C1'-C2'-O2'
4	B	4005	FAD	N10-C1'-C2'-C3'
6	A	5005	GOL	O1-C1-C2-O2
6	A	5005	GOL	O1-C1-C2-C3
6	B	5002	GOL	O1-C1-C2-C3
6	B	5002	GOL	C1-C2-C3-O3
6	B	5003	GOL	O1-C1-C2-C3
4	A	3005	FAD	C2'-C3'-C4'-C5'
4	B	4005	FAD	C2'-C3'-C4'-C5'
4	A	3005	FAD	C2'-C3'-C4'-O4'
4	B	4005	FAD	C2'-C3'-C4'-O4'
6	B	5002	GOL	O1-C1-C2-O2
9	A	5302	EAK	C3'-C4'-O4'-P
4	A	3005	FAD	O3'-C3'-C4'-O4'
4	B	4005	FAD	O3'-C3'-C4'-O4'
4	A	3005	FAD	O3'-C3'-C4'-C5'
4	B	4005	FAD	O3'-C3'-C4'-C5'
9	B	5303	EAK	C3'-C4'-O4'-P
6	B	5002	GOL	O2-C2-C3-O3
6	B	5003	GOL	O1-C1-C2-O2
6	A	5005	GOL	O2-C2-C3-O3
6	B	5004	GOL	O2-C2-C3-O3
6	A	5005	GOL	C1-C2-C3-O3

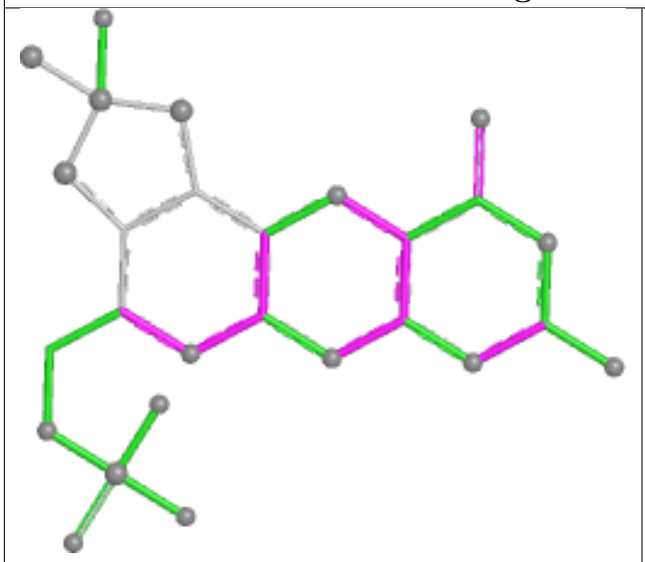
There are no ring outliers.

8 monomers are involved in 13 short contacts:

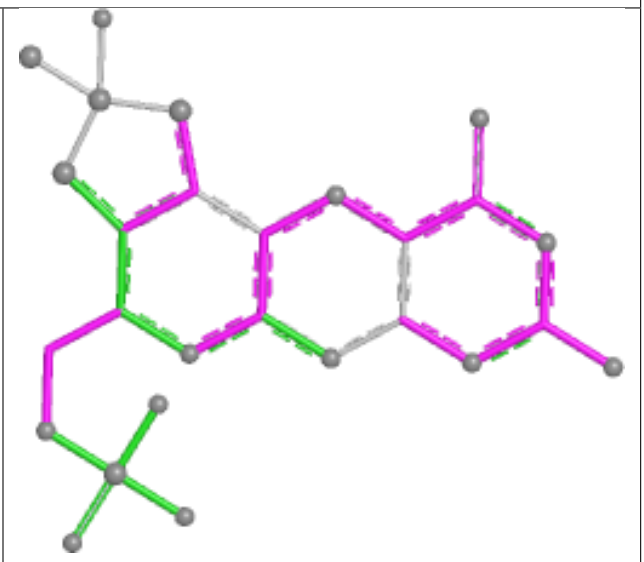
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4002	FES	2	0
9	B	5303	EAK	2	0
5	B	5102	141	2	0
6	B	5003	GOL	1	0
3	A	3002	FES	1	0
4	A	3005	FAD	1	0
5	A	5101	141	2	0
9	A	5302	EAK	2	0

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.

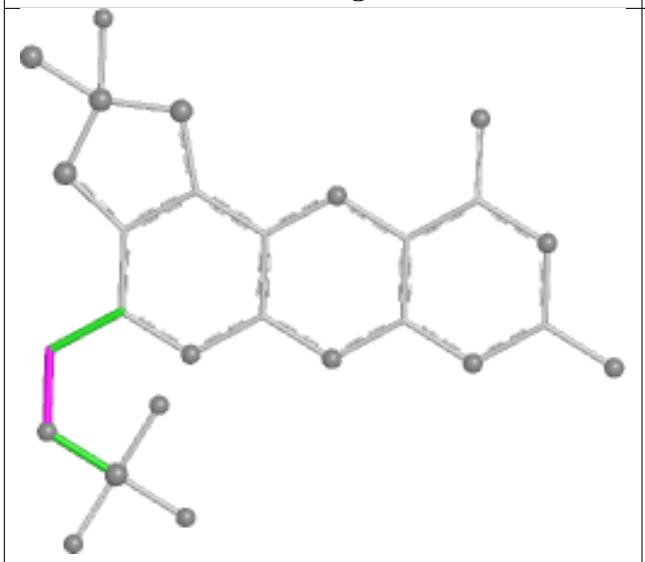
Ligand EAK B 5303



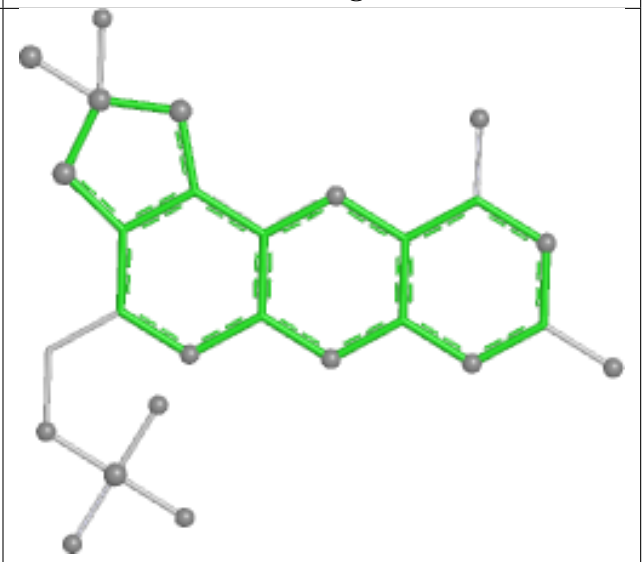
Bond lengths



Bond angles

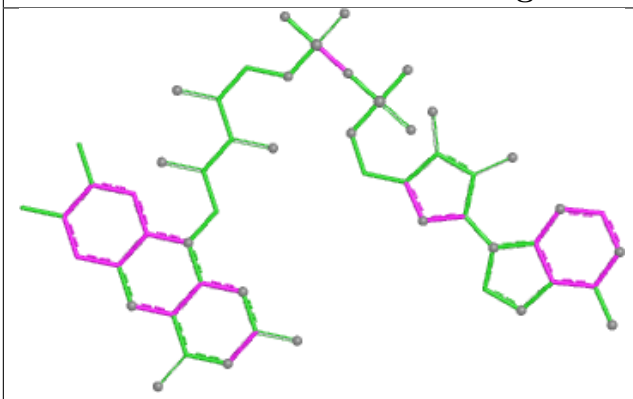


Torsions

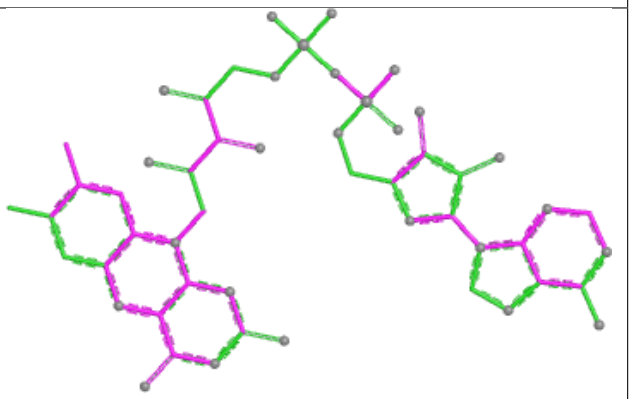


Rings

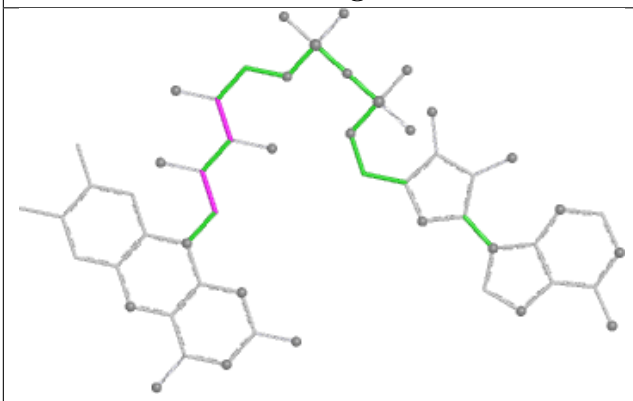
Ligand FAD B 4005



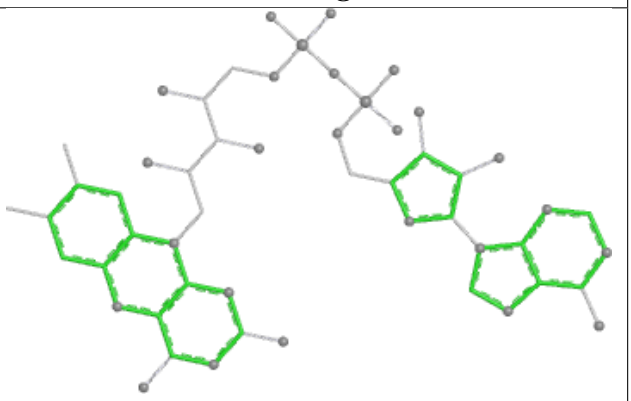
Bond lengths



Bond angles

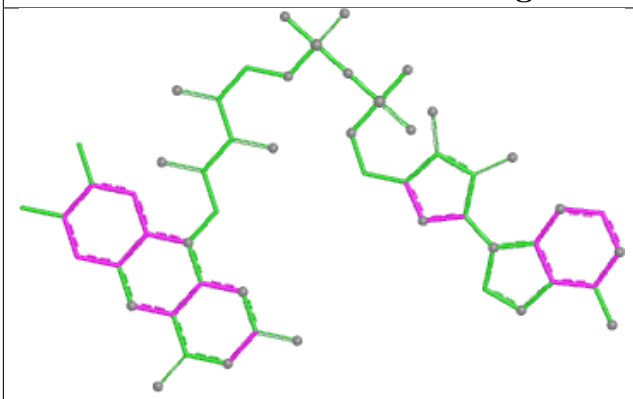


Torsions

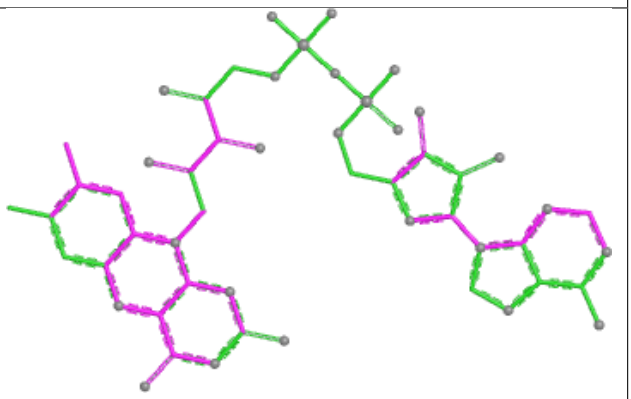


Rings

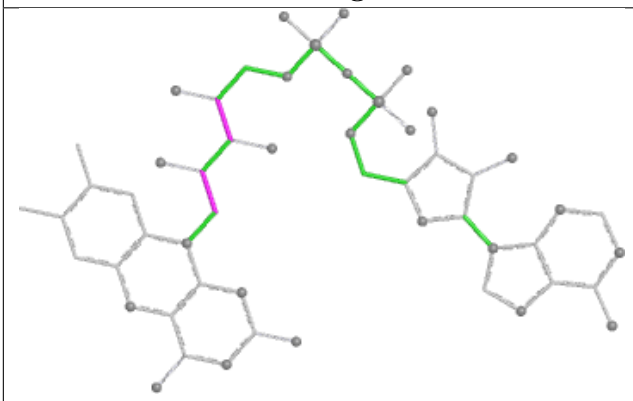
Ligand FAD A 3005



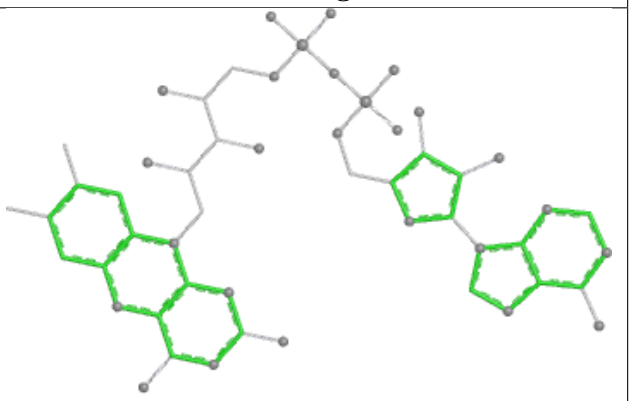
Bond lengths



Bond angles

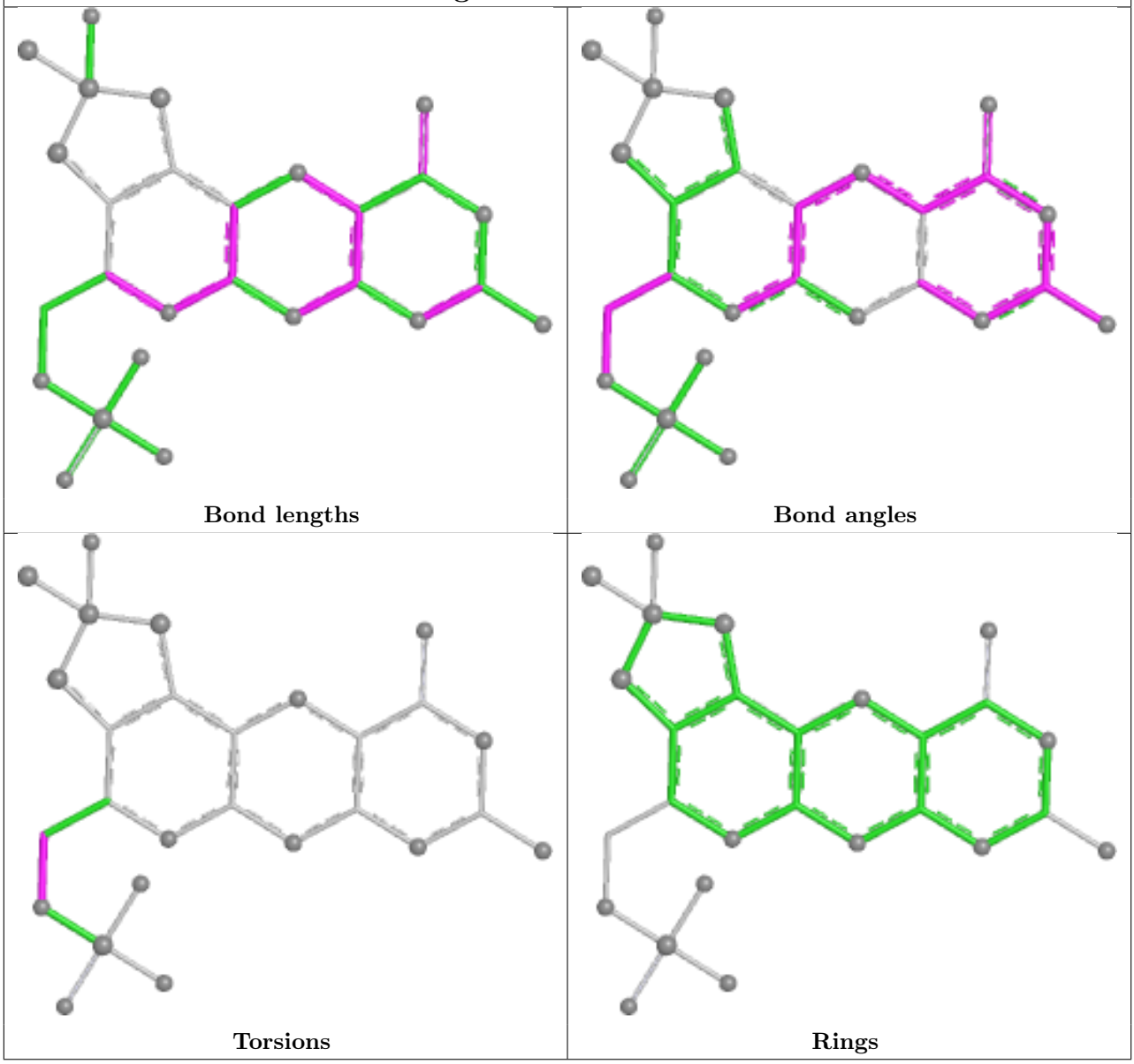


Torsions



Rings

Ligand EAK A 5302



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	1286/1332 (96%)	-0.29	13 (1%)	79	79	10, 19, 34, 57	0
1	B	1286/1332 (96%)	-0.25	14 (1%)	78	77	8, 19, 34, 56	0
All	All	2572/2664 (96%)	-0.27	27 (1%)	79	79	8, 19, 34, 57	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	565	ASN	4.0
1	B	566	GLY	4.0
1	A	528	GLY	3.9
1	B	528	GLY	3.6
1	A	1317	CYS	3.3
1	A	1286	THR	3.1
1	B	377	ARG	3.0
1	B	1288	ASN	3.0
1	B	552	HIS	2.9
1	A	1288	ASN	2.8
1	A	378	GLY	2.8
1	B	1286	THR	2.8
1	B	318	LYS	2.7
1	B	564	PRO	2.6
1	A	565	ASN	2.5
1	B	538	LEU	2.4
1	B	724	SER	2.3
1	A	552	HIS	2.3
1	B	222	VAL	2.2
1	A	219	LEU	2.2
1	B	537	LYS	2.2
1	A	222	VAL	2.1
1	A	1287	ASN	2.1
1	A	538	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	699	GLU	2.1
1	A	537	LYS	2.0
1	A	223	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
6	GOL	B	5004	6/6	0.87	0.12	21,28,29,34	0
6	GOL	A	5006	6/6	0.88	0.10	28,28,29,31	0
6	GOL	B	5002	6/6	0.89	0.10	20,23,25,25	0
6	GOL	B	5003	6/6	0.90	0.11	29,30,31,33	0
6	GOL	A	5005	6/6	0.91	0.09	18,19,19,20	0
6	GOL	B	5001	6/6	0.93	0.08	24,26,28,29	0
6	GOL	A	5007	6/6	0.94	0.08	22,26,27,27	0
5	141	A	5101	11/11	0.96	0.06	12,14,15,16	0
4	FAD	A	3005	53/53	0.97	0.05	12,16,20,23	0
5	141	B	5102	11/11	0.97	0.05	13,15,16,16	0
4	FAD	B	4005	53/53	0.97	0.05	12,15,20,22	0
7	CO3	B	5202	4/4	0.97	0.06	14,15,15,17	0
2	CA	B	5302	1/1	0.98	0.06	15,15,15,15	0
3	FES	A	3001	4/4	0.99	0.02	11,11,13,13	0
7	CO3	A	5201	4/4	0.99	0.03	12,13,13,15	0
3	FES	A	3002	4/4	0.99	0.02	11,11,11,12	0
9	EAK	A	5302	27/27	0.99	0.04	10,13,15,17	0
9	EAK	B	5303	27/27	0.99	0.05	9,13,16,18	0
2	CA	A	5301	1/1	1.00	0.02	15,15,15,15	0
3	FES	B	4001	4/4	1.00	0.02	11,12,12,14	0

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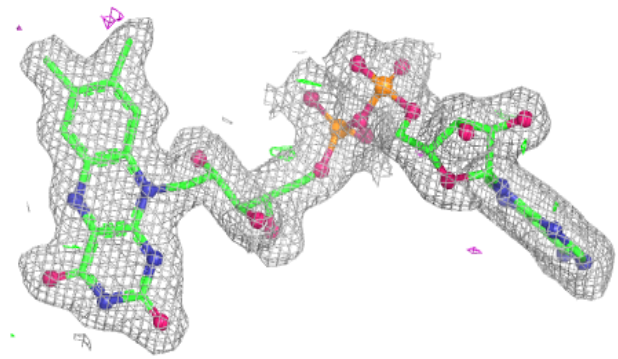
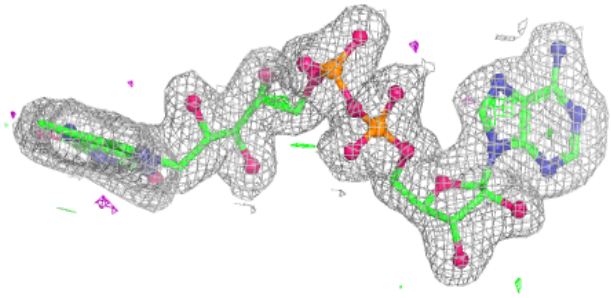
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FES	B	4002	4/4	1.00	0.01	11,12,12,12	0

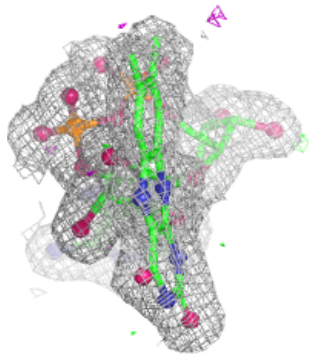
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

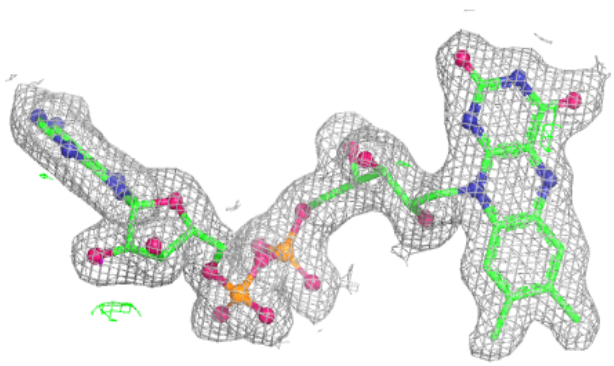


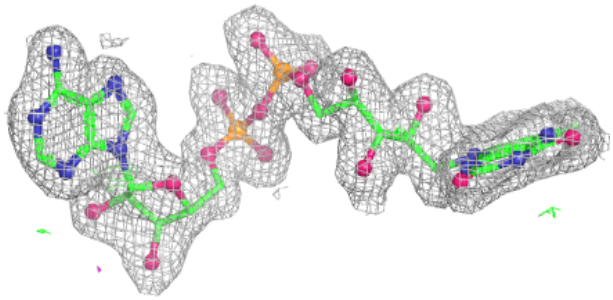




Electron density around FAD B 4005:

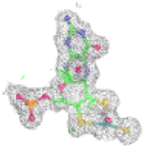
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around EAK A 5302:

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



Electron density around EAK B 5303: $2mF_o$-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.