



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:34 PM GMT

PDB ID : 1VDV
Title : Bovine Milk Xanthine Dehydrogenase Y-700 Bound Form
Authors : Fukunari, A.; Okamoto, K.; Nishino, T.; Eger, B.T.; Pai, E.F.; Kamezawa, M.; Yamada, I.; Kato, N.
Deposited on : 2004-03-25
Resolution : 1.98 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

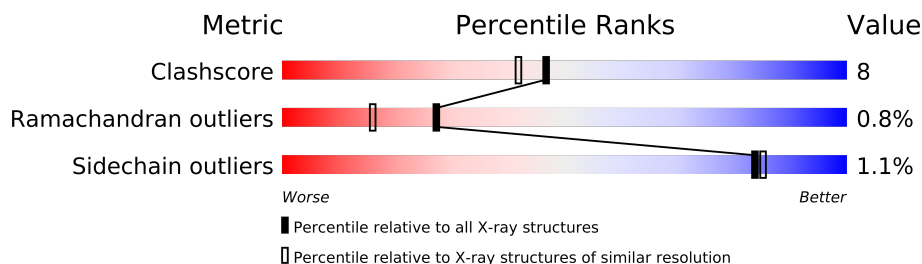
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.98 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))
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1332	
1	B	1332	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22610 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	1299	Total	C	N	O	S	0	0	0
			10077	6404	1728	1884	61			
1	B	1296	Total	C	N	O	S	0	0	0
			10054	6391	1724	1878	61			

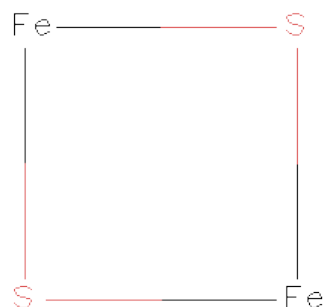
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P80457
B	1	MET	-	INITIATING METHIONINE	UNP P80457

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

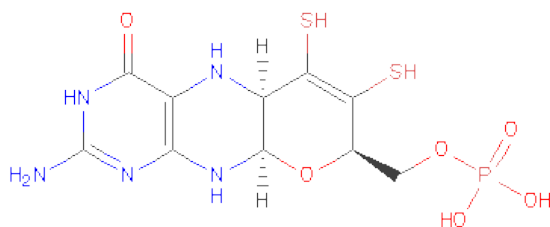
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



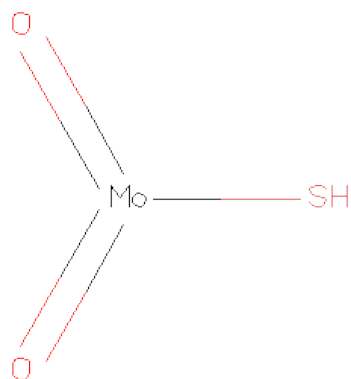
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



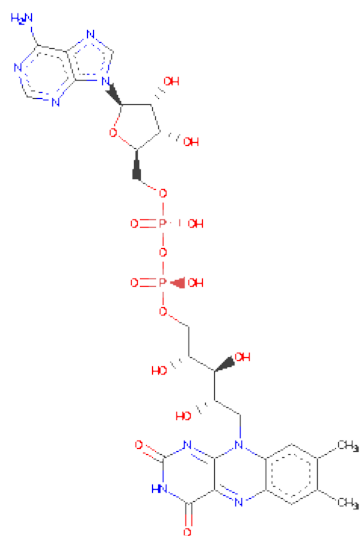
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI)ION (three-letter code: MOS) (formula: HMoO_2S).



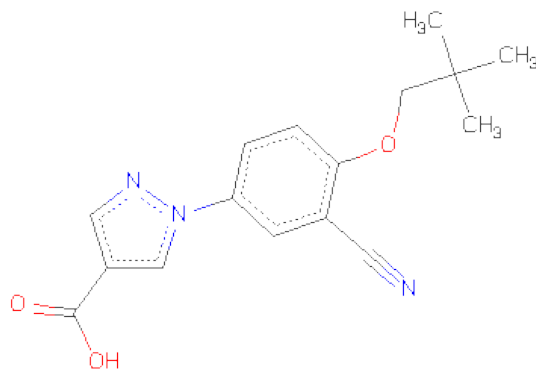
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 7 is 1-[3-CYANO-4-(NEOPENTYLOXY)PHENYL]-1H-PYRAZOLE-4-CARBOXYLICACID (three-letter code: YSH) (formula: C₁₆H₁₇N₃O₃).



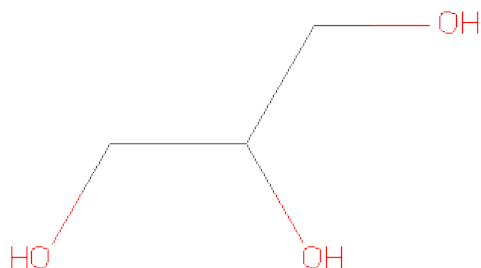
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			22	16	3	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			22	16	3	3		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



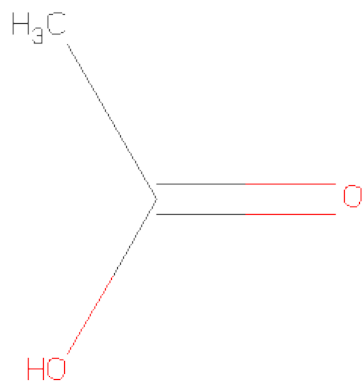
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total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

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

- Molecule 9 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1086	Total 1086	O 1086	0	0
10	B	1033	Total 1033	O 1033	0	0

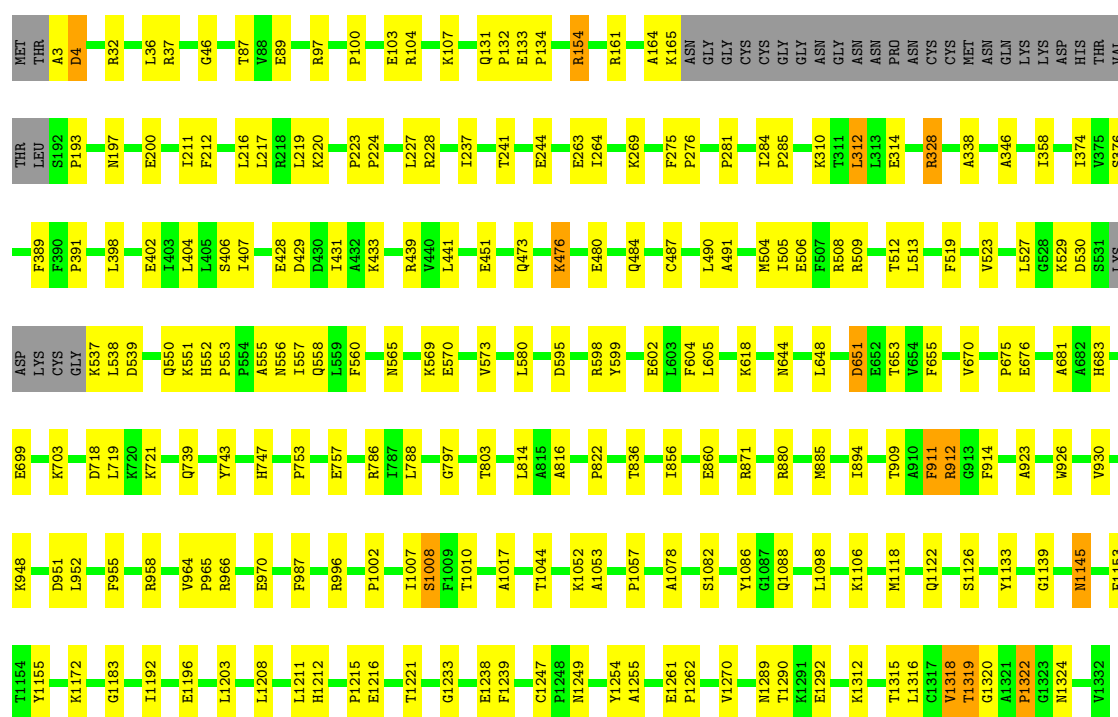
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

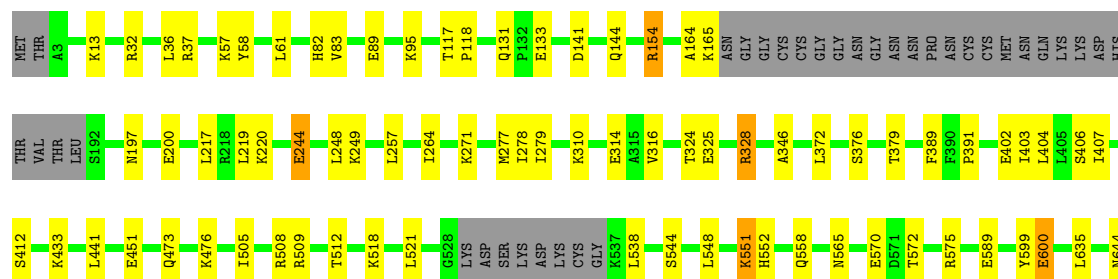
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:



L1316	G1087	R895	G896	T653	G897	T654	G898	F655	A656	K657	D658	E676	E699	L712	K713	L719	F723	A726	I736	Y743	H747	P753	E757	K778	R786	G797	L814	A815	A816	G817	K818	M826	T836	K847	V857	E860	R871	H875	R880					
G1317	Q1088	T896	L1088	N1108	P1109	F1132	Y1133	G1139	N1145	K1172	N1173	I1192	E1196	L952	F1199	L1203	T1221	T1226	P1236	T1237	E1238	F1239	N1249	A1255	E1261	P1262	G1267	A1281	Q1284	H1285	T1286	N1287	N1288	N1289	T1290	K1291	E1292	S1298	K1312					
V1318	T1319	G1320	A1321	P1322	G1323	N1324	C1325	K1326	V1332	R899	T909	A910	F911	R912	G913	F914	W926	Y930	K948	D951	L952	F955	R958	V964	P965	F987	C992	W993	K994	K995	R996	P1002	I1007	S1008	F1009	T1010	A1017	L1030	Q1048	A1053	P1057	A1078	S1082	Y1086

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.82Å 123.94Å 148.89Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	20.00 – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.178 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22610	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, YSH, MOS, CA, FES, ACY, FAD, MTE

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	0.32	0/10298	0.60	0/13939
1	B	0.31	0/10275	0.60	0/13909
All	All	0.32	0/20573	0.60	0/27848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10077	0	10076	172	0
1	B	10054	0	10053	155	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
4	A	24	0	10	1	0
4	B	24	0	10	1	0
5	A	4	0	0	1	0
5	B	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	53	0	31	4	0
6	B	53	0	31	3	0
7	A	22	0	16	3	0
7	B	22	0	16	3	0
8	A	66	0	88	8	0
8	B	60	0	80	8	0
9	A	4	0	3	4	0
9	B	4	0	3	4	0
10	A	1086	0	0	9	0
10	B	1033	0	0	7	0
All	All	22610	0	20417	331	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (331) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:B:5102:YSH:C1	7:B:5102:YSH:N2	1.70	1.52
7:A:5101:YSH:C1	7:A:5101:YSH:N2	1.68	1.51
1:A:3:ALA:HB1	1:A:228:ARG:H	1.20	1.06
1:A:537:LYS:HG2	1:A:538:LEU:H	1.28	0.98
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.30	0.97
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.32	0.94
1:A:439:ARG:HB3	1:A:439:ARG:HH11	1.32	0.93
1:A:131:GLN:HE21	1:A:133:GLU:H	1.14	0.90
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.36	0.89
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.56	0.87
1:A:1211:LEU:HA	1:A:1221:THR:HG21	1.57	0.86
1:B:404:LEU:HD21	1:B:407:ILE:HD11	1.57	0.86
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.57	0.84
1:A:3:ALA:HB1	1:A:228:ARG:N	1.93	0.83
1:B:131:GLN:HE21	1:B:133:GLU:H	1.26	0.83
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.15	0.82
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.45	0.80
1:B:551:LYS:NZ	1:B:551:LYS:HA	1.96	0.80
1:A:719:LEU:HD21	1:A:860:GLU:HG2	1.65	0.79
1:A:358:ILE:HD12	1:A:431:ILE:HG23	1.64	0.78
1:A:718:ASP:HB3	1:A:721:LYS:HE2	1.69	0.75
1:A:537:LYS:HG2	1:A:538:LEU:N	2.03	0.73
1:B:551:LYS:HZ2	1:B:552:HIS:H	1.32	0.73
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.71	0.73
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.25	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:551:LYS:HZ2	1:B:551:LYS:HA	1.54	0.70
1:A:1118:MET:O	1:A:1122:GLN:HG2	1.92	0.70
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.05	0.69
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.92	0.69
1:B:552:HIS:CE1	1:B:1172:LYS:HZ3	2.09	0.69
1:A:406:SER:C	1:A:407:ILE:HD12	2.13	0.68
1:A:264:ILE:HD11	6:A:3005:FAD:H3B	1.75	0.68
1:B:1078:ALA:HB1	5:B:4004:MOS:O1	1.94	0.68
1:A:217:LEU:O	1:A:220:LYS:HG2	1.93	0.68
1:A:911:PHE:H	9:A:5201:ACY:H3	1.59	0.67
1:B:376:SER:HB3	1:B:379:THR:OG1	1.95	0.66
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.76	0.66
1:B:719:LEU:HD11	1:B:895:ARG:HB2	1.78	0.66
1:A:948:LYS:HG2	1:A:951:ASP:OD2	1.95	0.65
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.97	0.65
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.96	0.65
1:A:538:LEU:HD12	8:A:5002:GOL:H31	1.77	0.65
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.32	0.65
1:A:428:GLU:OE2	1:A:1233:GLY:HA3	1.96	0.65
1:B:1312:LYS:O	1:B:1316:LEU:HD13	1.97	0.65
1:B:406:SER:O	1:B:407:ILE:HD12	1.97	0.65
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.79	0.65
1:A:131:GLN:HE21	1:A:133:GLU:N	1.92	0.64
1:A:439:ARG:HB3	1:A:439:ARG:NH1	2.09	0.64
1:B:551:LYS:HZ2	1:B:552:HIS:N	1.96	0.64
1:B:911:PHE:H	9:B:5202:ACY:H3	1.63	0.64
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.28	0.63
1:A:580:LEU:HD13	1:A:1044:THR:HG23	1.80	0.63
1:A:358:ILE:CD1	1:A:431:ILE:HG23	2.28	0.63
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.63	0.63
1:A:217:LEU:HD12	1:A:220:LYS:HD3	1.82	0.62
1:A:164:ALA:O	1:A:165:LYS:HB2	2.00	0.61
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.11	0.61
1:A:197:ASN:O	1:A:200:GLU:HG2	2.01	0.61
1:A:788:LEU:HB2	8:A:5011:GOL:H12	1.83	0.60
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.66	0.60
5:B:4004:MOS:O2	5:B:4004:MOS:MO	1.73	0.60
1:B:911:PHE:N	9:B:5202:ACY:H3	2.16	0.59
1:B:310:LYS:O	1:B:314:GLU:HG3	2.02	0.59
7:A:5101:YSH:C6	7:A:5101:YSH:C1	2.78	0.59
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.83	0.59
1:A:4:ASP:HB3	10:A:5928:HOH:O	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:439:ARG:CB	1:A:439:ARG:HH11	2.13	0.59
1:A:911:PHE:N	9:A:5201:ACY:H3	2.18	0.59
1:B:1318:VAL:HG22	1:B:1321:ALA:HB2	1.85	0.59
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.59
1:A:328:ARG:HG2	10:A:5679:HOH:O	2.03	0.59
1:A:966:ARG:O	1:A:970:GLU:HG3	2.02	0.58
1:B:570:GLU:OE2	1:B:1057:PRO:HG3	2.03	0.58
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.32	0.58
1:A:1010:THR:HG23	7:A:5101:YSH:O22	2.04	0.58
1:A:1203:LEU:HD13	1:A:1270:VAL:HG21	1.85	0.58
1:A:1172:LYS:HG3	8:A:5001:GOL:H31	1.87	0.57
1:B:1289:ASN:O	1:B:1290:THR:HB	2.05	0.57
1:B:372:LEU:HD23	1:B:407:ILE:HG13	1.86	0.57
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.05	0.57
1:A:914:PHE:HA	9:A:5201:ACY:H2	1.87	0.56
1:B:713:LYS:HD3	1:B:897:THR:HG22	1.88	0.56
1:B:473:GLN:O	1:B:476:LYS:HB2	2.05	0.56
1:B:346:ALA:HB1	6:B:4005:FAD:H4'	1.86	0.56
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.40	0.56
1:B:1326:LYS:HG3	10:B:5861:HOH:O	2.04	0.56
1:B:197:ASN:O	1:B:200:GLU:HG2	2.04	0.56
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.06	0.56
1:A:154:ARG:HD2	10:A:5453:HOH:O	2.06	0.56
1:A:1312:LYS:O	1:A:1316:LEU:HD23	2.06	0.56
1:A:651:ASP:CG	1:A:871:ARG:HH11	2.09	0.55
1:A:433:LYS:HE3	1:A:504:MET:SD	2.46	0.55
1:A:569:LYS:NZ	1:A:569:LYS:HB3	2.21	0.55
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.72	0.55
1:A:1318:VAL:HB	1:A:1322:PRO:HB3	1.88	0.55
1:B:404:LEU:HD21	1:B:407:ILE:CD1	2.33	0.55
1:B:1323:GLY:O	1:B:1325:CYS:N	2.41	0.54
1:A:1212:HIS:H	1:A:1221:THR:HG22	1.72	0.54
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.90	0.54
1:A:909:THR:O	9:A:5201:ACY:H1	2.08	0.54
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.08	0.54
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.90	0.53
1:A:269:LYS:HE3	10:A:6386:HOH:O	2.09	0.53
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.23	0.53
1:B:1010:THR:HG23	7:B:5102:YSH:O22	2.08	0.53
1:A:87:THR:HG1	1:A:89:GLU:HG2	1.74	0.53
1:B:1312:LYS:HG2	10:B:6326:HOH:O	2.10	0.52
1:B:909:THR:O	9:B:5202:ACY:H1	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1322:PRO:C	1:A:1324:ASN:H	2.12	0.52
1:A:473:GLN:O	1:A:476:LYS:HB2	2.09	0.52
1:A:599:TYR:HA	1:B:599:TYR:HA	1.91	0.52
1:A:131:GLN:NE2	1:A:133:GLU:H	1.96	0.52
1:B:521:LEU:HD22	1:B:538:LEU:HD11	1.91	0.52
1:B:551:LYS:HZ3	1:B:551:LYS:HA	1.73	0.52
1:B:264:ILE:HD11	6:B:4005:FAD:H3B	1.90	0.52
7:B:5102:YSH:C6	7:B:5102:YSH:C1	2.81	0.52
1:A:389:PHE:O	1:A:391:PRO:HD3	2.10	0.52
1:B:154:ARG:HD2	10:B:5493:HOH:O	2.08	0.52
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.13	0.52
1:A:1082:SER:HB2	4:A:3003:MTE:O3P	2.10	0.52
1:B:164:ALA:O	1:B:165:LYS:HB2	2.09	0.52
1:B:406:SER:C	1:B:407:ILE:HD12	2.30	0.51
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.93	0.51
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.11	0.51
1:A:537:LYS:CG	1:A:538:LEU:H	2.12	0.51
1:A:1078:ALA:HB1	5:A:3004:MOS:O1	2.09	0.51
1:B:376:SER:HB2	1:B:402:GLU:HG2	1.92	0.51
1:A:505:ILE:HD12	1:A:505:ILE:N	2.25	0.51
1:A:1318:VAL:HG12	1:A:1319:THR:H	1.76	0.51
1:B:548:LEU:HA	8:B:5022:GOL:H12	1.93	0.50
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.92	0.50
1:A:1319:THR:HG23	1:A:1320:GLY:N	2.26	0.50
1:B:723:PHE:CD2	1:B:847:LYS:HE2	2.47	0.50
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.12	0.50
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.11	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.47	0.50
1:A:480:GLU:O	1:A:484:GLN:HG3	2.11	0.50
1:B:914:PHE:HA	9:B:5202:ACY:H2	1.92	0.50
1:A:1318:VAL:HG12	1:A:1319:THR:N	2.26	0.50
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.94	0.50
1:A:1289:ASN:HD22	1:A:1292:GLU:HB2	1.77	0.50
1:A:161:ARG:HD3	10:A:5307:HOH:O	2.11	0.49
1:A:598:ARG:HG3	1:B:600:GLU:HG2	1.94	0.49
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.46	0.49
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.48	0.49
1:B:1172:LYS:HG3	8:B:5008:GOL:H31	1.95	0.49
1:B:551:LYS:CA	1:B:551:LYS:HZ2	2.23	0.49
1:B:58:TYR:CD2	1:B:220:LYS:HB2	2.47	0.49
1:B:165:LYS:NZ	1:B:165:LYS:HB2	2.27	0.49
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1007:ILE:O	1:A:1008:SER:CB	2.61	0.49
1:B:699:GLU:CD	1:B:699:GLU:H	2.14	0.49
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.48	0.49
1:A:237:ILE:N	1:A:237:ILE:HD12	2.28	0.49
1:A:644:ASN:O	1:A:653:THR:HA	2.13	0.49
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.78	0.49
1:A:856:ILE:N	1:A:856:ILE:HD12	2.27	0.49
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.48	0.49
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.95	0.49
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.47	0.48
1:A:1106:LYS:NZ	1:A:1106:LYS:HB3	2.27	0.48
1:B:1082:SER:HB2	4:B:4003:MTE:O3P	2.13	0.48
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.47	0.48
1:B:826:MET:HB3	8:B:5014:GOL:H31	1.94	0.48
1:B:1007:ILE:O	1:B:1008:SER:CB	2.61	0.48
1:A:508:ARG:O	1:A:512:THR:HG23	2.13	0.48
1:A:527:LEU:C	1:A:529:LYS:H	2.17	0.48
1:B:719:LEU:HD13	1:B:860:GLU:OE2	2.14	0.48
1:B:1323:GLY:O	1:B:1324:ASN:C	2.51	0.48
8:A:5011:GOL:O3	1:B:1030:LEU:HD22	2.14	0.48
1:A:346:ALA:HB1	6:A:3005:FAD:H4'	1.96	0.48
1:A:1318:VAL:HG21	1:A:1322:PRO:CB	2.44	0.48
1:B:726:ALA:HB2	1:B:857:VAL:CG2	2.44	0.48
1:A:211:ILE:HG12	1:A:212:PHE:N	2.29	0.48
1:B:1321:ALA:HB1	1:B:1322:PRO:CD	2.38	0.48
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.78	0.48
1:B:952:LEU:HD23	1:B:958:ARG:HA	1.94	0.48
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	1.96	0.47
1:A:310:LYS:O	1:A:314:GLU:HG3	2.14	0.47
1:A:604:PHE:HE2	8:A:5006:GOL:H31	1.79	0.47
1:B:433:LYS:HG3	10:B:5852:HOH:O	2.14	0.47
1:A:1215:PRO:HD2	1:A:1216:GLU:OE2	2.15	0.47
1:B:544:SER:HB2	1:B:994:LYS:HD2	1.97	0.47
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.95	0.47
1:A:529:LYS:O	1:A:530:ASP:HB2	2.14	0.47
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.45	0.47
1:A:1318:VAL:CB	1:A:1322:PRO:HB3	2.44	0.47
1:A:505:ILE:H	1:A:505:ILE:HD12	1.80	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.47
1:B:325:GLU:HB2	1:B:412:SER:HB3	1.96	0.47
1:B:1318:VAL:O	1:B:1320:GLY:N	2.47	0.47
1:A:885:MET:CE	1:A:894:ILE:HD11	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:987:PHE:CD2	1:A:996:ARG:HG3	2.50	0.47
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	1.96	0.46
1:A:926:TRP:O	1:A:930:VAL:HG23	2.14	0.46
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.80	0.46
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.20	0.46
1:B:736:ILE:O	1:B:736:ILE:HG23	2.16	0.46
1:B:994:LYS:HE3	8:B:5008:GOL:O2	2.15	0.46
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.51	0.46
1:B:217:LEU:O	1:B:220:LYS:HG2	2.15	0.46
1:A:1322:PRO:C	1:A:1324:ASN:N	2.68	0.46
1:B:1203:LEU:HD11	10:B:5736:HOH:O	2.14	0.46
1:B:117:THR:HB	1:B:118:PRO:HD3	1.97	0.46
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.86	0.46
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.16	0.46
1:B:726:ALA:HB2	1:B:857:VAL:HG21	1.98	0.46
1:A:648:LEU:HD11	1:A:803:THR:HG21	1.97	0.46
1:A:37:ARG:HD3	1:A:595:ASP:O	2.16	0.46
1:A:911:PHE:O	1:A:912:ARG:C	2.53	0.46
1:B:635:LEU:HD21	1:B:818:LYS:HG2	1.97	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.79	0.45
1:B:37:ARG:HD3	8:B:5013:GOL:O3	2.15	0.45
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.80	0.45
1:A:407:ILE:N	1:A:407:ILE:HD12	2.31	0.45
1:B:57:LYS:HE2	1:B:83:VAL:HG22	1.98	0.45
1:B:1221:THR:HG22	1:B:1226:THR:HB	1.98	0.45
1:A:602:GLU:HA	1:A:822:PRO:HG2	1.99	0.45
1:A:193:PRO:HG2	1:A:560:PHE:CZ	2.52	0.45
1:B:389:PHE:O	1:B:391:PRO:HD3	2.16	0.45
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.98	0.45
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.52	0.45
1:A:164:ALA:O	1:A:165:LYS:CB	2.64	0.45
1:B:736:ILE:HG13	1:B:1298:SER:HB3	1.99	0.45
1:B:987:PHE:CD2	1:B:996:ARG:HG3	2.52	0.45
1:A:605:LEU:C	1:A:605:LEU:HD23	2.37	0.45
1:B:508:ARG:O	1:B:512:THR:HG23	2.17	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.52	0.45
1:A:952:LEU:HD23	1:A:958:ARG:HA	2.00	0.44
1:A:699:GLU:H	1:A:699:GLU:CD	2.21	0.44
1:A:604:PHE:CE2	8:A:5006:GOL:H31	2.52	0.44
1:B:1324:ASN:O	1:B:1325:CYS:C	2.56	0.44
1:A:683:HIS:HA	8:A:5019:GOL:H12	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:573:VAL:HG21	1:A:1052:LYS:HD2	2.00	0.44
1:B:644:ASN:O	1:B:653:THR:HA	2.18	0.44
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.52	0.43
1:B:1088:GLN:HG3	10:B:5797:HOH:O	2.18	0.43
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.19	0.43
1:A:161:ARG:HH12	1:A:556:ASN:ND2	2.16	0.43
1:B:403:ILE:C	1:B:403:ILE:HD12	2.38	0.43
1:B:95:LYS:HG3	1:B:589:GLU:OE1	2.18	0.43
6:B:4005:FAD:HM73	10:B:5428:HOH:O	2.18	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.53	0.43
1:A:911:PHE:HD2	1:A:912:ARG:N	2.17	0.43
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.52	0.43
1:B:871:ARG:HH11	1:B:871:ARG:HG3	1.83	0.43
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.65	0.43
6:A:3005:FAD:HM73	10:A:5425:HOH:O	2.18	0.43
1:A:374:ILE:HG21	1:A:398:LEU:HD22	2.00	0.43
1:B:61:LEU:HD23	1:B:61:LEU:C	2.38	0.43
1:B:141:ASP:O	1:B:144:GLN:HG3	2.18	0.43
1:A:328:ARG:HG3	10:A:5888:HOH:O	2.17	0.43
1:A:651:ASP:OD1	1:A:871:ARG:NH1	2.52	0.43
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.19	0.43
1:A:487:CYS:HB3	1:A:513:LEU:HD13	2.00	0.43
1:B:955:PHE:CA	1:B:1145:ASN:HD21	2.20	0.43
1:A:1315:THR:O	1:A:1318:VAL:HG22	2.19	0.43
1:B:926:TRP:O	1:B:930:VAL:HG23	2.19	0.43
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.49	0.43
1:B:826:MET:H	8:B:5014:GOL:C3	2.30	0.43
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.53	0.43
1:A:1290:THR:HG22	1:A:1290:THR:O	2.19	0.43
1:B:82:HIS:NE2	1:B:219:LEU:HD13	2.33	0.43
1:B:948:LYS:HG2	1:B:951:ASP:CG	2.39	0.43
1:B:992:CYS:SG	1:B:1285:HIS:NE2	2.92	0.43
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.40	0.43
1:A:131:GLN:O	1:A:134:PRO:HD3	2.19	0.42
1:B:909:THR:OG1	1:B:910:ALA:N	2.51	0.42
1:A:100:PRO:O	1:A:104:ARG:HG3	2.19	0.42
1:A:216:LEU:HD23	1:A:219:LEU:HD12	2.00	0.42
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.19	0.42
1:B:1108:ASN:N	1:B:1109:PRO:HD3	2.34	0.42
1:B:753:PRO:HD3	1:B:816:ALA:HB1	2.01	0.42
1:A:491:ALA:O	1:A:509:ARG:NH2	2.52	0.42
1:B:257:LEU:HA	1:B:279:ILE:O	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:275:PHE:HA	1:A:276:PRO:HD2	1.91	0.42
1:B:719:LEU:HD11	1:B:895:ARG:HB3	2.00	0.42
1:B:249:LYS:HG3	1:B:403:ILE:CG2	2.50	0.42
1:B:572:THR:HA	1:B:575:ARG:HD2	2.01	0.42
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.19	0.42
1:A:519:PHE:O	1:A:523:VAL:HG23	2.20	0.42
1:A:651:ASP:OD2	1:A:871:ARG:HG3	2.19	0.42
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.19	0.42
1:A:103:GLU:HG3	1:A:107:LYS:HE2	2.02	0.42
1:A:703:LYS:HB3	1:A:703:LYS:NZ	2.35	0.42
1:A:46:GLY:HA2	3:A:3002:FES:S1	2.60	0.42
1:A:376:SER:HB3	1:A:402:GLU:HG2	2.02	0.42
1:B:473:GLN:NE2	1:B:473:GLN:HA	2.35	0.42
1:B:325:GLU:HB2	1:B:412:SER:CB	2.50	0.42
1:B:316:VAL:HA	1:B:324:THR:HG21	2.01	0.42
1:B:271:LYS:NZ	8:B:5020:GOL:H32	2.35	0.41
1:A:312:LEU:HA	1:A:312:LEU:HD12	1.89	0.41
1:B:551:LYS:NZ	1:B:552:HIS:H	2.09	0.41
1:B:217:LEU:HA	1:B:217:LEU:HD12	1.93	0.41
1:A:1319:THR:HG23	1:A:1320:GLY:H	1.85	0.41
1:B:518:LYS:HZ3	8:B:5022:GOL:C3	2.32	0.41
1:B:505:ILE:N	1:B:505:ILE:HD12	2.36	0.41
1:B:1325:CYS:O	1:B:1326:LYS:CB	2.67	0.41
1:A:1318:VAL:HG11	1:A:1322:PRO:HA	2.02	0.41
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.01	0.41
1:B:244:GLU:O	1:B:248:LEU:HG	2.19	0.41
1:B:13:LYS:C	1:B:13:LYS:HD3	2.41	0.41
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.67	0.41
1:B:552:HIS:HB2	1:B:1237:THR:HG21	2.03	0.41
1:A:1216:GLU:CD	1:A:1216:GLU:H	2.23	0.41
1:B:657:LYS:O	1:B:658:ASP:HB2	2.21	0.41
1:B:899:ARG:HD2	1:B:899:ARG:HA	1.87	0.41
1:A:1088:GLN:HG3	10:A:5686:HOH:O	2.19	0.41
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.36	0.41
1:B:1289:ASN:O	1:B:1290:THR:CB	2.69	0.41
1:B:992:CYS:HA	1:B:1284:GLN:HE21	1.86	0.41
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.79	0.40
1:B:1325:CYS:O	1:B:1326:LYS:HB3	2.20	0.40
1:A:433:LYS:HA	1:A:433:LYS:HD3	1.81	0.40
1:B:58:TYR:CZ	1:B:220:LYS:HD2	2.56	0.40
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.24	0.40
1:A:284:ILE:HA	1:A:285:PRO:HD2	1.91	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:712:LEU:HD21	1:B:875:HIS:CE1	2.56	0.40
1:A:1212:HIS:H	1:A:1221:THR:CG2	2.34	0.40
1:A:3:ALA:HA	1:A:227:LEU:HD23	2.04	0.40
1:A:539:ASP:H	8:A:5002:GOL:C3	2.35	0.40
1:A:556:ASN:O	1:A:557:ILE:HD13	2.21	0.40
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.57	0.40
1:A:490:LEU:HB2	1:A:513:LEU:CD2	2.52	0.40
1:A:551:LYS:HE3	10:A:6123:HOH:O	2.21	0.40
1:A:131:GLN:HA	1:A:132:PRO:HD2	1.95	0.40
1:A:263:GLU:HB2	6:A:3005:FAD:H52A	2.02	0.40
1:B:277:MET:HE3	1:B:278:ILE:N	2.35	0.40
1:A:506:GLU:CD	1:A:506:GLU:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	1293/1332 (97%)	1244 (96%)	41 (3%)	8 (1%)	33	23
1	B	1290/1332 (97%)	1234 (96%)	44 (3%)	12 (1%)	25	13
All	All	2583/2664 (97%)	2478 (96%)	85 (3%)	20 (1%)	27	16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	B	1008	SER
1	B	1287	ASN
1	B	1324	ASN
1	B	1326	LYS
1	A	1319	THR
1	B	244	GLU

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Mol	Chain	Res	Type
1	B	1325	CYS
1	A	912	ARG
1	A	1322	PRO
1	B	912	ARG
1	B	1139	GLY
1	B	1319	THR
1	A	797	GLY
1	A	1318	VAL
1	B	797	GLY
1	B	1322	PRO
1	B	1323	GLY
1	A	1139	GLY

5.3.2 Protein sidechains ⓘ

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	1101/1128 (98%)	1086 (99%)	15 (1%)	78	79
1	B	1098/1128 (97%)	1088 (99%)	10 (1%)	87	89
All	All	2199/2256 (98%)	2174 (99%)	25 (1%)	84	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ARG
1	A	281	PRO
1	A	312	LEU
1	A	328	ARG
1	A	476	LYS
1	A	550	GLN
1	A	565	ASN
1	A	618	LYS
1	A	651	ASP
1	A	743	TYR
1	A	911	PHE
1	A	1002	PRO
1	A	1145	ASN

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Mol	Chain	Res	Type
1	A	1208	LEU
1	A	1239	PHE
1	B	154	ARG
1	B	328	ARG
1	B	551	LYS
1	B	565	ASN
1	B	600	GLU
1	B	743	TYR
1	B	911	PHE
1	B	1002	PRO
1	B	1145	ASN
1	B	1239	PHE

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

Mol	Chain	Res	Type
1	A	131	GLN
1	A	252	HIS
1	A	272	ASN
1	A	351	ASN
1	A	471	GLN
1	A	473	GLN
1	A	550	GLN
1	A	556	ASN
1	A	565	ASN
1	A	626	GLN
1	A	650	ASN
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1289	ASN
1	A	1324	ASN
1	B	131	GLN
1	B	146	ASN
1	B	351	ASN
1	B	471	GLN
1	B	473	GLN
1	B	484	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	875	HIS

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Mol	Chain	Res	Type
1	B	976	GLN
1	B	1145	ASN
1	B	1284	GLN
1	B	1287	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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	$\# Z > 2$
3	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	A	3003	5	26,26,26	4.74	16 (61%)	34,40,40	3.43	17 (50%)
5	MOS	A	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	A	3005	-	58,58,58	2.35	20 (34%)	85,89,89	2.69	30 (35%)
8	GOL	A	5001	-	5,5,5	0.22	0	5,5,5	0.42	0
8	GOL	A	5002	-	5,5,5	0.16	0	5,5,5	0.37	0
8	GOL	A	5003	-	5,5,5	0.24	0	5,5,5	0.35	0
8	GOL	A	5004	-	5,5,5	0.21	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	5005	-	5,5,5	0.23	0	5,5,5	0.35	0
8	GOL	A	5006	-	5,5,5	0.15	0	5,5,5	0.44	0
8	GOL	A	5011	-	5,5,5	0.14	0	5,5,5	0.36	0
8	GOL	A	5016	-	5,5,5	0.19	0	5,5,5	0.51	0
8	GOL	A	5017	-	5,5,5	0.20	0	5,5,5	0.33	0
8	GOL	A	5018	-	5,5,5	0.28	0	5,5,5	0.29	0
8	GOL	A	5019	-	5,5,5	0.25	0	5,5,5	0.31	0
7	YSH	A	5101	-	23,23,23	6.69	14 (60%)	33,33,33	3.73	12 (36%)
9	ACY	A	5201	-	3,3,3	0.85	0	3,3,3	1.58	1 (33%)
3	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	B	4003	5	26,26,26	4.56	17 (65%)	34,40,40	4.19	18 (52%)
5	MOS	B	4004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	B	4005	-	58,58,58	2.47	24 (41%)	85,89,89	2.65	29 (34%)
8	GOL	B	5007	-	5,5,5	0.20	0	5,5,5	0.34	0
8	GOL	B	5008	-	5,5,5	0.17	0	5,5,5	0.40	0
8	GOL	B	5009	-	5,5,5	0.24	0	5,5,5	0.31	0
8	GOL	B	5012	-	5,5,5	0.15	0	5,5,5	0.46	0
8	GOL	B	5013	-	5,5,5	0.16	0	5,5,5	0.30	0
8	GOL	B	5014	-	5,5,5	0.14	0	5,5,5	0.40	0
8	GOL	B	5015	-	5,5,5	0.19	0	5,5,5	0.32	0
8	GOL	B	5020	-	5,5,5	0.18	0	5,5,5	0.35	0
8	GOL	B	5021	-	5,5,5	0.19	0	5,5,5	0.40	0
8	GOL	B	5022	-	5,5,5	0.16	0	5,5,5	0.37	0
7	YSH	B	5102	-	23,23,23	6.83	14 (60%)	33,33,33	3.71	12 (36%)
9	ACY	B	5202	-	3,3,3	0.94	0	3,3,3	1.52	1 (33%)

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
3	FES	A	3001	1	-	0/0/4/4	0/0/1/1
3	FES	A	3002	1	-	0/0/4/4	0/0/1/1
4	MTE	A	3003	5	-	0/6/34/34	0/0/3/3
5	MOS	A	3004	4	-	0/0/0/0	0/0/0/0
6	FAD	A	3005	-	-	0/34/50/50	0/1/6/6
8	GOL	A	5001	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5002	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5003	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	5004	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5005	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5006	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5011	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5016	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5017	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5018	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5019	-	-	0/4/4/4	0/0/0/0
7	YSH	A	5101	-	-	0/16/16/16	0/2/2/2
9	ACY	A	5201	-	-	0/0/0/0	0/0/0/0
3	FES	B	4001	1	-	0/0/4/4	0/0/1/1
3	FES	B	4002	1	-	0/0/4/4	0/0/1/1
4	MTE	B	4003	5	-	0/6/34/34	0/0/3/3
5	MOS	B	4004	4	-	0/0/0/0	0/0/0/0
6	FAD	B	4005	-	-	0/34/50/50	0/1/6/6
8	GOL	B	5007	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5008	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5009	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5012	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5013	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5014	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5015	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5020	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5021	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5022	-	-	0/4/4/4	0/0/0/0
7	YSH	B	5102	-	-	0/16/16/16	0/2/2/2
9	ACY	B	5202	-	-	0/0/0/0	0/0/0/0

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	5102	YSH	C1-N2	21.26	1.70	1.36
7	A	5101	YSH	C1-N2	20.58	1.68	1.36
7	B	5102	YSH	C11-C6	14.26	1.62	1.38
7	A	5101	YSH	C11-C6	14.18	1.62	1.38
4	A	3003	MTE	C9-C10	13.70	1.61	1.41
4	B	4003	MTE	C9-C10	13.68	1.61	1.41
7	B	5102	YSH	C1-C5	13.61	1.71	1.37
7	A	5101	YSH	C1-C5	13.42	1.71	1.37
7	B	5102	YSH	C10-C9	8.52	1.57	1.39
4	A	3003	MTE	C7-C6	8.50	1.68	1.53
7	A	5101	YSH	C10-C9	8.30	1.57	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4003	MTE	C7-C6	8.30	1.68	1.53
6	B	4005	FAD	C1'-C2'	7.47	1.58	1.51
4	A	3003	MTE	C9-N5	7.19	1.62	1.38
4	B	4003	MTE	C9-N5	7.07	1.61	1.38
6	A	3005	FAD	C1'-C2'	6.88	1.58	1.51
4	A	3003	MTE	C6-N5	-6.48	1.36	1.45
4	B	4003	MTE	P-O4'	-6.42	1.37	1.60
6	A	3005	FAD	C9A-N10	6.37	1.48	1.38
6	B	4005	FAD	C9A-N10	6.35	1.48	1.38
4	A	3003	MTE	P-O4'	-6.26	1.38	1.60
7	B	5102	YSH	C6-N2	6.04	1.55	1.43
4	B	4003	MTE	C6-C1'	-5.74	1.42	1.50
4	A	3003	MTE	C6-C1'	-5.68	1.42	1.50
7	A	5101	YSH	C6-N2	5.59	1.54	1.43
7	A	5101	YSH	C8-C12	5.58	1.53	1.44
4	A	3003	MTE	C2-N1	5.56	1.40	1.33
7	B	5102	YSH	C8-C12	5.41	1.53	1.44
7	A	5101	YSH	O22-C20	5.40	1.39	1.23
6	A	3005	FAD	C10-N1	5.37	1.45	1.35
7	B	5102	YSH	O22-C20	5.31	1.39	1.23
4	B	4003	MTE	P-O3P	-5.28	1.35	1.54
4	A	3003	MTE	P-O3P	-5.22	1.35	1.54
6	B	4005	FAD	C10-N1	5.07	1.44	1.35
4	B	4003	MTE	C3'-C2'	4.96	1.60	1.51
4	B	4003	MTE	C2-N1	4.95	1.39	1.33
4	A	3003	MTE	C3'-C2'	4.62	1.59	1.51
6	B	4005	FAD	C4-N3	4.52	1.44	1.37
7	B	5102	YSH	O14-C9	4.45	1.46	1.37
6	A	3005	FAD	C4-N3	4.39	1.44	1.37
6	B	4005	FAD	C1'-N10	4.38	1.53	1.48
6	B	4005	FAD	C10-N10	4.06	1.47	1.38
7	A	5101	YSH	O14-C9	4.04	1.45	1.37
4	B	4003	MTE	C4'-C3'	-4.03	1.45	1.52
4	A	3003	MTE	C4'-C3'	-3.88	1.46	1.52
6	A	3005	FAD	C1'-N10	3.76	1.52	1.48
6	A	3005	FAD	C10-N10	3.68	1.46	1.38
6	B	4005	FAD	C4A-N3A	3.65	1.41	1.35
4	A	3003	MTE	O4-C4	3.51	1.31	1.24
4	B	4003	MTE	C4-C9	3.45	1.47	1.41
6	A	3005	FAD	C4A-N3A	3.42	1.40	1.35
4	A	3003	MTE	C4-C9	3.41	1.47	1.41
6	B	4005	FAD	C5X-N5	3.24	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4005	FAD	C9A-C5X	3.17	1.49	1.42
6	B	4005	FAD	C6-C5X	3.14	1.45	1.41
4	B	4003	MTE	C6-N5	-3.14	1.40	1.45
6	A	3005	FAD	C6-C5X	3.13	1.45	1.41
4	B	4003	MTE	O4-C4	3.12	1.30	1.24
4	A	3003	MTE	O4'-C4'	-3.07	1.32	1.44
6	B	4005	FAD	O4B-C1B	3.07	1.46	1.41
6	B	4005	FAD	C9-C9A	3.06	1.46	1.40
6	A	3005	FAD	O4B-C1B	3.03	1.46	1.41
6	B	4005	FAD	C2-N3	3.03	1.43	1.37
6	B	4005	FAD	C4X-C10	3.02	1.46	1.40
7	B	5102	YSH	C4-N3	3.01	1.40	1.33
6	A	3005	FAD	C2-N3	2.98	1.43	1.37
6	A	3005	FAD	C5X-N5	2.96	1.39	1.35
6	A	3005	FAD	C9-C9A	2.96	1.46	1.40
7	B	5102	YSH	C7-C6	2.93	1.42	1.38
7	A	5101	YSH	C4-N3	2.92	1.39	1.33
7	B	5102	YSH	O14-C15	2.88	1.53	1.43
6	A	3005	FAD	C4X-C10	2.86	1.45	1.40
6	B	4005	FAD	C6-C7	2.81	1.45	1.37
7	A	5101	YSH	O14-C15	2.80	1.53	1.43
7	A	5101	YSH	C7-C6	2.79	1.42	1.38
6	A	3005	FAD	C9A-C5X	2.74	1.48	1.42
7	A	5101	YSH	C11-C10	-2.74	1.33	1.38
6	B	4005	FAD	C2A-N3A	2.70	1.37	1.32
6	A	3005	FAD	C6-C7	2.67	1.45	1.37
6	A	3005	FAD	C2A-N1A	2.66	1.39	1.33
6	A	3005	FAD	C4A-N9A	-2.64	1.33	1.37
4	B	4003	MTE	C10-N8	2.63	1.40	1.35
4	A	3003	MTE	C10-N8	2.62	1.40	1.35
6	A	3005	FAD	C2A-N3A	2.61	1.37	1.32
6	B	4005	FAD	C4A-N9A	-2.61	1.33	1.37
6	B	4005	FAD	C8-C7	2.61	1.48	1.40
6	A	3005	FAD	C8-C7	2.59	1.48	1.40
4	A	3003	MTE	C1'-S1'	-2.50	1.65	1.74
6	B	4005	FAD	C2A-N1A	2.50	1.38	1.33
7	B	5102	YSH	O21-C20	-2.47	1.22	1.30
4	B	4003	MTE	C1'-S1'	-2.47	1.65	1.74
6	B	4005	FAD	C5'-C4'	2.46	1.55	1.51
7	A	5101	YSH	O21-C20	-2.46	1.22	1.30
6	B	4005	FAD	C4'-C3'	2.36	1.58	1.53
4	B	4003	MTE	O3'-C3'	2.25	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3003	MTE	P-O2P	-2.21	1.46	1.54
4	B	4003	MTE	P-O2P	-2.19	1.46	1.54
7	B	5102	YSH	C8-C9	2.18	1.44	1.40
6	B	4005	FAD	C2'-C3'	2.17	1.58	1.53
7	A	5101	YSH	C8-C9	2.08	1.44	1.40
7	B	5102	YSH	C11-C10	-2.07	1.34	1.38
4	B	4003	MTE	C2'-C1'	2.06	1.48	1.35
6	A	3005	FAD	C4'-C3'	2.04	1.57	1.53
6	B	4005	FAD	C2-N1	2.02	1.41	1.35
6	B	4005	FAD	P-O1P	2.01	1.59	1.51

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	5102	YSH	C4-N3-N2	15.05	114.44	103.70
7	A	5101	YSH	C4-N3-N2	14.56	114.09	103.70
6	A	3005	FAD	N3A-C2A-N1A	-13.20	117.67	128.71
6	B	4005	FAD	N3A-C2A-N1A	-13.04	117.81	128.71
7	A	5101	YSH	C6-N2-N3	11.21	128.73	118.87
4	B	4003	MTE	P-O4'-C4'	10.59	148.82	118.19
7	B	5102	YSH	C6-N2-N3	10.55	128.15	118.87
4	B	4003	MTE	C4'-C3'-C2'	8.82	121.38	110.98
4	B	4003	MTE	O3'-C3'-C4'	-8.57	86.71	108.81
6	B	4005	FAD	C1'-N10-C9A	8.17	126.81	118.87
6	A	3005	FAD	C1'-N10-C9A	8.08	126.73	118.87
4	A	3003	MTE	C4-C9-N5	7.65	130.22	119.10
4	B	4003	MTE	C4-C9-N5	7.46	129.94	119.10
6	A	3005	FAD	C4X-N5-C5X	7.14	124.71	116.69
6	B	4005	FAD	C4X-N5-C5X	7.06	124.62	116.69
4	B	4003	MTE	C2-N1-C10	7.01	127.58	117.61
6	B	4005	FAD	C2-N1-C10	6.81	121.85	114.98
4	A	3003	MTE	C2-N1-C10	6.75	127.21	117.61
7	A	5101	YSH	C5-C1-N2	-6.72	90.97	108.85
7	B	5102	YSH	C5-C1-N2	-6.69	91.05	108.85
4	A	3003	MTE	N8-C10-N1	6.48	126.68	116.51
6	A	3005	FAD	C2-N1-C10	6.43	121.45	114.98
4	A	3003	MTE	P-O4'-C4'	6.41	136.73	118.19
4	B	4003	MTE	N8-C10-N1	6.37	126.50	116.51
4	B	4003	MTE	C7-O3'-C3'	5.98	123.72	112.03
4	B	4003	MTE	N2-C2-N3	5.75	124.19	117.86
4	A	3003	MTE	N2-C2-N3	5.54	123.96	117.86
4	A	3003	MTE	C6-C7-N8	5.45	117.45	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3005	FAD	O4B-C1B-N9A	-5.21	103.59	108.44
4	B	4003	MTE	C6-C7-N8	5.19	117.09	110.01
4	A	3003	MTE	C7-O3'-C3'	5.11	122.03	112.03
4	B	4003	MTE	C9-C10-N1	-4.88	113.71	121.50
4	A	3003	MTE	C9-C10-N1	-4.81	113.81	121.50
6	A	3005	FAD	C2B-C1B-N9A	4.61	125.10	113.27
6	B	4005	FAD	C2B-C1B-N9A	4.50	124.83	113.27
4	A	3003	MTE	C1'-C6-N5	4.28	119.77	111.70
6	B	4005	FAD	O4B-C1B-N9A	-4.26	104.47	108.44
4	A	3003	MTE	O3'-C3'-C4'	4.05	119.24	108.81
6	A	3005	FAD	C1'-N10-C10	-4.02	113.47	119.17
6	B	4005	FAD	O4'-C4'-C3'	4.00	119.01	109.05
6	A	3005	FAD	O4'-C4'-C3'	3.91	118.79	109.05
6	A	3005	FAD	N3A-C4A-N9A	3.89	132.46	125.43
6	B	4005	FAD	N3A-C4A-N9A	3.89	132.46	125.43
6	B	4005	FAD	C1'-N10-C10	-3.87	113.68	119.17
6	A	3005	FAD	C3B-C2B-C1B	3.55	106.47	100.91
6	B	4005	FAD	C3B-C2B-C1B	3.41	106.25	100.91
4	B	4003	MTE	C1'-C6-N5	3.41	118.13	111.70
6	A	3005	FAD	C5'-C4'-C3'	-3.31	105.80	112.06
4	A	3003	MTE	C10-C9-N5	-3.28	113.99	118.50
7	A	5101	YSH	C10-C11-C6	-3.27	115.90	119.29
7	A	5101	YSH	C1-N2-C6	-3.16	119.15	124.77
7	B	5102	YSH	C10-C11-C6	-3.14	116.03	119.29
6	B	4005	FAD	C5'-C4'-C3'	-3.13	106.15	112.06
4	A	3003	MTE	O3'-C7-N8	-3.10	105.19	109.22
6	B	4005	FAD	C4X-C10-N1	-3.09	119.64	122.73
6	A	3005	FAD	C4X-C10-N10	-3.00	119.01	120.51
6	A	3005	FAD	C4X-C10-N1	-2.96	119.78	122.73
4	B	4003	MTE	N2-C2-N1	-2.94	116.33	120.31
7	A	5101	YSH	C1-C5-C4	2.91	112.35	104.57
6	A	3005	FAD	C2A-N3A-C4A	2.80	121.99	114.01
4	A	3003	MTE	N2-C2-N1	-2.78	116.54	120.31
6	B	4005	FAD	C2A-N3A-C4A	2.77	121.89	114.01
4	B	4003	MTE	C10-C9-N5	-2.76	114.71	118.50
7	B	5102	YSH	C1-C5-C4	2.75	111.94	104.57
6	A	3005	FAD	O3'-C3'-C4'	2.72	115.62	108.74
4	B	4003	MTE	C9-C4-N3	2.70	120.99	114.06
7	A	5101	YSH	O22-C20-C5	-2.70	114.01	121.25
7	B	5102	YSH	C1-N2-C6	-2.66	120.04	124.77
4	A	3003	MTE	C9-C4-N3	2.63	120.81	114.06
7	B	5102	YSH	C7-C6-N2	-2.62	115.94	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	5102	YSH	O22-C20-C5	-2.57	114.36	121.25
7	A	5101	YSH	C11-C6-C7	2.53	123.78	121.55
6	A	3005	FAD	O3B-C3B-C4B	-2.47	103.80	111.08
6	A	3005	FAD	C2'-C1'-N10	-2.47	109.18	112.45
6	B	4005	FAD	O3B-C3B-C4B	-2.47	103.81	111.08
6	B	4005	FAD	O2B-C2B-C3B	2.43	119.74	111.83
6	B	4005	FAD	O3'-C3'-C4'	2.41	114.83	108.74
7	A	5101	YSH	C10-C9-C8	2.40	122.78	119.57
4	B	4003	MTE	O3'-C7-N8	-2.40	106.10	109.22
6	A	3005	FAD	O2'-C2'-C1'	2.40	115.66	109.71
6	A	3005	FAD	C9A-C5X-N5	-2.39	118.70	122.37
6	B	4005	FAD	O2'-C2'-C1'	2.38	115.61	109.71
6	A	3005	FAD	C8M-C8-C9	-2.35	114.71	120.38
6	B	4005	FAD	C9A-N10-C10	-2.33	119.48	121.77
6	B	4005	FAD	C9A-C5X-N5	-2.33	118.80	122.37
6	A	3005	FAD	O5B-PA-O1A	2.32	118.47	109.37
6	B	4005	FAD	C8M-C8-C9	-2.31	114.81	120.38
6	B	4005	FAD	C4X-C10-N10	-2.31	119.36	120.51
6	B	4005	FAD	C2'-C1'-N10	-2.31	109.39	112.45
6	B	4005	FAD	C2A-N1A-C6A	2.29	122.90	118.77
6	A	3005	FAD	C2A-N1A-C6A	2.29	122.90	118.77
7	A	5101	YSH	C7-C6-N2	-2.29	116.35	119.13
6	A	3005	FAD	O2B-C2B-C3B	2.28	119.27	111.83
7	B	5102	YSH	C10-C9-C8	2.24	122.56	119.57
7	A	5101	YSH	O21-C20-C5	2.22	120.89	115.01
7	B	5102	YSH	O21-C20-C5	2.22	120.89	115.01
4	A	3003	MTE	C7-C6-N5	2.21	111.25	108.44
7	B	5102	YSH	C11-C6-C7	2.19	123.48	121.55
6	A	3005	FAD	C8M-C8-C7	2.18	125.77	120.74
4	B	4003	MTE	O2P-P-O4'	2.18	112.66	106.65
7	B	5102	YSH	C15-O14-C9	-2.17	112.86	117.71
6	B	4005	FAD	C5A-C4A-N3A	-2.16	120.99	125.70
6	B	4005	FAD	O5B-PA-O1A	2.16	117.83	109.37
9	A	5201	ACY	O-C-CH3	-2.15	112.69	122.06
6	B	4005	FAD	C4A-C5A-N7A	-2.14	107.69	109.52
6	A	3005	FAD	C5A-C4A-N3A	-2.13	121.07	125.70
4	B	4003	MTE	O3'-C7-C6	-2.10	106.64	109.50
6	A	3005	FAD	C7M-C7-C6	-2.09	115.34	120.38
4	B	4003	MTE	C7-C6-N5	2.08	111.08	108.44
6	A	3005	FAD	O2'-C2'-C3'	2.07	114.21	109.05
6	B	4005	FAD	C4-N3-C2	-2.07	121.14	125.39
6	B	4005	FAD	C8M-C8-C7	2.07	125.52	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3005	FAD	O5'-P-O1P	2.06	117.45	109.37
4	A	3003	MTE	C4-N3-C2	2.06	123.12	119.51
7	A	5101	YSH	C15-O14-C9	-2.06	113.09	117.71
6	A	3005	FAD	C9A-N10-C10	-2.06	119.75	121.77
9	B	5202	ACY	O-C-CH3	-2.05	113.10	122.06
6	B	4005	FAD	C1B-N9A-C4A	-2.05	123.10	126.64
4	A	3003	MTE	O3'-C7-C6	-2.04	106.73	109.50
6	A	3005	FAD	C4-N3-C2	-2.02	121.24	125.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.