Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:40 PM EDT

PDB ID	:	3UNI / pdb_00003uni
Title	:	Crystal Structure of Bovine Milk Xanthine Dehydrogenase with NADH Bound
Authors	:	Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.
Deposited on	:	2011-11-15
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:

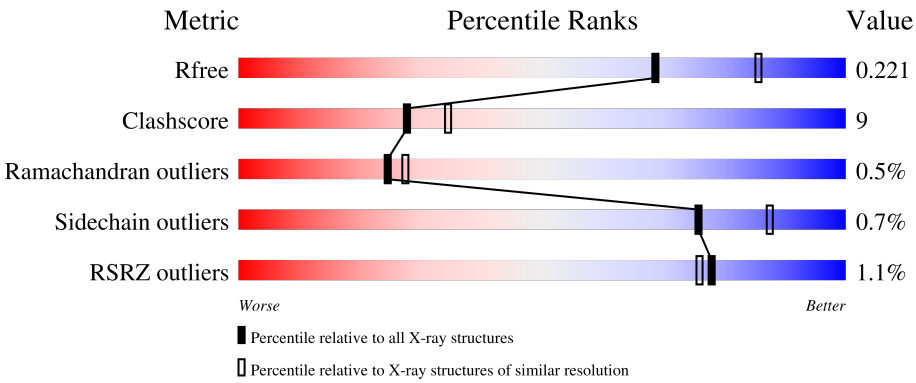
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.20 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	1332	% 75% 20% • •
1	B	1332	% 75% 20% • •

2 Entry composition (i)

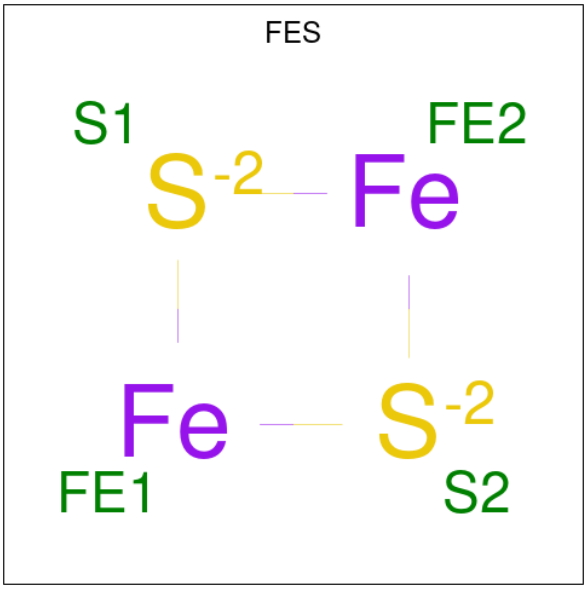
There are 10 unique types of molecules in this entry. The entry contains 21491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

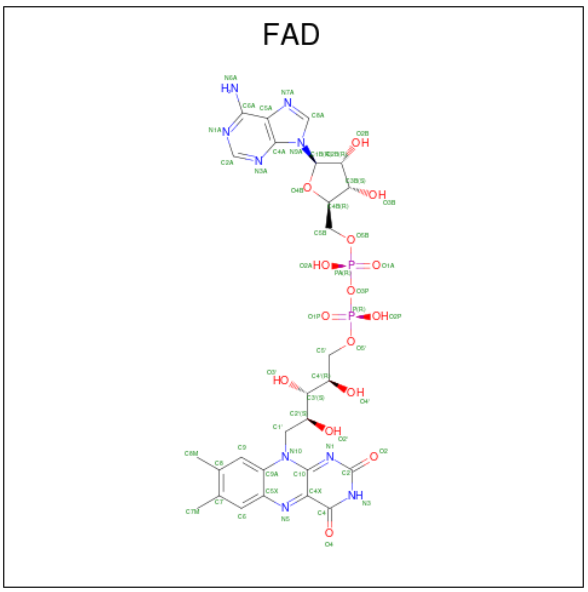
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1289	10003	6360	1712	1871	60	0	0	0
1	B	1288	9998	6357	1711	1870	60	0	0	0

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



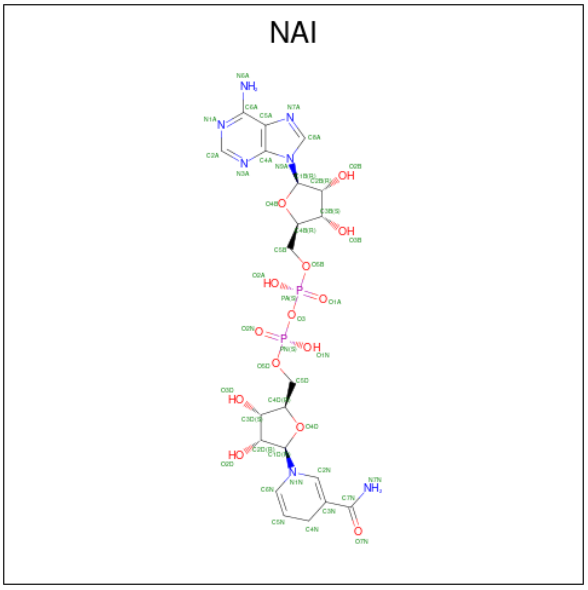
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0
2	B	1	4	2	2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



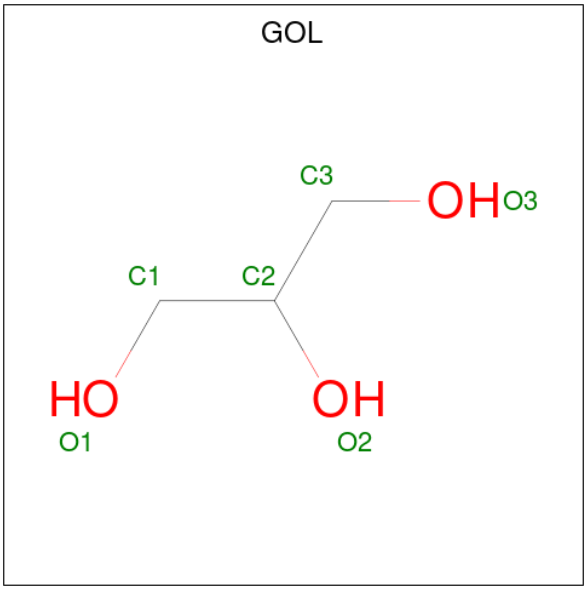
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
3	B	1	53	27	9	15	2	0	0

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



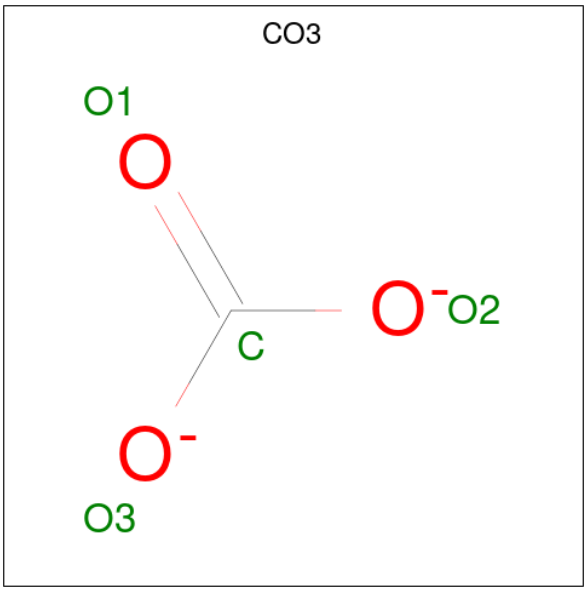
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



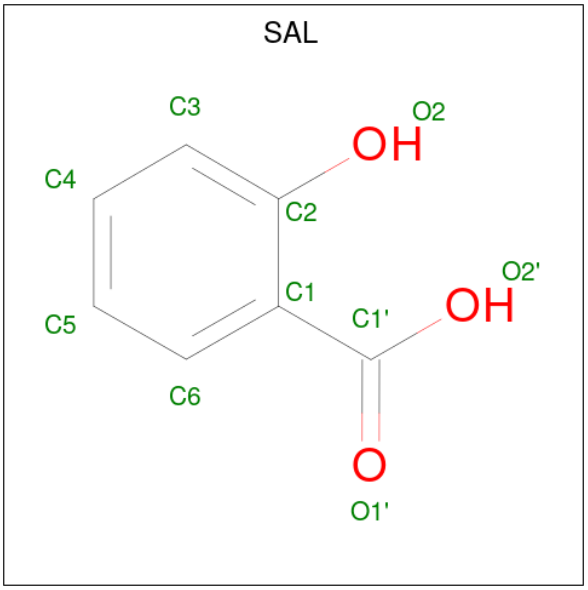
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			6	3	3			
5	A	1	Total	C	O		0	0
			6	3	3			
5	A	1	Total	C	O		0	0
			6	3	3			
5	A	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6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

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



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

- Molecule 7 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$).

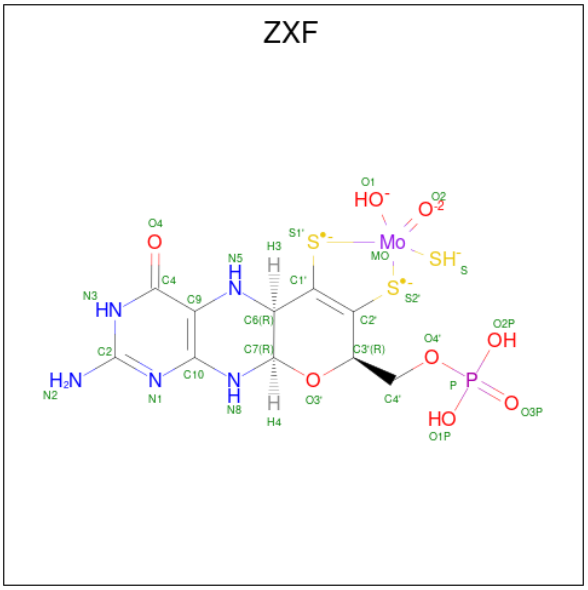


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	10	7	3	0	0
			Total	C	O		
7	B	1	10	7	3	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is Molybdopterin hydoxy-oxo-thiol-molybdenum (CCD ID: ZXF) (formula: $C_{10}H_{14}MoN_5O_8PS_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C Mo N O P S 28 10 1 5 8 1 3	0	0
9	B	1	Total C Mo N O P S 28 10 1 5 8 1 3	0	0

- Molecule 10 is water.

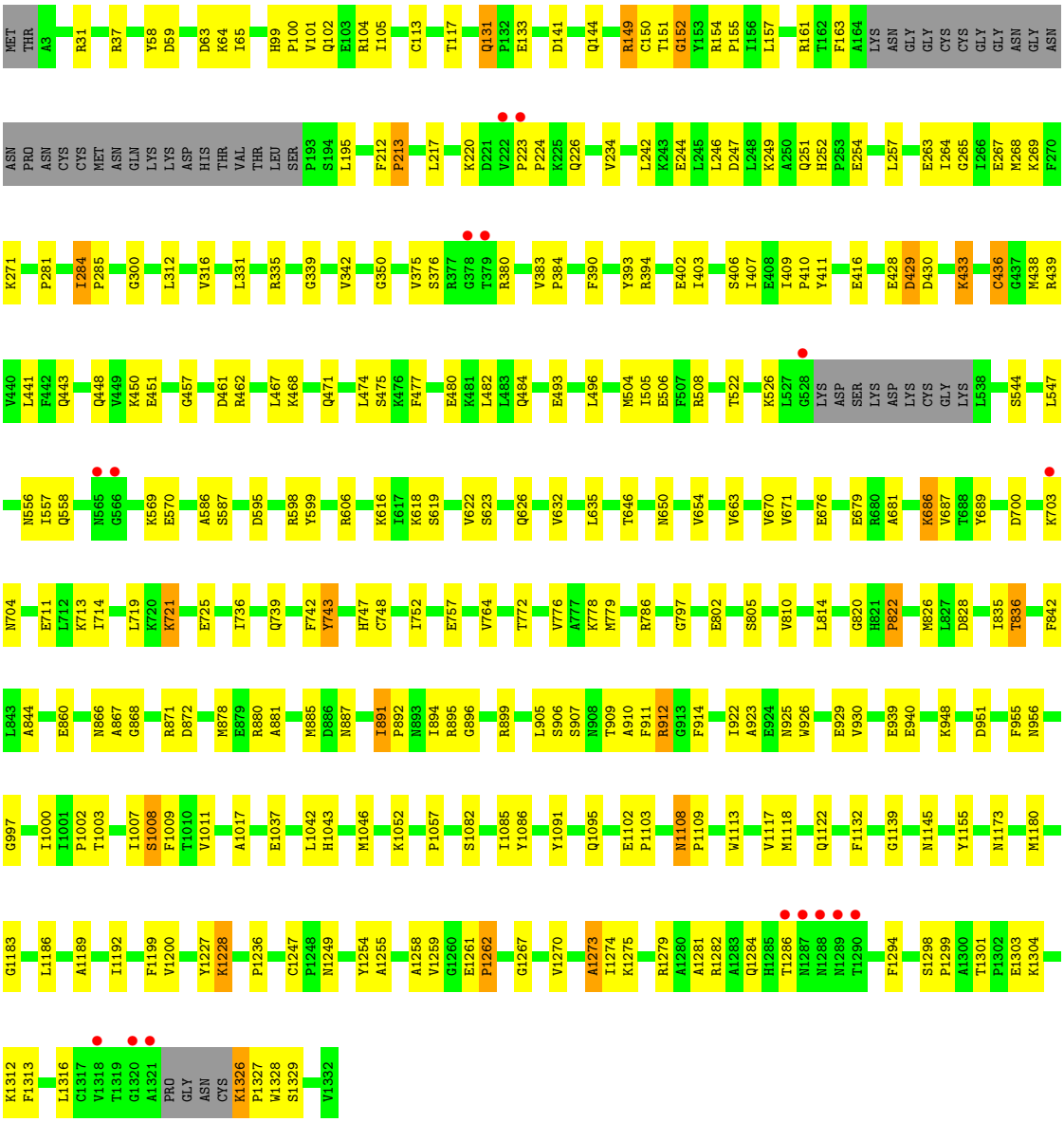
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	587	Total O 587 587	0	0
10	B	553	Total O 553 553	0	0

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.

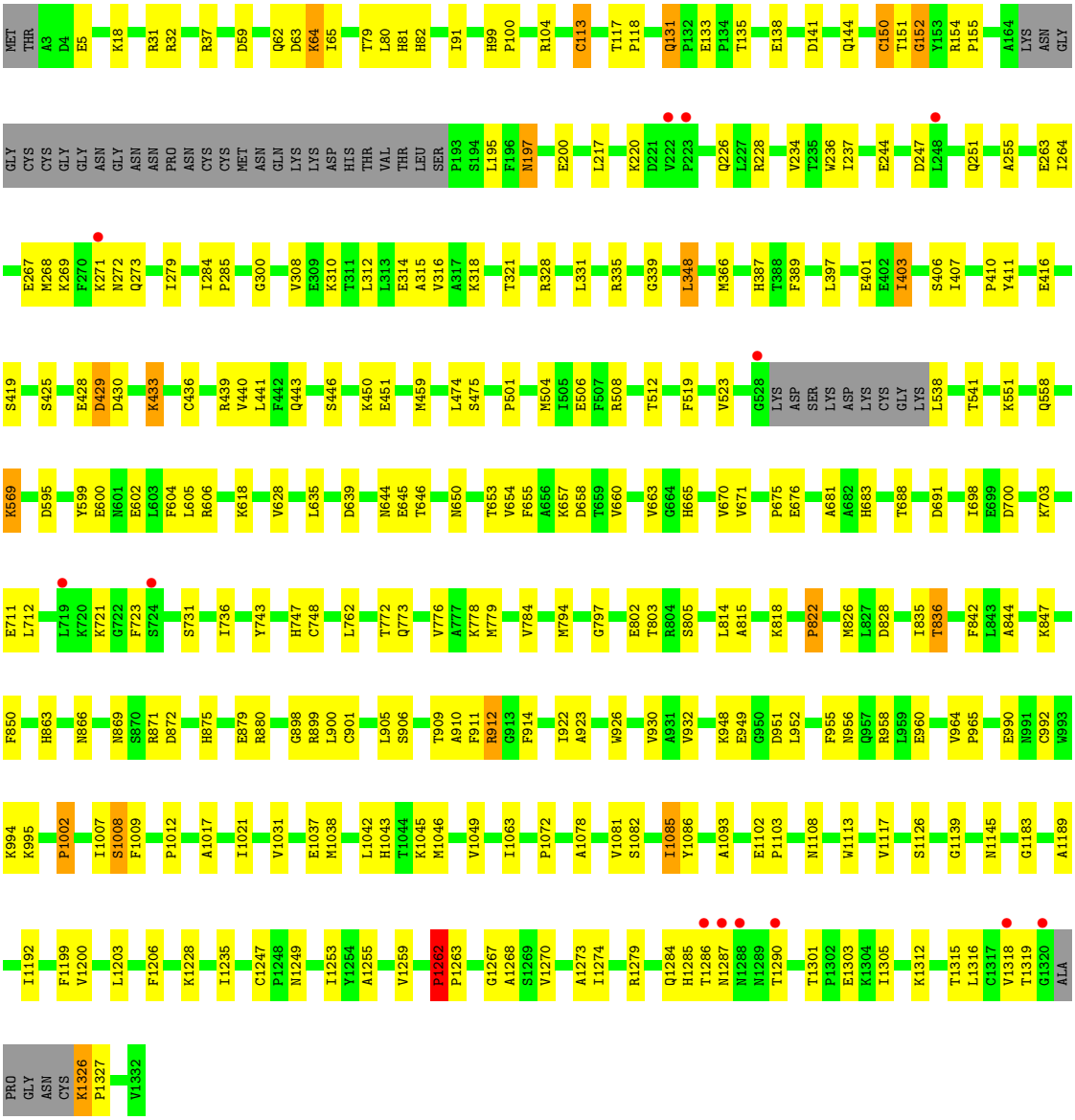
- Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.04Å 146.70Å 107.02Å 90.00° 106.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 95.7 (20.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.240 0.181 , 0.221	Depositor DCC
R_{free} test set	2293 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21491	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: SAL, GOL, NAI, FES, FAD, ZXF, CO3, 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	0.38	0/10221	0.93	44/13835 (0.3%)
1	B	0.38	0/10216	0.93	37/13828 (0.3%)
All	All	0.38	0/20437	0.93	81/27663 (0.3%)

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	835	ILE	N-CA-C	12.72	123.16	110.82
1	A	151	THR	N-CA-C	10.29	125.20	112.23
1	A	835	ILE	N-CA-C	10.04	122.22	111.58
1	B	151	THR	N-CA-C	8.83	123.35	112.23
1	B	1262	PRO	N-CA-C	8.25	120.77	110.70
1	A	1262	PRO	N-CA-C	8.24	120.75	110.70
1	B	836	THR	N-CA-C	8.12	122.85	113.19
1	A	1011	VAL	N-CA-C	-8.02	99.61	107.55
1	A	836	THR	N-CA-C	7.87	122.72	113.20
1	A	433	LYS	N-CA-C	-7.80	102.10	111.69
1	B	433	LYS	N-CA-C	-7.75	100.88	112.04
1	B	1273	ALA	N-CA-C	-7.19	102.85	111.69
1	A	152	GLY	N-CA-C	-7.13	105.38	115.43
1	B	956	ASN	N-CA-C	7.12	121.35	112.24
1	A	663	VAL	N-CA-C	-6.99	100.56	109.30
1	A	654	VAL	N-CA-C	-6.89	103.48	111.00
1	A	743	TYR	N-CA-C	-6.81	100.20	110.28
1	A	956	ASN	N-CA-C	6.78	120.92	112.24
1	B	1085	ILE	N-CA-C	6.54	117.32	110.72
1	A	411	TYR	N-CA-C	-6.46	100.93	110.48
1	B	869	ASN	N-CA-C	6.42	120.60	113.21
1	A	1273	ALA	N-CA-C	-6.42	104.36	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	436	CYS	N-CA-C	6.25	117.72	108.60
1	A	828	ASP	N-CA-C	-6.24	102.29	110.53
1	B	828	ASP	N-CA-C	-6.22	102.32	110.53
1	B	450	LYS	N-CA-C	-6.17	105.41	113.12
1	B	654	VAL	N-CA-C	-6.14	104.52	110.72
1	B	152	GLY	N-CA-C	-6.08	106.85	115.30
1	B	663	VAL	N-CA-C	-6.00	100.92	108.84
1	A	891	ILE	CA-C-N	5.97	126.13	119.32
1	A	891	ILE	C-N-CA	5.97	126.13	119.32
1	B	269	LYS	N-CA-C	5.93	117.83	111.36
1	B	131	GLN	CA-C-N	5.87	126.01	119.32
1	B	131	GLN	C-N-CA	5.87	126.01	119.32
1	A	1085	ILE	N-CA-C	5.79	117.32	111.00
1	A	234	VAL	N-CA-C	5.78	117.08	108.46
1	B	197	ASN	CA-C-N	5.77	126.16	119.47
1	B	197	ASN	C-N-CA	5.77	126.16	119.47
1	A	450	LYS	N-CA-C	-5.73	106.83	113.88
1	A	150	CYS	N-CA-C	5.73	120.41	112.45
1	B	300	GLY	N-CA-C	-5.69	105.39	111.93
1	B	113	CYS	N-CA-C	-5.65	105.27	111.82
1	A	31	ARG	N-CA-C	5.64	118.63	111.69
1	A	1108	ASN	CA-C-N	5.63	125.74	119.32
1	A	1108	ASN	C-N-CA	5.63	125.74	119.32
1	A	820	GLY	N-CA-C	-5.60	107.91	115.36
1	B	1108	ASN	CA-C-N	5.60	125.70	119.32
1	B	1108	ASN	C-N-CA	5.60	125.70	119.32
1	B	234	VAL	N-CA-C	5.59	116.79	108.46
1	B	822	PRO	N-CA-C	-5.56	102.54	111.38
1	A	113	CYS	N-CA-C	-5.56	105.38	111.82
1	B	80	LEU	N-CA-C	5.55	119.14	112.93
1	B	31	ARG	N-CA-C	5.48	117.34	111.36
1	A	867	ALA	N-CA-C	5.46	118.15	111.82
1	B	1326	LYS	CA-C-N	5.45	125.39	119.78
1	B	1326	LYS	C-N-CA	5.45	125.39	119.78
1	A	443	GLN	N-CA-C	-5.42	102.59	110.08
1	A	835	ILE	CB-CA-C	-5.42	105.11	111.94
1	B	1009	PHE	N-CA-C	-5.39	101.87	109.96
1	A	764	VAL	N-CA-C	5.38	116.47	108.46
1	A	284	ILE	CA-C-N	5.38	124.83	119.24
1	A	284	ILE	C-N-CA	5.38	124.83	119.24
1	A	131	GLN	CA-C-N	5.36	125.02	119.56
1	A	131	GLN	C-N-CA	5.36	125.02	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	150	CYS	N-CA-C	5.33	119.71	112.04
1	A	822	PRO	N-CA-C	-5.30	102.95	111.38
1	B	410	PRO	N-CA-C	5.28	120.50	111.68
1	A	457	GLY	N-CA-C	-5.23	102.04	111.19
1	A	300	GLY	N-CA-C	-5.22	105.41	112.14
1	B	436	CYS	N-CA-C	5.22	116.73	108.96
1	A	410	PRO	N-CA-C	5.18	119.62	111.38
1	A	409	ILE	CA-C-N	5.15	125.05	119.85
1	A	409	ILE	C-N-CA	5.15	125.05	119.85
1	A	1228	LYS	N-CA-C	5.15	117.10	107.99
1	A	872	ASP	CB-CA-C	-5.12	110.65	116.54
1	B	411	TYR	N-CA-C	-5.12	102.91	110.48
1	B	872	ASP	CB-CA-C	-5.06	110.76	116.63
1	B	79	THR	N-CA-C	-5.06	107.16	113.38
1	A	1009	PHE	N-CA-C	-5.04	102.40	109.96
1	B	691	ASP	N-CA-C	5.04	116.79	110.24
1	A	1186	LEU	N-CA-C	-5.02	105.90	112.23

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	10003	0	9999	184	0
1	B	9998	0	9994	182	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	53	0	31	3	0
3	B	53	0	31	2	0
4	A	44	0	27	0	0
4	B	44	0	27	1	0
5	A	24	0	32	0	0
5	B	30	0	40	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	10	0	4	1	0
7	B	10	0	4	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	28	0	0	0	0
9	B	28	0	0	0	0
10	A	587	0	0	8	0
10	B	553	0	0	8	0
All	All	21491	0	20189	364	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 9.

All (364) 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:955:PHE:HA	1:B:1145:ASN:HD21	1.28	0.97
1:A:131:GLN:HE21	1:A:133:GLU:H	1.11	0.96
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.31	0.94
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.36	0.91
1:A:700:ASP:HA	1:A:703:LYS:HE3	1.53	0.89
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.37	0.85
1:A:506:GLU:CD	1:A:506:GLU:H	1.90	0.79
1:A:264:ILE:HG22	1:A:268:MET:HE2	1.65	0.78
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.53	0.73
1:A:1118:MET:O	1:A:1122:GLN:HG2	1.90	0.72
1:A:556:ASN:C	1:A:557:ILE:HD12	2.15	0.72
1:B:131:GLN:HE21	1:B:133:GLU:H	1.38	0.71
1:A:1279:ARG:HG2	1:A:1294:PHE:CE2	2.25	0.71
1:B:1249:ASN:O	1:B:1255:ALA:HA	1.95	0.67
1:A:844:ALA:HB2	1:A:922:ILE:HD13	1.77	0.66
10:A:1346:ZXF:O2	10:A:1346:ZXF:MO	1.66	0.65
1:A:622:VAL:O	1:A:626:GLN:HG3	1.96	0.65
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.96	0.65
1:B:312:LEU:O	1:B:316:VAL:HG23	1.98	0.64
1:B:267:GLU:HA	1:B:271:LYS:HG2	1.80	0.64
10:B:1347:ZXF:O2	10:B:1347:ZXF:MO	1.68	0.64
1:B:639:ASP:HB3	1:B:818:LYS:HE3	1.81	0.63
1:A:131:GLN:HE21	1:A:133:GLU:N	1.91	0.63
1:A:1326:LYS:HA	1:A:1326:LYS:HE3	1.80	0.63
1:A:635:LEU:HD13	1:A:814:LEU:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLN:NE2	1:A:133:GLU:H	1.91	0.63
1:B:618:LYS:HE2	1:B:618:LYS:HA	1.79	0.63
1:A:1249:ASN:O	1:A:1255:ALA:HA	1.97	0.63
1:B:994:LYS:HE3	5:B:1342:GOL:O2	1.99	0.63
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.09	0.63
1:A:1299:PRO:O	1:A:1304:LYS:HE2	1.98	0.62
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.81	0.61
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	1.82	0.61
1:A:1316:LEU:HD23	1:A:1316:LEU:O	2.00	0.60
1:B:1315:THR:O	1:B:1318:VAL:HG22	2.01	0.60
1:A:58:TYR:CE2	1:A:220:LYS:HD2	2.36	0.60
1:A:939:GLU:HG2	1:A:940:GLU:N	2.17	0.59
1:B:64:LYS:HG2	1:B:65:ILE:N	2.16	0.59
1:A:598:ARG:O	1:B:600:GLU:HG2	2.02	0.59
1:A:375:VAL:HG12	1:A:380:ARG:HG3	1.83	0.59
1:A:141:ASP:O	1:A:144:GLN:HG3	2.03	0.59
1:A:504:MET:HE2	1:A:1303:GLU:OE1	2.02	0.59
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.38	0.59
1:B:712:LEU:HD21	1:B:879:GLU:HG2	1.85	0.58
1:B:264:ILE:O	1:B:268:MET:HG2	2.04	0.58
1:A:474:LEU:O	1:A:475:SER:HB2	2.04	0.58
1:B:1318:VAL:HG23	1:B:1319:THR:N	2.20	0.57
1:B:1279:ARG:HG3	1:B:1279:ARG:HH11	1.70	0.57
1:B:712:LEU:HD21	1:B:879:GLU:CG	2.33	0.57
1:B:932:VAL:HG13	1:B:1279:ARG:NH2	2.19	0.57
1:A:635:LEU:HD13	1:A:814:LEU:HD12	1.86	0.56
1:B:1262:PRO:HB2	1:B:1263:PRO:HD3	1.87	0.56
1:A:406:SER:C	1:A:407:ILE:HD12	2.29	0.56
1:A:100:PRO:O	1:A:104:ARG:HG3	2.05	0.56
1:A:149:ARG:HG3	1:A:742:PHE:O	2.05	0.56
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.21	0.56
1:A:713:LYS:HG2	1:A:714:ILE:N	2.19	0.56
1:B:366:MET:HE2	1:B:387:HIS:HA	1.87	0.56
1:B:37:ARG:HD3	1:B:595:ASP:O	2.06	0.56
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.06	0.55
1:A:911:PHE:O	1:A:912:ARG:C	2.49	0.55
1:B:433:LYS:HE2	1:B:504:MET:SD	2.47	0.55
1:B:618:LYS:HB2	1:B:688:THR:HG22	1.88	0.55
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.89	0.55
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.42	0.54
1:B:911:PHE:O	1:B:912:ARG:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HG2	1:A:65:ILE:N	2.22	0.54
1:A:814:LEU:C	1:A:814:LEU:HD13	2.32	0.54
1:A:1279:ARG:HB3	1:A:1279:ARG:NH1	2.22	0.54
1:B:310:LYS:O	1:B:314:GLU:HG3	2.08	0.54
1:B:605:LEU:C	1:B:605:LEU:HD23	2.32	0.54
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	1.90	0.54
1:B:635:LEU:HD11	1:B:815:ALA:HA	1.88	0.54
1:A:599:TYR:HA	1:B:599:TYR:HA	1.88	0.53
1:A:157:LEU:O	1:A:161:ARG:HG3	2.08	0.53
1:A:195:LEU:HD22	1:A:1189:ALA:HA	1.90	0.53
1:A:508:ARG:HD3	10:A:1547:HOH:O	2.09	0.53
1:A:1082:SER:HB2	10:A:1346:ZXF:O1P	2.08	0.53
1:A:1282:ARG:O	1:A:1286:THR:HB	2.09	0.53
1:A:461:ASP:OD1	1:A:462:ARG:HG2	2.08	0.53
1:A:217:LEU:O	1:A:220:LYS:HG2	2.08	0.53
1:A:748:CYS:HB2	1:A:826:MET:HG3	1.90	0.53
1:B:1316:LEU:O	1:B:1316:LEU:HD23	2.08	0.53
1:B:506:GLU:CD	1:B:506:GLU:H	2.17	0.53
1:A:430:ASP:CG	1:A:1228:LYS:HE2	2.34	0.53
1:B:263:GLU:HB2	3:B:1337:FAD:H52A	1.91	0.52
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.74	0.52
1:B:676:GLU:H	1:B:676:GLU:CD	2.17	0.52
1:A:247:ASP:HB3	1:A:251:GLN:NE2	2.24	0.52
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.44	0.52
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.07	0.52
1:A:249:LYS:HD3	1:A:257:LEU:HD11	1.92	0.52
1:A:407:ILE:HD12	1:A:407:ILE:N	2.24	0.52
1:B:419:SER:HB2	1:B:519:PHE:CD1	2.45	0.52
1:B:794:MET:HE3	1:B:1038:MET:HB3	1.92	0.52
1:B:1007:ILE:O	1:B:1008:SER:CB	2.58	0.52
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.73	0.52
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.75	0.52
1:A:448:GLN:HB2	1:A:477:PHE:CE2	2.44	0.51
1:A:264:ILE:HD11	3:A:1337:FAD:H3B	1.93	0.51
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.92	0.51
1:B:863:HIS:O	1:B:898:GLY:HA2	2.11	0.51
1:B:1270:VAL:O	1:B:1274:ILE:HG13	2.11	0.51
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.40	0.51
1:A:948:LYS:HG2	1:A:951:ASP:OD2	2.10	0.51
1:B:443:GLN:HB2	1:B:446:SER:OG	2.10	0.51
1:B:197:ASN:HD22	1:B:200:GLU:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:SER:HB3	10:B:1525:HOH:O	2.09	0.51
1:B:459:MET:HE2	1:B:512:THR:HG21	1.92	0.51
1:B:1312:LYS:HG2	10:B:1856:HOH:O	2.11	0.50
1:B:504:MET:HE2	1:B:1303:GLU:OE1	2.11	0.50
1:B:312:LEU:HB2	1:B:331:LEU:HD21	1.93	0.50
1:B:1279:ARG:NH2	1:B:1290:THR:O	2.45	0.50
1:A:144:GLN:HB2	1:A:339:GLY:HA2	1.94	0.50
1:B:416:GLU:OE1	1:B:439:ARG:HD2	2.12	0.50
1:A:390:PHE:HB3	10:A:1552:HOH:O	2.10	0.50
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.93	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.47	0.50
1:A:1007:ILE:O	1:A:1008:SER:CB	2.60	0.50
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.75	0.50
1:B:389:PHE:HA	1:B:397:LEU:HG	1.94	0.50
1:B:197:ASN:ND2	1:B:200:GLU:HG3	2.27	0.49
1:B:711:GLU:HA	1:B:899:ARG:CD	2.42	0.49
1:B:267:GLU:HA	1:B:271:LYS:CG	2.41	0.49
1:B:403:ILE:C	1:B:403:ILE:HD13	2.37	0.49
1:B:474:LEU:O	1:B:475:SER:HB2	2.13	0.49
1:B:569:LYS:NZ	1:B:569:LYS:HB3	2.28	0.49
1:B:1046:MET:HE2	1:B:1046:MET:HA	1.93	0.49
1:A:1052:LYS:HD3	1:A:1254:TYR:CE1	2.48	0.49
1:A:506:GLU:CD	1:A:506:GLU:N	2.67	0.49
1:B:698:ILE:HG23	1:B:901:CYS:SG	2.53	0.49
1:A:1326:LYS:HB3	1:A:1327:PRO:HD3	1.94	0.49
1:A:544:SER:HA	1:A:547:LEU:HD12	1.93	0.49
1:A:686:LYS:HD3	1:A:686:LYS:C	2.38	0.49
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.48	0.49
1:B:154:ARG:HD2	1:B:154:ARG:C	2.38	0.49
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.93	0.49
1:B:871:ARG:HG3	1:B:871:ARG:HH11	1.78	0.48
1:B:308:VAL:HG21	1:B:348:LEU:HG	1.95	0.48
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.48	0.48
1:A:467:LEU:O	1:A:471:GLN:HB2	2.14	0.48
1:A:154:ARG:C	1:A:154:ARG:HD2	2.38	0.48
1:A:249:LYS:HD3	1:A:257:LEU:CD1	2.44	0.48
1:A:871:ARG:HH11	1:A:871:ARG:HG3	1.78	0.48
1:A:686:LYS:HD3	1:A:687:VAL:N	2.29	0.48
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.13	0.48
1:B:1007:ILE:HG22	1:B:1081:VAL:HG12	1.95	0.48
1:A:254:GLU:H	1:A:254:GLU:CD	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:SER:HB2	10:B:1347:ZXF:O1P	2.14	0.48
1:A:1279:ARG:HB3	1:A:1279:ARG:CZ	2.44	0.47
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.96	0.47
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.49	0.47
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.95	0.47
1:A:711:GLU:HB2	1:A:899:ARG:HD3	1.97	0.47
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.15	0.47
1:A:721:LYS:NZ	1:A:721:LYS:HB3	2.29	0.47
1:B:508:ARG:HD3	10:B:1785:HOH:O	2.13	0.47
1:A:265:GLY:O	1:A:269:LYS:HB2	2.13	0.47
1:A:281:PRO:HB2	1:A:284:ILE:HD12	1.97	0.47
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.95	0.47
1:A:480:GLU:O	1:A:484:GLN:HG3	2.15	0.47
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	1.97	0.47
1:B:646:THR:O	1:B:650:ASN:HA	2.14	0.47
1:A:154:ARG:N	1:A:155:PRO:HD2	2.30	0.47
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.44	0.47
1:A:926:TRP:O	1:A:930:VAL:HG23	2.15	0.47
1:A:1227:TYR:C	1:A:1228:LYS:HD2	2.39	0.47
1:B:723:PHE:CZ	1:B:847:LYS:HE3	2.50	0.47
1:B:909:THR:OG1	1:B:910:ALA:N	2.47	0.47
1:A:267:GLU:O	1:A:271:LYS:HB2	2.15	0.47
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.96	0.47
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.12	0.47
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.50	0.47
1:B:335:ARG:HH21	1:B:551:LYS:NZ	2.13	0.47
1:B:905:LEU:O	1:B:906:SER:C	2.56	0.47
1:B:1279:ARG:HG3	1:B:1279:ARG:NH1	2.28	0.47
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.51	0.46
1:A:866:ASN:C	1:A:866:ASN:HD22	2.23	0.46
1:B:644:ASN:O	1:B:653:THR:HA	2.16	0.46
1:A:1270:VAL:O	1:A:1274:ILE:HG13	2.16	0.46
1:B:773:GLN:HG2	1:B:784:VAL:HG13	1.97	0.46
1:A:263:GLU:HB3	3:A:1337:FAD:H52A	1.96	0.46
1:A:416:GLU:OE1	1:A:439:ARG:HD2	2.16	0.46
1:B:401:GLU:OE2	1:B:401:GLU:N	2.39	0.46
1:B:660:VAL:HA	1:B:665:HIS:ND1	2.31	0.46
1:B:949:GLU:OE2	1:B:960:GLU:HA	2.16	0.46
1:B:1017:ALA:HB2	1:B:1085:ILE:HD12	1.96	0.46
1:A:403:ILE:C	1:A:403:ILE:HD12	2.39	0.46
1:A:955:PHE:CA	1:A:1145:ASN:HD21	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:LYS:HB3	1:A:1327:PRO:CD	2.46	0.46
1:B:272:ASN:CG	1:B:683:HIS:HE1	2.24	0.46
1:A:99:HIS:CE1	1:A:101:VAL:HG23	2.51	0.46
1:B:236:TRP:CD1	1:B:236:TRP:C	2.93	0.46
1:B:1206:PHE:CE1	1:B:1268:ALA:HB2	2.51	0.46
1:B:772:THR:O	1:B:776:VAL:HG23	2.16	0.46
1:A:99:HIS:CE1	1:A:100:PRO:HD2	2.50	0.45
1:B:255:ALA:HB1	1:B:279:ILE:HG13	1.97	0.45
1:B:700:ASP:HA	1:B:703:LYS:NZ	2.32	0.45
1:A:242:LEU:O	1:A:246:LEU:HG	2.16	0.45
1:A:885:MET:SD	1:A:896:GLY:HA3	2.56	0.45
1:A:1155:TYR:O	1:A:1180:MET:HE3	2.16	0.45
1:B:226:GLN:HB2	1:B:244:GLU:OE1	2.17	0.45
1:A:428:GLU:O	1:A:429:ASP:C	2.60	0.45
1:B:321:THR:O	1:B:328:ARG:NH2	2.49	0.45
1:A:342:VAL:HG23	10:A:1746:HOH:O	2.16	0.45
1:A:618:LYS:O	1:A:619:SER:HB3	2.17	0.45
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.16	0.45
1:A:104:ARG:HD2	1:A:163:PHE:CE1	2.51	0.45
1:A:350:GLY:C	3:A:1337:FAD:H5'1	2.42	0.45
1:A:646:THR:O	1:A:650:ASN:HA	2.16	0.45
1:B:144:GLN:HB2	1:B:339:GLY:HA2	1.99	0.45
1:B:541:THR:HA	1:B:990:GLU:O	2.17	0.45
1:B:992:CYS:O	1:B:1285:HIS:HE1	2.00	0.45
1:A:1042:LEU:O	1:A:1046:MET:HG2	2.17	0.45
1:B:195:LEU:HD22	1:B:1189:ALA:HA	1.99	0.45
1:B:1301:THR:O	1:B:1305:ILE:HG13	2.16	0.45
1:A:725:GLU:O	1:A:725:GLU:HG2	2.16	0.44
1:A:1312:LYS:HE3	1:A:1313:PHE:CZ	2.52	0.44
1:B:141:ASP:O	1:B:144:GLN:HG3	2.17	0.44
1:B:1045:LYS:O	1:B:1049:VAL:HG23	2.17	0.44
1:A:312:LEU:O	1:A:316:VAL:HG23	2.17	0.44
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.17	0.44
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.98	0.44
1:B:602:GLU:HG3	1:B:822:PRO:HB2	2.00	0.44
1:A:376:SER:HB3	1:A:402:GLU:HG2	1.99	0.44
1:A:703:LYS:NZ	1:A:704:ASN:HD21	2.16	0.44
1:B:440:VAL:HG13	1:B:440:VAL:O	2.17	0.44
1:B:1183:GLY:HA2	1:B:1247:CYS:O	2.18	0.44
1:B:721:LYS:C	1:B:721:LYS:HD2	2.43	0.44
1:B:1312:LYS:O	1:B:1316:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:HIS:HA	1:B:900:LEU:HD11	1.99	0.44
1:A:1108:ASN:N	1:A:1109:PRO:HD3	2.33	0.44
1:B:154:ARG:N	1:B:155:PRO:HD2	2.33	0.44
1:A:496:LEU:HB2	1:A:505:ILE:HG23	1.99	0.44
1:A:736:ILE:O	1:A:736:ILE:HG23	2.18	0.44
1:B:315:ALA:HA	1:B:318:LYS:NZ	2.31	0.44
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.44
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	0.44
1:A:736:ILE:HG13	1:A:1298:SER:HB3	2.00	0.43
1:B:519:PHE:O	1:B:523:VAL:HG23	2.18	0.43
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.00	0.43
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.48	0.43
1:A:779:MET:HG3	1:A:810:VAL:CG1	2.48	0.43
1:A:1281:ALA:O	1:A:1284:GLN:HB3	2.18	0.43
1:B:721:LYS:HD2	1:B:721:LYS:O	2.18	0.43
1:A:117:THR:CG2	1:A:586:ALA:HA	2.48	0.43
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.00	0.43
1:A:772:THR:O	1:A:776:VAL:HG23	2.19	0.43
1:A:226:GLN:HB2	1:A:244:GLU:OE1	2.18	0.43
1:A:383:VAL:HA	1:A:384:PRO:HD3	1.91	0.43
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.01	0.43
1:A:1000:ILE:HG23	1:A:1000:ILE:O	2.17	0.43
1:B:428:GLU:O	1:B:429:ASP:C	2.61	0.43
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.84	0.43
1:A:616:LYS:O	1:A:689:TYR:HA	2.18	0.43
1:B:59:ASP:O	1:B:63:ASP:N	2.51	0.43
1:B:762:LEU:N	1:B:762:LEU:HD12	2.32	0.43
1:B:779:MET:SD	1:B:779:MET:C	3.01	0.43
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.54	0.43
1:B:228:ARG:HG3	1:B:237:ILE:CD1	2.49	0.43
1:A:267:GLU:HA	1:A:271:LYS:HB2	1.99	0.43
1:B:113:CYS:HB3	1:B:150:CYS:SG	2.58	0.43
1:B:1008:SER:HA	1:B:1081:VAL:HG11	2.01	0.43
1:B:1253:ILE:O	1:B:1253:ILE:HG23	2.18	0.43
1:A:152:GLY:CA	1:A:1200:VAL:HG21	2.47	0.43
1:A:284:ILE:HA	1:A:285:PRO:HD3	1.88	0.43
1:A:522:THR:HG22	1:A:526:LYS:HE3	2.00	0.43
1:A:752:ILE:HD13	1:A:822:PRO:HB3	2.00	0.43
1:A:844:ALA:CB	1:A:922:ILE:HD13	2.47	0.43
1:B:731:SER:OG	1:B:847:LYS:HG3	2.19	0.43
1:B:866:ASN:C	1:B:866:ASN:HD22	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.67	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CE2	2.54	0.43
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.43	0.43
1:B:802:GLU:HG2	1:B:803:THR:HG23	2.01	0.43
1:B:1113:TRP:O	1:B:1117:VAL:HG23	2.19	0.43
1:B:217:LEU:O	1:B:220:LYS:HG2	2.19	0.42
1:B:247:ASP:O	1:B:251:GLN:HG3	2.19	0.42
1:B:366:MET:CE	1:B:387:HIS:HA	2.49	0.42
1:B:736:ILE:CG2	1:B:842:PHE:HB2	2.49	0.42
1:A:312:LEU:HB2	1:A:331:LEU:HD21	2.00	0.42
1:B:1042:LEU:O	1:B:1046:MET:HG2	2.19	0.42
1:A:37:ARG:HD2	1:A:595:ASP:O	2.19	0.42
1:A:58:TYR:CZ	1:A:220:LYS:HD2	2.54	0.42
1:A:868:GLY:HA3	1:A:907:SER:HA	2.02	0.42
1:A:59:ASP:O	1:A:63:ASP:N	2.50	0.42
1:A:331:LEU:O	1:A:335:ARG:HG3	2.19	0.42
1:A:606:ARG:HG2	1:A:679:GLU:HA	2.00	0.42
1:B:850:PHE:CD2	1:B:850:PHE:N	2.87	0.42
1:B:1259:VAL:HG22	1:B:1259:VAL:O	2.18	0.42
1:B:331:LEU:O	1:B:335:ARG:HG3	2.20	0.42
1:B:1012:PRO:HB2	10:B:1817:HOH:O	2.18	0.42
1:A:878:MET:O	1:A:881:ALA:HB3	2.19	0.42
1:A:911:PHE:C	10:A:1346:ZXF:S	3.03	0.42
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.55	0.42
1:B:747:HIS:ND1	1:B:805:SER:HA	2.35	0.42
1:A:102:GLN:NE2	1:A:587:SER:HA	2.35	0.42
1:A:909:THR:OG1	1:A:910:ALA:N	2.51	0.42
1:A:1007:ILE:HD12	1:A:1258:ALA:HB3	2.01	0.42
1:B:117:THR:HB	1:B:118:PRO:HD3	2.01	0.42
1:B:1031:VAL:HB	1:B:1063:ILE:HG12	2.01	0.42
1:A:912:ARG:N	10:A:1346:ZXF:S	2.93	0.42
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.19	0.42
1:B:407:ILE:HD12	1:B:407:ILE:N	2.35	0.42
1:A:393:TYR:CE2	1:A:394:ARG:HD2	2.55	0.42
1:A:1275:LYS:O	1:A:1279:ARG:HG3	2.20	0.42
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	2.02	0.42
1:B:272:ASN:CG	1:B:272:ASN:O	2.63	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.90	0.41
1:A:436:CYS:SG	1:A:438:MET:HE3	2.60	0.41
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	2.02	0.41
1:A:905:LEU:O	1:A:906:SER:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLN:O	1:B:63:ASP:C	2.62	0.41
1:B:712:LEU:HD21	1:B:879:GLU:HG3	2.02	0.41
1:B:952:LEU:HD23	1:B:958:ARG:HA	2.01	0.41
1:A:105:ILE:HA	10:A:1766:HOH:O	2.20	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD2	1.87	0.41
1:A:1199:PHE:CE1	1:A:1267:GLY:HA2	2.55	0.41
1:B:748:CYS:HB2	1:B:826:MET:HG3	2.02	0.41
1:B:926:TRP:O	1:B:930:VAL:HG23	2.20	0.41
1:A:721:LYS:HD2	1:A:721:LYS:O	2.21	0.41
1:A:1328:TRP:CE3	1:A:1329:SER:HB3	2.55	0.41
1:B:131:GLN:HE21	1:B:133:GLU:N	2.13	0.41
1:B:406:SER:C	1:B:407:ILE:HD12	2.45	0.41
1:B:429:ASP:OD1	3:B:1337:FAD:H6	2.20	0.41
1:A:676:GLU:CD	1:A:676:GLU:H	2.27	0.41
1:A:802:GLU:OE1	7:A:1344:SAL:H3	2.20	0.41
1:B:91:ILE:O	1:B:99:HIS:HB2	2.20	0.41
1:B:1078:ALA:HB1	10:B:1347:ZXF:O1	2.21	0.41
1:A:598:ARG:HG3	1:B:600:GLU:HG2	2.03	0.41
1:A:623:SER:HA	1:A:626:GLN:HE21	1.86	0.41
1:B:284:ILE:HA	1:B:285:PRO:HD3	1.91	0.41
1:B:430:ASP:CG	1:B:1228:LYS:HE2	2.46	0.41
1:A:252:HIS:HB3	1:A:254:GLU:OE2	2.21	0.41
1:B:5:GLU:OE2	1:B:18:LYS:HE2	2.21	0.41
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	2.03	0.41
1:A:468:LYS:HB2	1:A:493:GLU:CD	2.45	0.41
1:A:632:VAL:HB	1:A:671:VAL:O	2.21	0.41
1:B:1326:LYS:CG	1:B:1327:PRO:HD2	2.50	0.41
1:A:468:LYS:HB2	1:A:493:GLU:OE2	2.21	0.41
1:A:899:ARG:HA	1:A:899:ARG:HD2	1.91	0.41
1:A:1113:TRP:O	1:A:1117:VAL:HG23	2.21	0.41
1:B:605:LEU:HD23	1:B:606:ARG:N	2.36	0.41
1:B:604:PHE:O	1:B:671:VAL:HA	2.20	0.41
1:B:1318:VAL:CG2	1:B:1319:THR:N	2.83	0.41
1:A:471:GLN:HA	1:A:471:GLN:NE2	2.36	0.40
1:B:100:PRO:O	1:B:104:ARG:HG3	2.22	0.40
1:B:1286:THR:CG2	1:B:1287:ASN:N	2.78	0.40
1:A:482:LEU:HD23	1:A:482:LEU:C	2.46	0.40
1:A:887:ASN:OD1	1:A:1003:THR:HA	2.21	0.40
1:A:212:PHE:O	1:A:213:PRO:C	2.64	0.40
1:A:433:LYS:HA	1:A:433:LYS:HD3	1.91	0.40
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:HIS:ND1	1:A:805:SER:HA	2.37	0.40
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.20	0.40
1:B:64:LYS:CB	1:B:64:LYS:NZ	2.84	0.40
1:B:81:HIS:O	1:B:82:HIS:HB2	2.21	0.40
1:B:501:PRO:HD2	4:B:1338:NAI:C6A	2.51	0.40
1:A:925:ASN:O	1:A:929:GLU:HG3	2.21	0.40
1:B:32:ARG:NH2	1:B:676:GLU:OE2	2.54	0.40
1:B:271:LYS:HB2	1:B:273:GLN:HG2	2.02	0.40
1:B:152:GLY:O	1:B:1235:ILE:HG21	2.22	0.40
1:B:912:ARG:N	10:B:1347:ZXF:S	2.95	0.40
1:B:1021:ILE:HD12	1:B:1093:ALA:HB3	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	1281/1332 (96%)	1229 (96%)	46 (4%)	6 (0%)	24 27
1	B	1280/1332 (96%)	1228 (96%)	46 (4%)	6 (0%)	24 27
All	All	2561/2664 (96%)	2457 (96%)	92 (4%)	12 (0%)	24 27

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	429	ASP
1	A	912	ARG
1	B	429	ASP
1	B	912	ARG
1	B	1002	PRO

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Mol	Chain	Res	Type
1	A	797	GLY
1	A	1139	GLY
1	B	1139	GLY
1	A	213	PRO
1	B	797	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1092/1128 (97%)	1085 (99%)	7 (1%)	78	89
1	B	1092/1128 (97%)	1083 (99%)	9 (1%)	73	85
All	All	2184/2256 (97%)	2168 (99%)	16 (1%)	76	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ARG
1	A	569	LYS
1	A	686	LYS
1	A	721	LYS
1	A	743	TYR
1	A	1002	PRO
1	A	1326	LYS
1	B	64	LYS
1	B	348	LEU
1	B	403	ILE
1	B	538	LEU
1	B	569	LYS
1	B	743	TYR
1	B	1002	PRO
1	B	1072	PRO
1	B	1262	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
1	A	226	GLN
1	A	251	GLN
1	A	252	HIS
1	A	471	GLN
1	A	484	GLN
1	A	565	ASN
1	A	626	GLN
1	A	650	ASN
1	A	683	HIS
1	A	704	ASN
1	A	1088	GLN
1	A	1108	ASN
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1289	ASN
1	B	62	GLN
1	B	71	ASN
1	B	131	GLN
1	B	144	GLN
1	B	197	ASN
1	B	226	GLN
1	B	272	ASN
1	B	471	GLN
1	B	473	GLN
1	B	556	ASN
1	B	626	GLN
1	B	650	ASN
1	B	683	HIS
1	B	866	ASN
1	B	869	ASN
1	B	925	ASN
1	B	1088	GLN
1	B	1095	GLN
1	B	1122	GLN
1	B	1145	ASN
1	B	1220	HIS
1	B	1284	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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
5	GOL	B	1339	-	5,5,5	0.35	0	5,5,5	0.19	0
5	GOL	A	1342	-	5,5,5	0.47	0	5,5,5	0.40	0
5	GOL	A	1339	-	5,5,5	0.46	0	5,5,5	0.32	0
5	GOL	A	1341	-	5,5,5	0.41	0	5,5,5	0.36	0
10	ZXF	B	1347	-	24,31,31	3.64	9 (37%)	22,52,52	2.95	10 (45%)
3	FAD	B	1337	-	58,58,58	2.36	18 (31%)	85,89,89	2.04	23 (27%)
5	GOL	A	1340	-	5,5,5	0.26	0	5,5,5	0.13	0
3	FAD	A	1337	-	58,58,58	2.35	17 (29%)	85,89,89	2.01	20 (23%)
7	SAL	B	1345	-	10,10,10	2.08	5 (50%)	13,13,13	2.17	4 (30%)
2	FES	B	1333	1	0,4,4	-	-	-		
4	NAI	B	1338	-	47,48,48	1.28	7 (14%)	64,73,73	1.61	9 (14%)
2	FES	B	1334	1	0,4,4	-	-	-		
2	FES	A	1333	1	0,4,4	-	-	-		
5	GOL	B	1343	-	5,5,5	0.40	0	5,5,5	0.31	0
7	SAL	A	1344	-	10,10,10	2.05	5 (50%)	13,13,13	2.11	4 (30%)
4	NAI	A	1338	-	47,48,48	1.33	7 (14%)	64,73,73	1.63	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	1341	-	5,5,5	0.35	0	5,5,5	0.31	0
6	CO3	B	1344	-	3,3,3	0.34	0	2,3,3	0.05	0
10	ZXF	A	1346	-	24,31,31	3.45	8 (33%)	22,52,52	2.93	9 (40%)
2	FES	A	1334	1	0,4,4	-	-	-		
5	GOL	B	1342	-	5,5,5	0.39	0	5,5,5	0.28	0
5	GOL	B	1340	-	5,5,5	0.46	0	5,5,5	0.35	0
6	CO3	A	1343	-	3,3,3	0.17	0	2,3,3	0.23	0

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
5	GOL	B	1339	-	-	0/4/4/4	-
5	GOL	A	1342	-	-	2/4/4/4	-
5	GOL	A	1339	-	-	3/4/4/4	-
5	GOL	A	1341	-	-	2/4/4/4	-
10	ZXF	B	1347	-	-	1/6/46/46	0/4/4/4
3	FAD	B	1337	-	-	6/34/50/50	0/6/6/6
3	FAD	A	1337	-	-	6/34/50/50	0/6/6/6
7	SAL	B	1345	-	-	0/4/4/4	0/1/1/1
2	FES	B	1333	1	-	-	0/1/1/1
4	NAI	B	1338	-	-	7/29/72/72	0/5/5/5
2	FES	B	1334	1	-	-	0/1/1/1
2	FES	A	1333	1	-	-	0/1/1/1
5	GOL	B	1343	-	-	0/4/4/4	-
7	SAL	A	1344	-	-	0/4/4/4	0/1/1/1
4	NAI	A	1338	-	-	7/29/72/72	0/5/5/5
5	GOL	B	1341	-	-	3/4/4/4	-
10	ZXF	A	1346	-	-	1/6/46/46	0/4/4/4
2	FES	A	1334	1	-	-	0/1/1/1
5	GOL	B	1342	-	-	2/4/4/4	-
5	GOL	B	1340	-	-	0/4/4/4	-
5	GOL	A	1340	-	-	0/4/4/4	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1347	ZXF	C10-N8	11.06	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1346	ZXF	C10-N8	10.67	1.46	1.35
10	B	1347	ZXF	MO-S2'	-7.64	2.28	2.39
10	B	1347	ZXF	O4-C4	6.06	1.35	1.23
3	A	1337	FAD	C9A-N10	6.06	1.51	1.41
10	A	1346	ZXF	O4-C4	6.02	1.35	1.23
3	B	1337	FAD	C9A-N10	5.87	1.51	1.41
10	A	1346	ZXF	MO-S2'	-5.73	2.31	2.39
3	B	1337	FAD	C9A-C5X	5.48	1.50	1.41
3	A	1337	FAD	C9A-C5X	5.33	1.49	1.41
3	B	1337	FAD	C9-C9A	5.18	1.48	1.39
10	B	1347	ZXF	C9-C10	5.01	1.47	1.38
10	A	1346	ZXF	C9-C10	4.98	1.47	1.38
10	A	1346	ZXF	C9-N5	4.91	1.49	1.37
3	A	1337	FAD	C9-C9A	4.75	1.47	1.39
10	B	1347	ZXF	C9-N5	4.74	1.49	1.37
3	A	1337	FAD	C4A-N3A	4.58	1.43	1.34
10	A	1346	ZXF	O3'-C3'	4.46	1.52	1.43
3	B	1337	FAD	C4A-N3A	4.45	1.42	1.34
3	A	1337	FAD	C2A-N1A	4.43	1.41	1.33
3	A	1337	FAD	C5A-C4A	4.43	1.47	1.39
3	A	1337	FAD	O4B-C1B	4.41	1.52	1.42
3	B	1337	FAD	C5A-C4A	4.41	1.47	1.39
3	B	1337	FAD	C6-C5X	4.36	1.46	1.40
3	B	1337	FAD	C2A-N1A	4.32	1.41	1.33
10	B	1347	ZXF	O3'-C3'	4.30	1.51	1.43
3	B	1337	FAD	O4B-C1B	4.15	1.51	1.42
3	A	1337	FAD	O4B-C4B	4.07	1.54	1.45
10	A	1346	ZXF	O3'-C7	4.07	1.49	1.43
3	A	1337	FAD	C6-C5X	4.05	1.46	1.40
3	B	1337	FAD	C8-C7	4.03	1.50	1.40
3	A	1337	FAD	C8-C7	3.93	1.50	1.40
10	B	1347	ZXF	O3'-C7	3.81	1.49	1.43
3	B	1337	FAD	C10-N1	3.74	1.40	1.33
3	A	1337	FAD	C10-N1	3.72	1.40	1.33
3	A	1337	FAD	C4X-N5	3.64	1.38	1.30
3	B	1337	FAD	C4X-N5	3.57	1.38	1.30
3	B	1337	FAD	O4B-C4B	3.56	1.52	1.45
7	B	1345	SAL	C5-C6	3.50	1.44	1.38
7	A	1344	SAL	C5-C6	3.34	1.44	1.38
3	B	1337	FAD	C5A-C6A	3.28	1.50	1.41
3	A	1337	FAD	C2A-N3A	3.27	1.39	1.33
4	A	1338	NAI	C5A-N7A	-3.24	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1337	FAD	C5A-C6A	3.21	1.49	1.41
4	B	1338	NAI	C5A-N7A	-3.17	1.33	1.39
3	B	1337	FAD	C2A-N3A	3.14	1.39	1.33
4	A	1338	NAI	PA-O3	3.13	1.62	1.59
4	A	1338	NAI	C4N-C5N	-3.10	1.41	1.49
7	A	1344	SAL	C1-C1'	-3.07	1.43	1.49
3	A	1337	FAD	C2-N3	3.06	1.45	1.39
4	B	1338	NAI	C4N-C3N	3.06	1.55	1.50
4	B	1338	NAI	C4N-C5N	-2.95	1.41	1.49
3	B	1337	FAD	C2-N3	2.93	1.45	1.39
4	A	1338	NAI	C4N-C3N	2.92	1.55	1.50
10	B	1347	ZXF	C7-C6	2.71	1.55	1.53
4	B	1338	NAI	C6N-C5N	2.66	1.41	1.33
7	B	1345	SAL	C6-C1	2.62	1.43	1.39
7	B	1345	SAL	C1-C1'	-2.54	1.44	1.49
7	B	1345	SAL	C3-C2	2.51	1.43	1.39
7	A	1344	SAL	O2'-C1'	-2.50	1.23	1.30
4	A	1338	NAI	C6N-C5N	2.45	1.40	1.33
4	B	1338	NAI	PA-O3	2.44	1.62	1.59
7	A	1344	SAL	C6-C1	2.43	1.43	1.39
7	B	1345	SAL	O2'-C1'	-2.39	1.23	1.30
3	B	1337	FAD	C6-C7	2.38	1.42	1.39
4	A	1338	NAI	PN-O3	2.37	1.62	1.59
3	B	1337	FAD	C4X-C10	2.30	1.51	1.44
10	B	1347	ZXF	C2-N1	2.28	1.38	1.33
3	A	1337	FAD	C4X-C10	2.27	1.50	1.44
7	A	1344	SAL	C3-C2	2.22	1.43	1.39
4	B	1338	NAI	C7N-C3N	2.14	1.53	1.48
3	A	1337	FAD	C6A-N1A	2.13	1.41	1.35
4	B	1338	NAI	C6N-N1N	2.13	1.42	1.37
10	A	1346	ZXF	C2-N1	2.07	1.38	1.33
4	A	1338	NAI	C6N-N1N	2.07	1.42	1.37
3	B	1337	FAD	P-O3P	2.02	1.61	1.59

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1346	ZXF	C2-N1-C10	6.93	125.60	113.36
10	B	1347	ZXF	C2-N1-C10	6.87	125.48	113.36
3	A	1337	FAD	C9-C9A-N10	6.85	131.07	121.85
3	B	1337	FAD	C5X-C9A-N10	-6.80	111.82	117.97
3	B	1337	FAD	C9-C9A-N10	6.79	130.99	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1337	FAD	C5X-C9A-N10	-6.57	112.03	117.97
4	B	1338	NAI	N3A-C2A-N1A	-5.27	120.60	128.58
4	A	1338	NAI	N3A-C2A-N1A	-5.19	120.72	128.58
4	A	1338	NAI	C5A-C4A-N3A	-5.14	119.64	126.72
10	B	1347	ZXF	O4-C4-C9	-5.13	114.89	127.26
3	B	1337	FAD	C4-C4X-N5	4.96	125.06	118.21
10	A	1346	ZXF	O4-C4-C9	-4.95	115.33	127.26
4	B	1338	NAI	C5A-C4A-N3A	-4.93	119.93	126.72
3	A	1337	FAD	C4-C4X-N5	4.85	124.91	118.21
4	B	1338	NAI	O4D-C1D-N1N	-4.80	98.92	108.08
10	A	1346	ZXF	C7-C6-N5	4.75	112.53	107.87
3	A	1337	FAD	N3A-C2A-N1A	-4.71	121.45	128.58
4	A	1338	NAI	O4D-C1D-N1N	-4.68	99.16	108.08
3	B	1337	FAD	N3A-C2A-N1A	-4.63	121.58	128.58
3	B	1337	FAD	O4B-C1B-N9A	-4.44	99.57	108.09
10	B	1347	ZXF	C7-C6-N5	4.41	112.20	107.87
7	B	1345	SAL	O2'-C1'-O1'	-4.20	114.33	123.35
3	A	1337	FAD	O4B-C1B-N9A	-4.13	100.15	108.09
10	A	1346	ZXF	C4-C9-N5	4.08	127.39	116.27
7	A	1344	SAL	O2'-C1'-O1'	-3.99	114.77	123.35
10	A	1346	ZXF	N2-C2-N3	3.95	125.10	116.76
10	B	1347	ZXF	C4-C9-N5	3.87	126.82	116.27
10	B	1347	ZXF	N2-C2-N3	3.87	124.92	116.76
10	A	1346	ZXF	O3'-C7-C6	-3.83	106.41	108.96
4	A	1338	NAI	C2A-N3A-C4A	3.76	121.01	111.83
4	B	1338	NAI	C2A-N3A-C4A	3.74	120.95	111.83
4	A	1338	NAI	N3A-C4A-N9A	3.73	133.51	127.17
3	B	1337	FAD	C10-N1-C2	3.72	124.91	116.85
3	A	1337	FAD	C10-N1-C2	3.72	124.90	116.85
4	B	1338	NAI	N3A-C4A-N9A	3.70	133.46	127.17
10	B	1347	ZXF	O3'-C7-C6	-3.70	106.50	108.96
3	B	1337	FAD	C8M-C8-C7	3.67	128.25	120.76
10	B	1347	ZXF	N3-C2-N1	-3.63	116.69	123.32
3	A	1337	FAD	C8M-C8-C7	3.58	128.08	120.76
10	A	1346	ZXF	N3-C2-N1	-3.55	116.82	123.32
7	B	1345	SAL	C3-C2-C1	3.49	123.52	119.89
7	A	1344	SAL	C3-C2-C1	3.48	123.51	119.89
10	B	1347	ZXF	C9-C4-N3	3.41	121.49	112.13
10	A	1346	ZXF	C9-C4-N3	3.37	121.38	112.13
10	B	1347	ZXF	O4'-C4'-C3'	3.28	116.67	108.58
3	B	1337	FAD	C8M-C8-C9	-3.27	113.81	119.57
3	B	1337	FAD	C9A-N10-C10	3.20	125.63	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1344	SAL	C2-C1-C1'	3.19	123.28	120.00
7	B	1345	SAL	C2-C1-C1'	3.19	123.28	120.00
3	A	1337	FAD	C8M-C8-C9	-3.17	113.99	119.57
10	A	1346	ZXF	O4'-C4'-C3'	3.03	116.07	108.58
3	A	1337	FAD	C9A-N10-C10	2.93	125.21	120.75
4	A	1338	NAI	C5A-N7A-C8A	2.79	107.84	103.45
10	B	1347	ZXF	C2'-C1'-S1'	-2.76	118.58	120.15
4	B	1338	NAI	C5A-N7A-C8A	2.75	107.78	103.45
3	A	1337	FAD	C4'-C3'-C2'	-2.70	109.08	113.57
4	A	1338	NAI	C3N-C2N-N1N	-2.65	119.31	123.20
3	A	1337	FAD	O3'-C3'-C4'	2.65	114.94	108.93
4	B	1338	NAI	N9A-C8A-N7A	-2.65	110.18	113.94
7	B	1345	SAL	O2'-C1'-C1	2.63	122.75	115.28
3	B	1337	FAD	C2A-N3A-C4A	2.62	118.23	111.83
3	B	1337	FAD	C4'-C3'-C2'	-2.61	109.23	113.57
3	B	1337	FAD	O3B-C3B-C4B	-2.58	103.67	111.08
3	A	1337	FAD	C2A-N3A-C4A	2.58	118.13	111.83
4	A	1338	NAI	N9A-C8A-N7A	-2.58	110.28	113.94
4	A	1338	NAI	C4A-C5A-N7A	-2.54	107.68	110.58
7	A	1344	SAL	O2'-C1'-C1	2.52	122.45	115.28
3	B	1337	FAD	O3'-C3'-C4'	2.50	114.62	108.93
4	B	1338	NAI	C3N-C2N-N1N	-2.49	119.55	123.20
3	A	1337	FAD	C5X-N5-C4X	2.48	122.10	118.09
4	B	1338	NAI	C4A-C5A-N7A	-2.46	107.77	110.58
3	A	1337	FAD	O3B-C3B-C4B	-2.45	104.05	111.08
3	B	1337	FAD	N3A-C4A-N9A	2.43	131.30	127.17
3	B	1337	FAD	O4-C4-C4X	-2.43	120.13	126.53
3	A	1337	FAD	O4-C4-C4X	-2.41	120.17	126.53
3	B	1337	FAD	C1'-N10-C9A	-2.41	115.95	120.63
3	B	1337	FAD	C10-C4X-N5	-2.39	119.94	124.81
3	A	1337	FAD	C10-C4X-N5	-2.38	119.94	124.81
3	A	1337	FAD	C1'-N10-C9A	-2.32	116.12	120.63
3	B	1337	FAD	C5X-N5-C4X	2.32	121.84	118.09
3	A	1337	FAD	N3A-C4A-N9A	2.26	131.01	127.17
3	B	1337	FAD	O4B-C4B-C5B	-2.19	102.31	109.33
3	B	1337	FAD	C4X-C4-N3	2.15	118.72	113.25
3	A	1337	FAD	C4X-C4-N3	2.12	118.65	113.25
3	B	1337	FAD	C2A-N1A-C6A	2.09	122.17	118.73
3	B	1337	FAD	C5A-C4A-N3A	-2.09	123.83	126.72
3	B	1337	FAD	N9A-C8A-N7A	2.09	116.90	113.94
3	A	1337	FAD	C2A-N1A-C6A	2.05	122.09	118.73
4	A	1338	NAI	C2D-C1D-N1N	2.04	118.31	113.31

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1337	FAD	N10-C1'-C2'-O2'
3	A	1337	FAD	N10-C1'-C2'-C3'
3	B	1337	FAD	N10-C1'-C2'-O2'
3	B	1337	FAD	N10-C1'-C2'-C3'
5	A	1339	GOL	C1-C2-C3-O3
5	A	1341	GOL	O1-C1-C2-C3
5	B	1341	GOL	C1-C2-C3-O3
5	B	1342	GOL	C1-C2-C3-O3
3	A	1337	FAD	C2'-C3'-C4'-C5'
3	B	1337	FAD	C2'-C3'-C4'-C5'
3	A	1337	FAD	C2'-C3'-C4'-O4'
3	B	1337	FAD	C2'-C3'-C4'-O4'
5	B	1342	GOL	O2-C2-C3-O3
10	A	1346	ZXF	C3'-C4'-O4'-P
10	B	1347	ZXF	C3'-C4'-O4'-P
3	A	1337	FAD	O3'-C3'-C4'-O4'
3	B	1337	FAD	O3'-C3'-C4'-O4'
4	A	1338	NAI	C2D-C1D-N1N-C6N
3	A	1337	FAD	O3'-C3'-C4'-C5'
3	B	1337	FAD	O3'-C3'-C4'-C5'
4	A	1338	NAI	C2D-C1D-N1N-C2N
4	B	1338	NAI	C2D-C1D-N1N-C2N
4	B	1338	NAI	C2D-C1D-N1N-C6N
5	A	1339	GOL	O2-C2-C3-O3
5	A	1341	GOL	O1-C1-C2-O2
5	B	1341	GOL	O1-C1-C2-O2
5	B	1341	GOL	O2-C2-C3-O3
4	A	1338	NAI	PA-O3-PN-O5D
4	B	1338	NAI	PA-O3-PN-O5D
5	A	1339	GOL	O1-C1-C2-O2
5	A	1342	GOL	O2-C2-C3-O3
4	B	1338	NAI	O4D-C1D-N1N-C6N
4	A	1338	NAI	O4D-C1D-N1N-C2N
4	A	1338	NAI	O4D-C1D-N1N-C6N
4	B	1338	NAI	O4D-C1D-N1N-C2N
5	A	1342	GOL	C1-C2-C3-O3
4	A	1338	NAI	C2N-C3N-C7N-N7N
4	B	1338	NAI	C2N-C3N-C7N-N7N
4	A	1338	NAI	O4D-C4D-C5D-O5D
4	B	1338	NAI	O4D-C4D-C5D-O5D

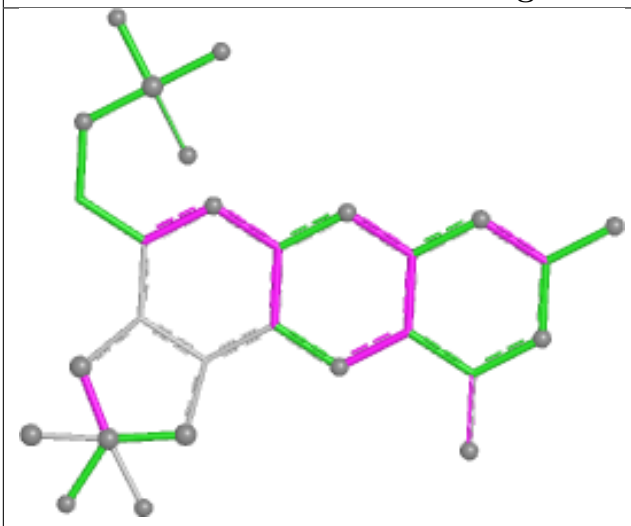
There are no ring outliers.

7 monomers are involved in 16 short contacts:

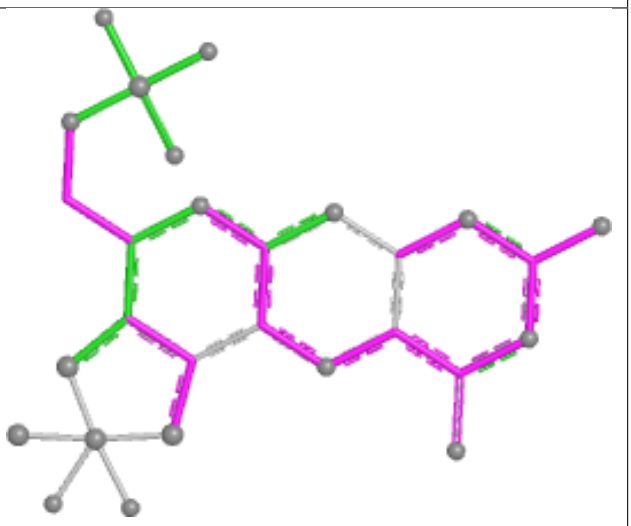
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1347	ZXF	4	0
3	B	1337	FAD	2	0
3	A	1337	FAD	3	0
4	B	1338	NAI	1	0
7	A	1344	SAL	1	0
10	A	1346	ZXF	4	0
5	B	1342	GOL	1	0

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.

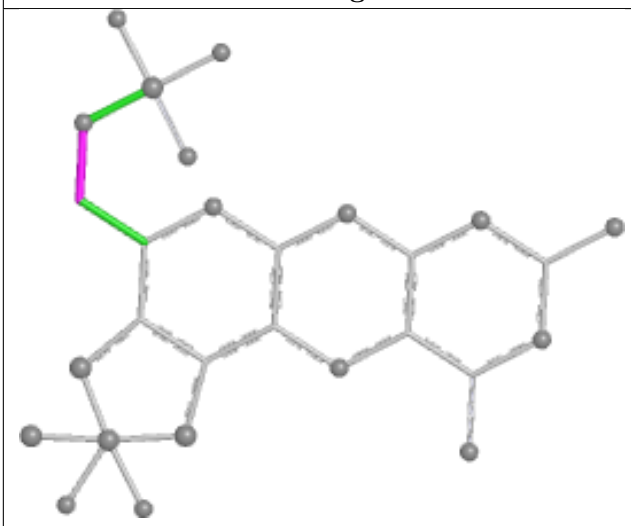
Ligand ZXF B 1347



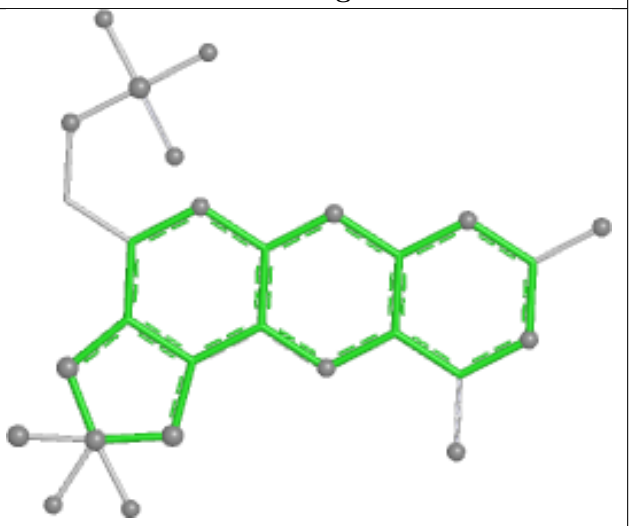
Bond lengths



Bond angles

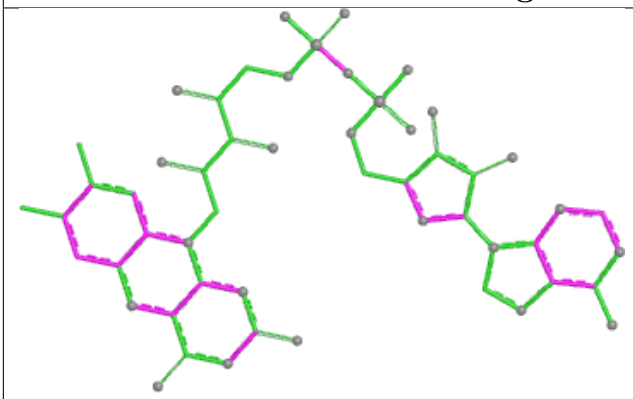


Torsions

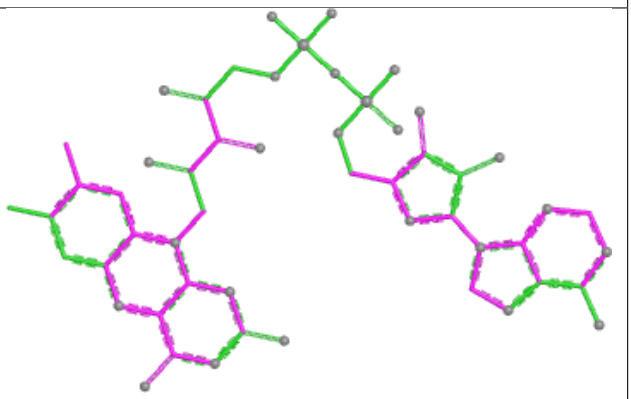


Rings

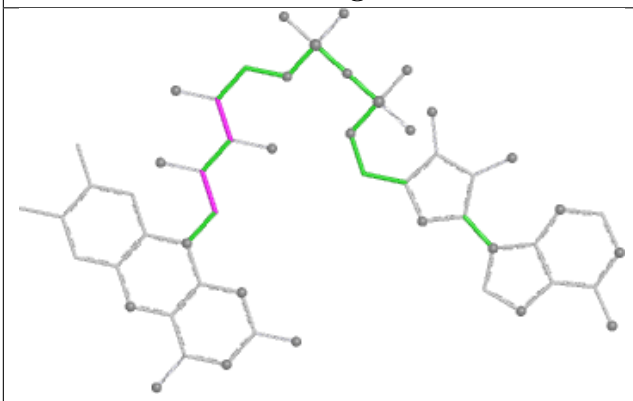
Ligand FAD B 1337



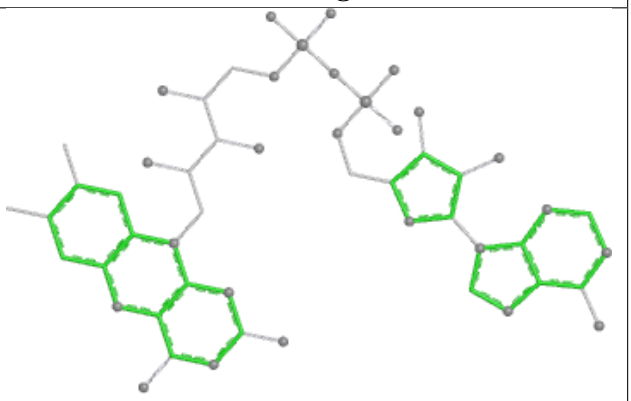
Bond lengths



Bond angles

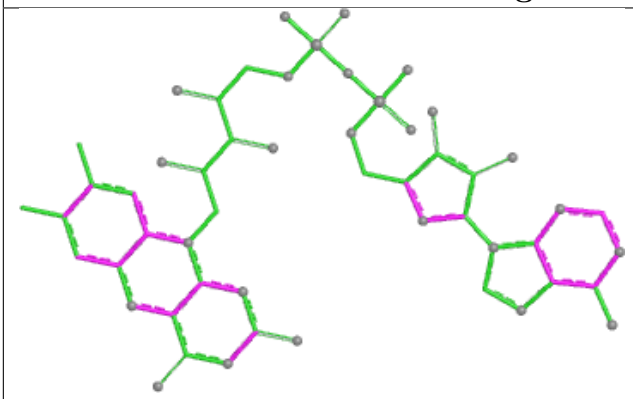


Torsions

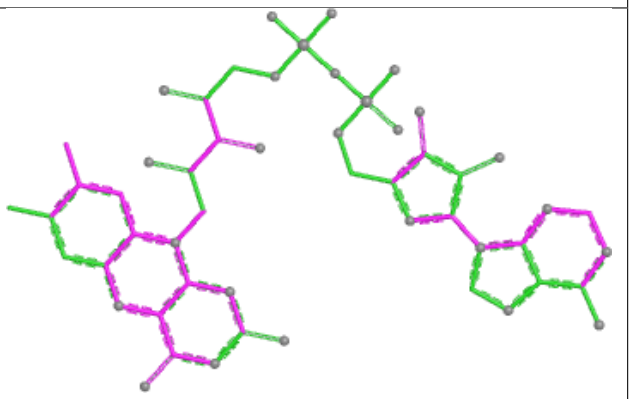


Rings

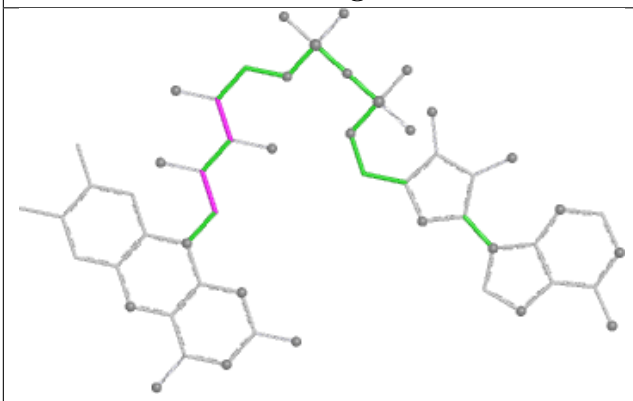
Ligand FAD A 1337



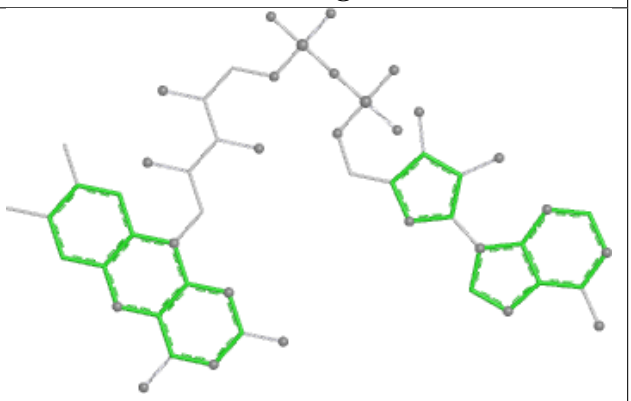
Bond lengths



Bond angles

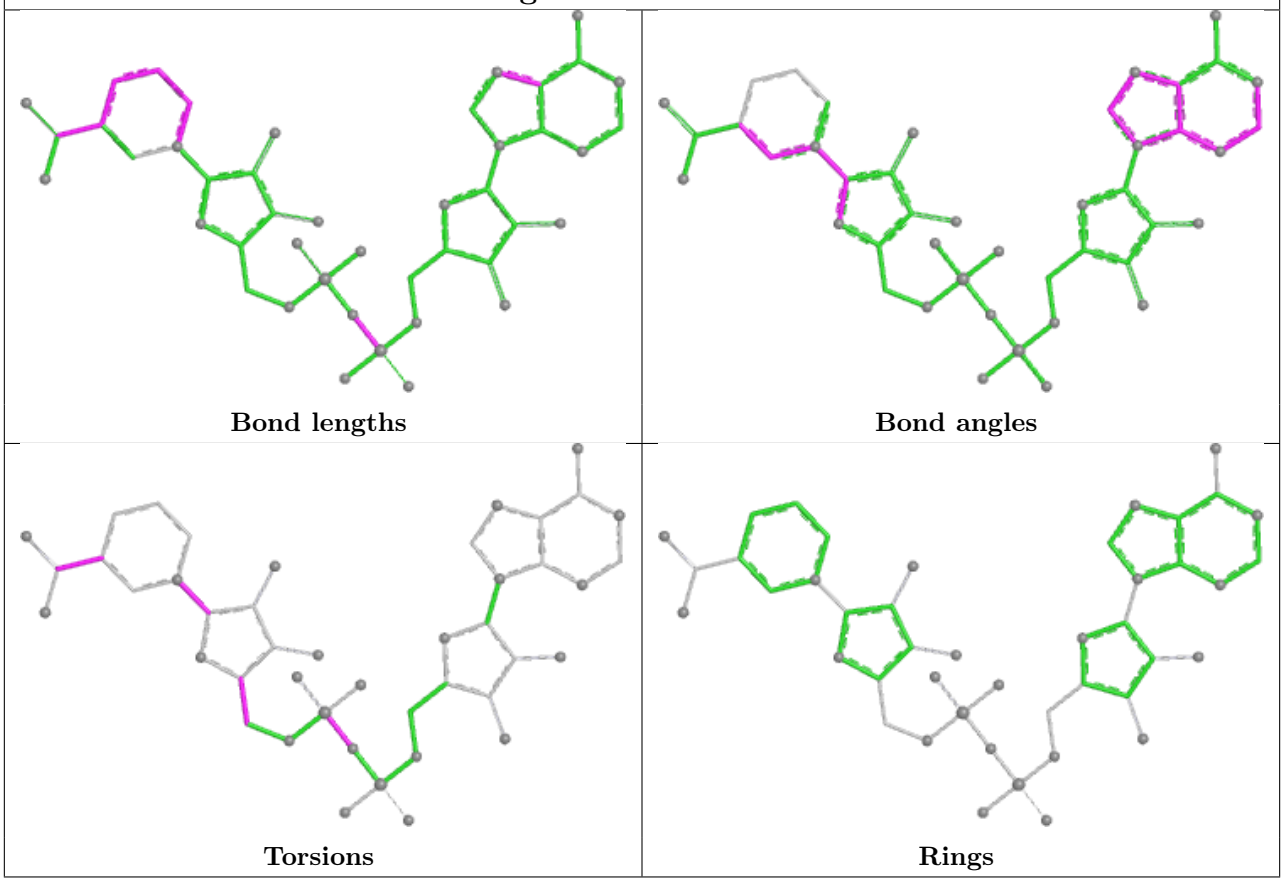


Torsions

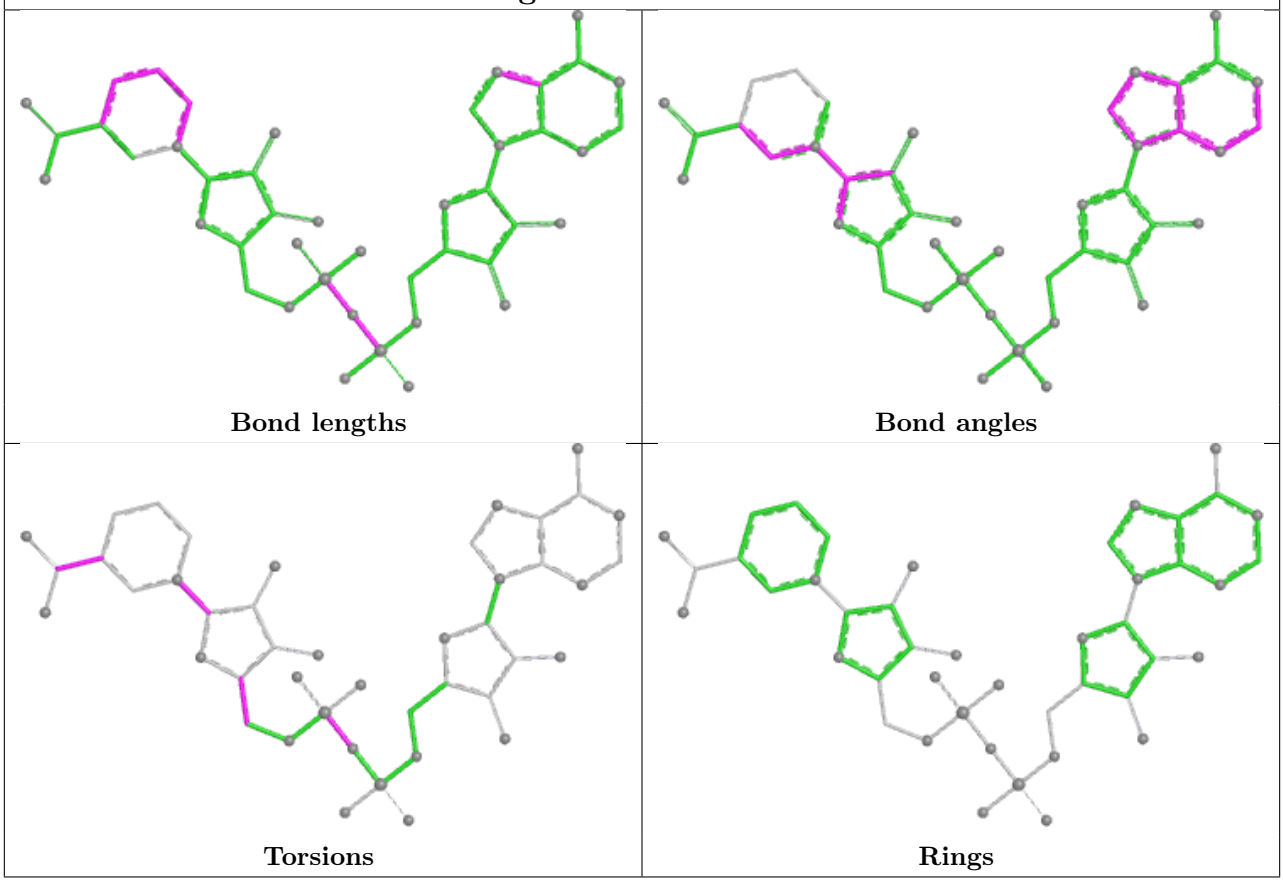


Rings

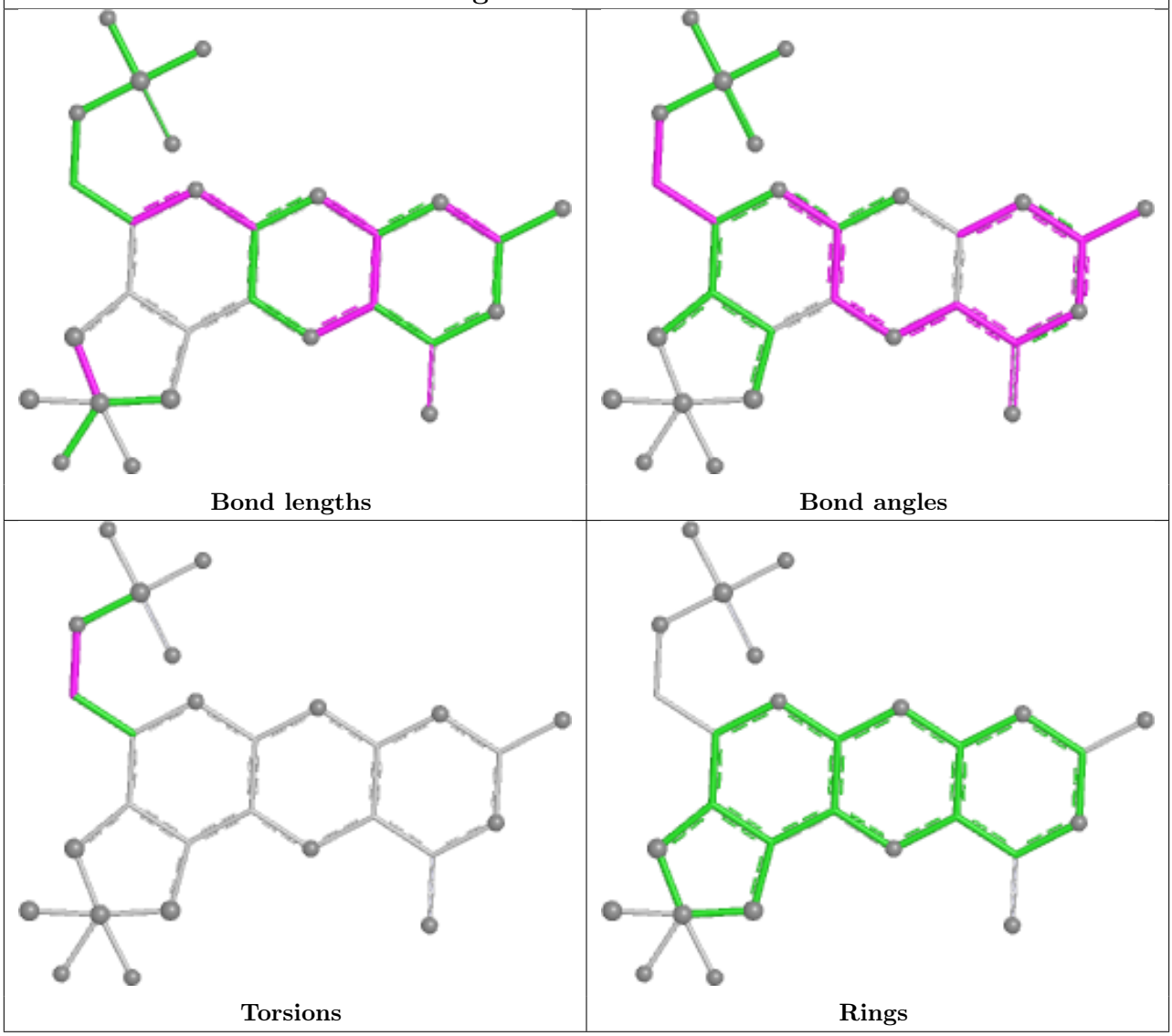
Ligand NAI B 1338



Ligand NAI A 1338



Ligand ZXF A 1346



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	1289/1332 (96%)	-0.23	16 (1%)	76	74	7, 22, 40, 65	0
1	B	1288/1332 (96%)	-0.21	13 (1%)	79	77	7, 23, 39, 65	0
All	All	2577/2664 (96%)	-0.22	29 (1%)	78	76	7, 22, 40, 65	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1286	THR	5.2
1	A	528	GLY	3.8
1	A	1320	GLY	3.8
1	B	1288	ASN	3.4
1	A	1318	VAL	3.3
1	A	566	GLY	3.2
1	B	1318	VAL	3.2
1	A	1288	ASN	3.2
1	B	1286	THR	3.2
1	A	565	ASN	3.1
1	B	1320	GLY	3.1
1	A	378	GLY	2.9
1	B	1287	ASN	2.9
1	B	719	LEU	2.6
1	A	379	THR	2.6
1	B	1290	THR	2.5
1	B	223	PRO	2.5
1	A	222	VAL	2.5
1	A	1290	THR	2.4
1	A	1289	ASN	2.3
1	A	703	LYS	2.3
1	A	1287	ASN	2.2
1	B	528	GLY	2.2
1	B	222	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1321	ALA	2.1
1	B	271	LYS	2.0
1	B	724	SER	2.0
1	A	223	PRO	2.0
1	B	248	LEU	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
5	GOL	A	1340	6/6	0.89	0.09	25,26,28,28	0
5	GOL	A	1342	6/6	0.90	0.11	28,30,31,34	0
5	GOL	A	1339	6/6	0.91	0.10	37,38,40,40	0
5	GOL	B	1339	6/6	0.91	0.10	22,23,25,25	0
7	SAL	B	1345	10/10	0.91	0.08	26,27,29,29	0
4	NAI	B	1338	44/44	0.92	0.09	16,23,27,31	0
4	NAI	A	1338	44/44	0.92	0.09	18,24,30,33	0
5	GOL	B	1340	6/6	0.93	0.09	25,29,29,33	0
5	GOL	B	1342	6/6	0.94	0.08	30,31,31,32	0
5	GOL	B	1343	6/6	0.94	0.07	30,33,35,38	0
5	GOL	A	1341	6/6	0.94	0.08	18,20,21,25	0
7	SAL	A	1344	10/10	0.95	0.06	17,21,23,25	0
5	GOL	B	1341	6/6	0.95	0.07	16,16,18,19	0
3	FAD	B	1337	53/53	0.96	0.07	16,20,24,26	0
3	FAD	A	1337	53/53	0.96	0.07	16,19,25,30	0
6	CO3	B	1344	4/4	0.97	0.05	12,13,14,16	0
6	CO3	A	1343	4/4	0.98	0.04	12,13,14,15	0
2	FES	B	1334	4/4	0.98	0.03	14,14,16,17	0

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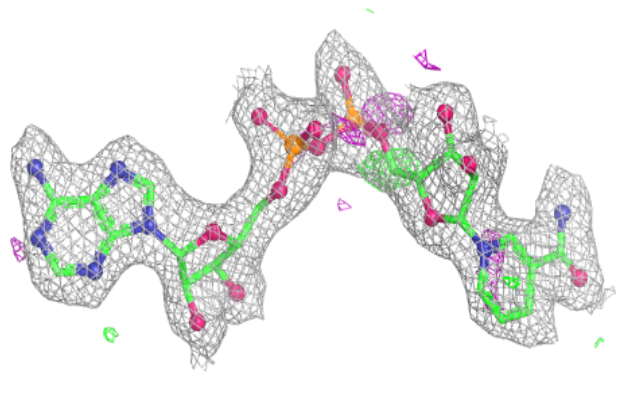
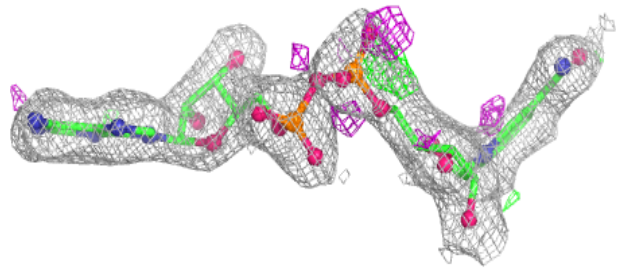
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FES	A	1333	4/4	0.99	0.02	12,13,13,13	0
2	FES	A	1334	4/4	0.99	0.03	14,15,16,17	0
2	FES	B	1333	4/4	0.99	0.03	11,11,12,13	0
8	CA	B	1346	1/1	0.99	0.02	21,21,21,21	0
10	ZXF	A	1346	28/28	0.99	0.05	9,16,23,28	0
10	ZXF	B	1347	28/28	0.99	0.05	12,18,22,29	0
8	CA	A	1345	1/1	1.00	0.01	17,17,17,17	0

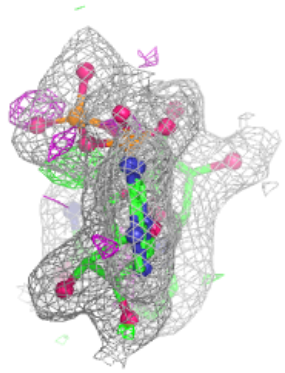
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI B 1338:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

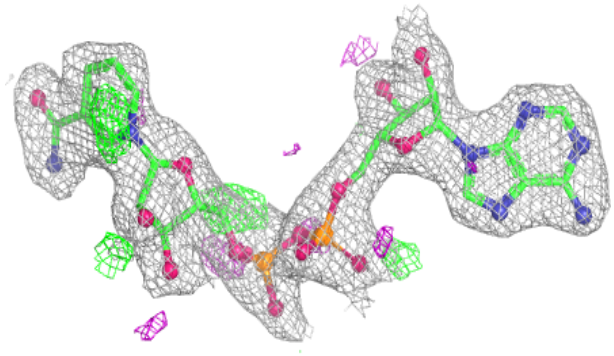


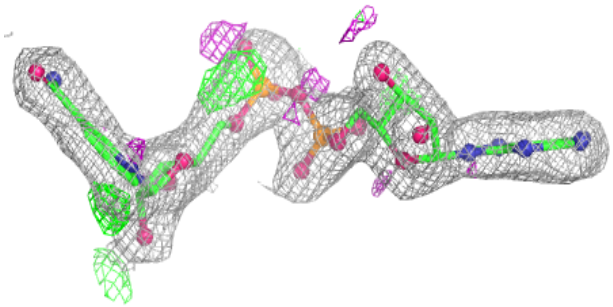


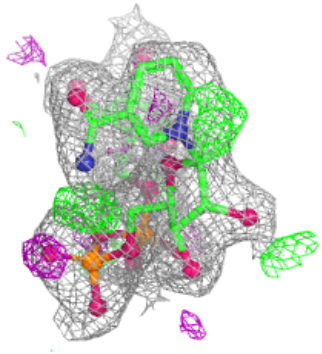


Electron density around NAI A 1338:

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

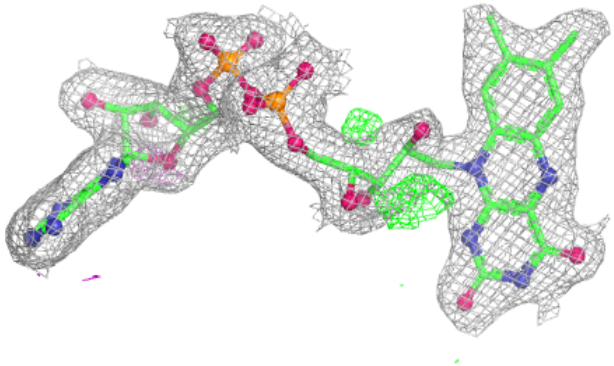


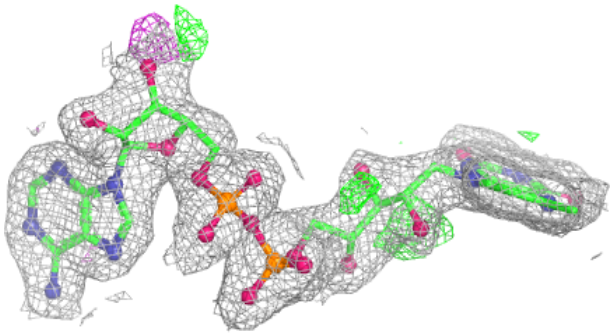


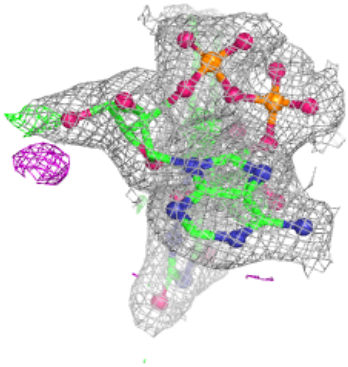


Electron density around FAD B 1337:

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

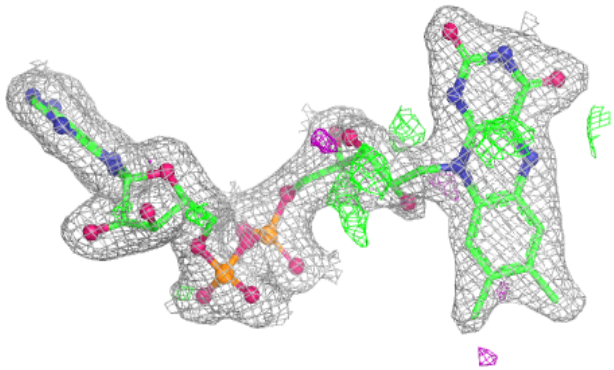


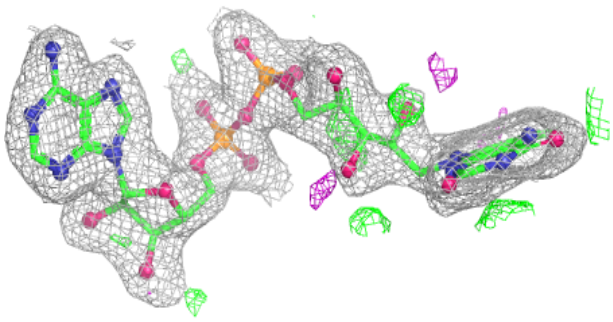


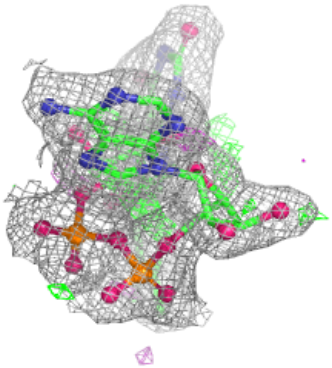


Electron density around FAD A 1337:

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

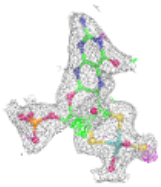






Electron density around ZXF A 1346:

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

Electron density around ZXF B 1347: $2mF_o$-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.