Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2017 – 09:05 PM EST

PDB ID	:	1FO4
Title	:	CRYSTAL STRUCTURE OF XANTHINE DEHYDROGENASE ISOLATED FROM BOVINE MILK
Authors	:	Enroth, C.; Eger, B.T.; Okamoto, K.; Nishino, T.; Nishino, T.; Pai, E.F.
Deposited on	:	2000-08-24
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

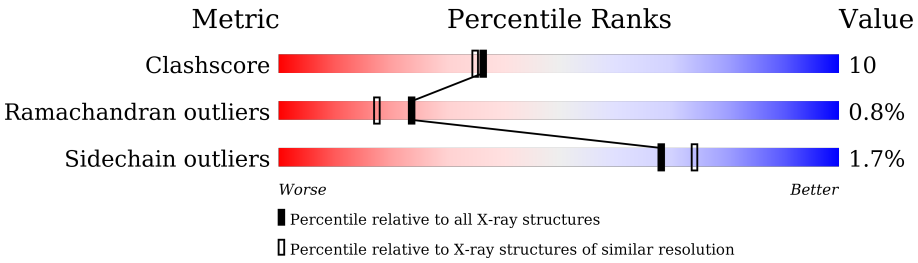
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1332	78% 18%
1	B	1332	79% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MOS	A	3004	-	-	X	-
5	MOS	B	4004	-	-	X	-
7	FAD	A	3006	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FAD	B	4006	X	-	-	-
8	GOL	A	3007	-	X	X	-
8	GOL	A	3008	-	X	-	-
8	GOL	B	4007	-	X	X	-
8	GOL	B	4008	-	X	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22402 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.

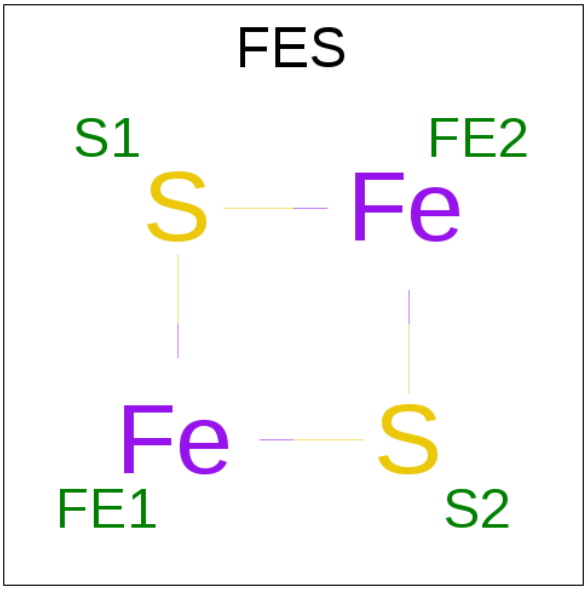
- Molecule 1 is a protein called XANTHINE DEHYDROGENASE.

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			

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

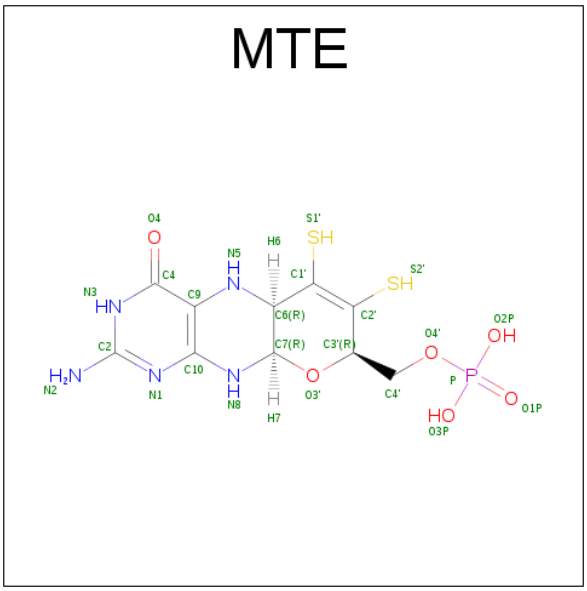
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



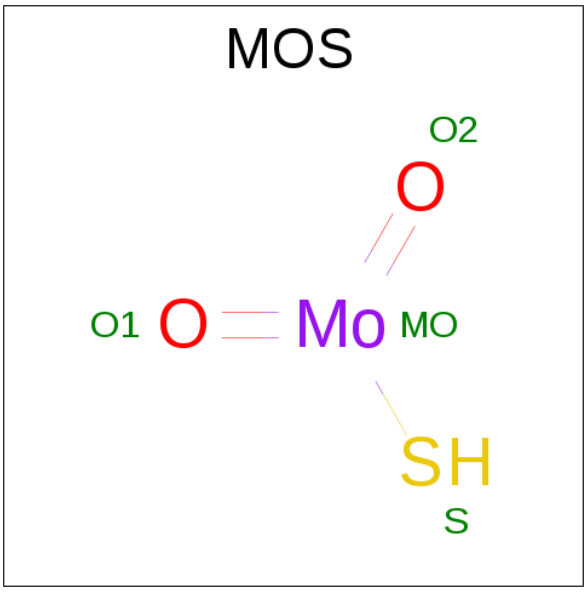
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0

- 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: $C_{10}H_{14}N_5O_6PS_2$).



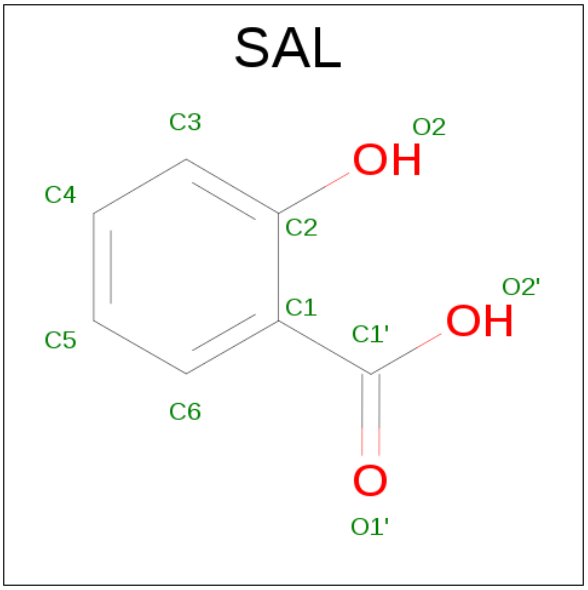
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 24 10 5 6 1 2	0	0
4	B	1	Total C N O P S 24 10 5 6 1 2	0	0

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



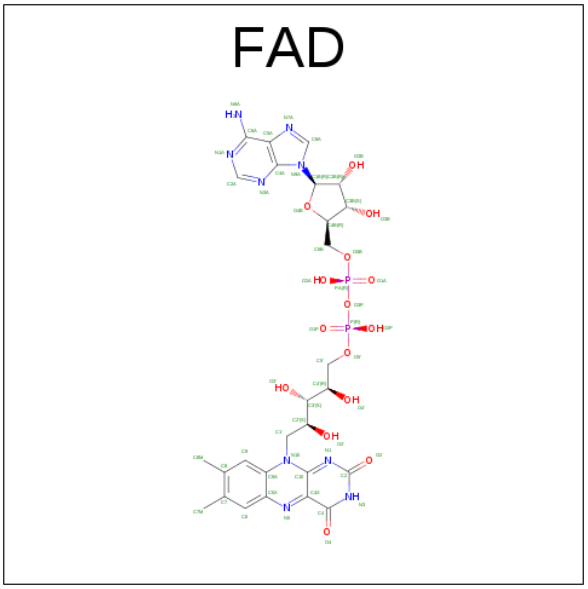
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 6 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



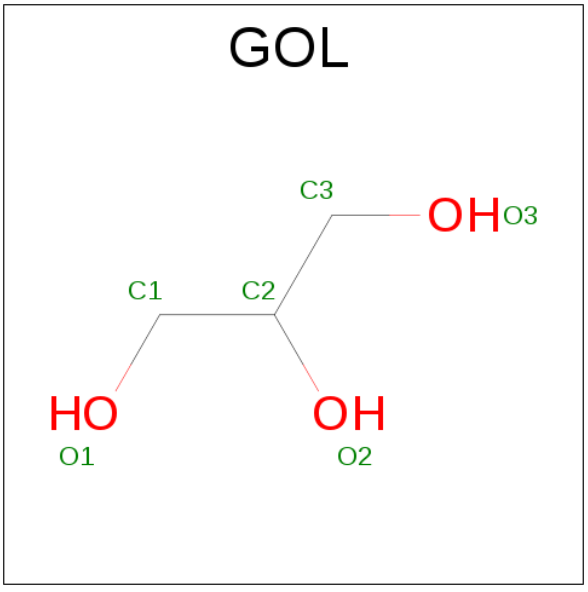
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- 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 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1047	Total O 1047 1047	0	0
9	B	1000	Total O 1000 1000	0	0

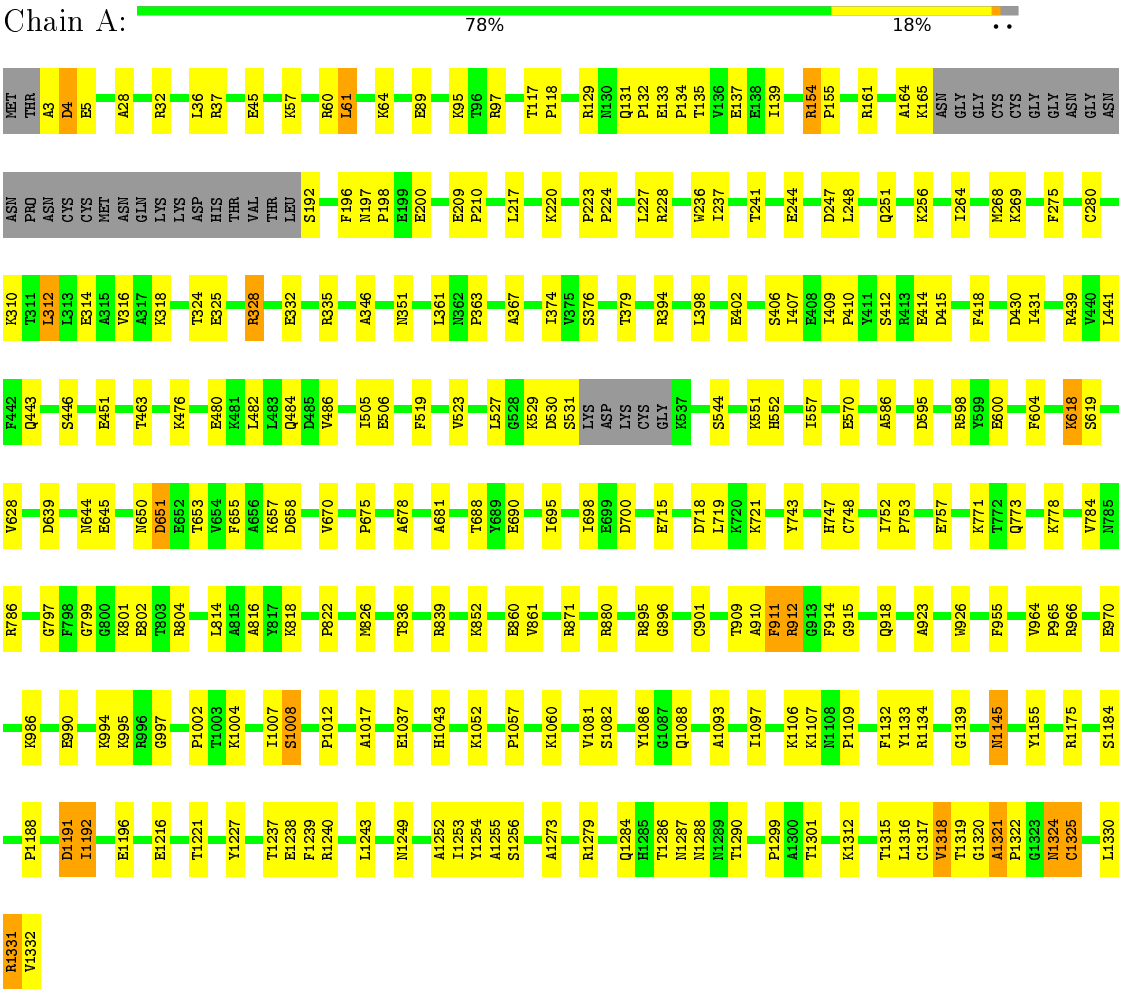
3 Residue-property plots (i)

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.

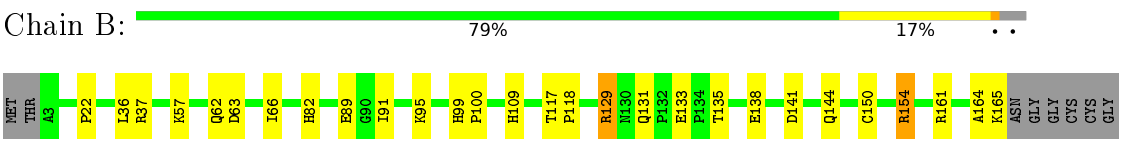
- Molecule 1: XANTHINE DEHYDROGENASE

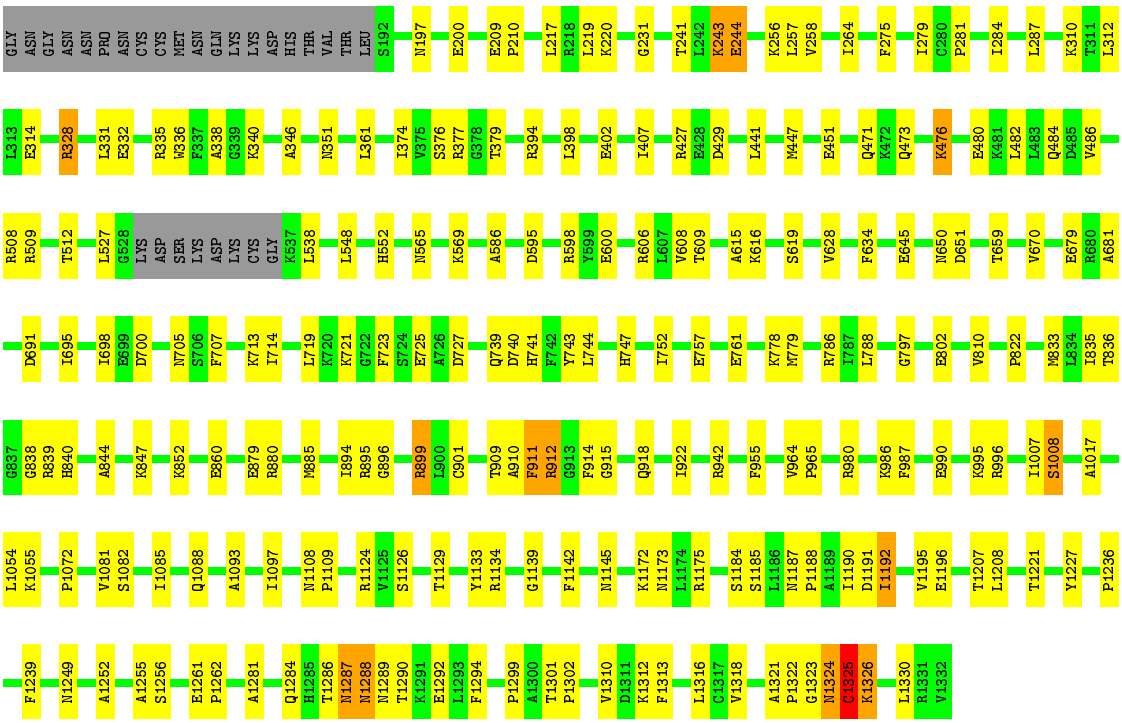
Chain A:



- Molecule 1: XANTHINE DEHYDROGENASE

Chain B:




GLY ASN GLY ASN ASN PRO ASN CYS CYS MET ASN GLN LYS LYS ASP HIS THR VAL THR LEU S192 N197 E200 E209 P210 L217 R218 L219 K220 G231 T241 L242 K243 E244 K256 L257 V258 I264 F275 I279 C280 P281 I284 L287 K310 T311 L312
L313 E314 R328 L331 E332 R335 W336 F337 A338 G339 K340 A346 N351 L361 I374 V375 S376 R377 G378 T379 R394 L398 E402 I407 R427 E428 D429 L441 M447 E451 Q471 K472 Q473 K476 E480 K481 L482 L483 Q484 D485 V486
R508 R509 T512 L527 G528 LYS ASP SER LYS ASP LYS CYS GLY K537 L538 L548 H552 N565 K569 A586 D595 R598 Y599 E600 R606 L607 V608 T609 A615 K616 S619 V628 F634 E645 N650 D651 T659 V670 E679 R680 A681
D691 I695 I698 E699 D700 N705 S706 F707 K713 I714 L719 K720 K721 G722 F723 S724 E725 A726 D727 Q739 D740 H741 F742 Y743 L744 H747 I752 E757 E761 K778 M779 R786 I787 L788 G797 E802 V810 P822 M833 L834 I835 T836
G837 G838 R839 H840 A844 K847 K852 E860 E879 R880 M885 I894 R895 G896 R899 L900 C901 T909 A910 F911 R912 G913 F914 G915 Q918 I922 R942 F955 V964 P965 R980 K986 F987 E990 K995 R996 I1007 S1008 A1017
L1054 K1055 P1072 V1081 S1082 I1085 Q1088 A1093 I1097 N1108 P1109 R1124 V1125 S1126 T1129 Y1133 R1134 G1139 F1142 N1145 K1172 N1173 L1174 R1175 S1184 S1185 L1186 N1187 P1188 A1189 I1190 D1191 I1192 V1195 E1196 T1207 L1208 T1221 Y1227 P1236
F1239 N1249 A1252 A1255 S1256 E1261 P1262 A1281 Q1284 H1285 T1286 N1287 N1288 N1289 T1290 K1291 E1292 L1293 F1294 P1299 A1300 T1301 P1302 V1310 D1311 K1312 F1313 L1316 G1317 V1318 A1321 P1322 G1323 N1324 C1325 K1326 L1330 R1331 V1332

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.45Å 124.49Å 148.33Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10	Depositor
% Data completeness (in resolution range)	86.9 (25.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22402	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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, SAL, MOS, CA, FES, 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	0.37	0/10298	0.64	1/13939 (0.0%)
1	B	0.37	0/10275	0.64	1/13909 (0.0%)
All	All	0.37	0/20573	0.64	2/27848 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1191	ASP	N-CA-C	-5.23	96.89	111.00
1	B	243	LYS	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	10077	0	10075	203	0
1	B	10054	0	10054	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	24	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	10	2	0
5	A	4	0	0	2	0
5	B	4	0	0	2	0
6	A	10	0	4	0	0
6	B	10	0	4	1	0
7	A	53	0	29	3	0
7	B	53	0	30	2	0
8	A	12	0	5	7	0
8	B	12	0	7	11	0
9	A	1047	0	0	21	0
9	B	1000	0	0	11	0
All	All	22402	0	20228	386	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 10.

All (386) 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)
8:A:3008:GOL:C1	8:A:3008:GOL:O1	1.68	1.39
8:B:4008:GOL:C1	8:B:4008:GOL:O1	1.71	1.36
1:A:3:ALA:HB1	1:A:228:ARG:H	1.19	1.07
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.19	1.07
5:B:4004:MOS:MO	5:B:4004:MOS:S	1.66	1.06
1:B:243:LYS:O	1:B:244:GLU:HB2	1.62	0.99
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.25	0.98
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.50	0.94
1:A:506:GLU:HG3	1:A:1319:THR:HB	1.47	0.93
5:A:3004:MOS:S	5:A:3004:MOS:MO	1.82	0.90
1:B:1312:LYS:O	1:B:1316:LEU:HD13	1.74	0.88
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.58	0.85
1:B:719:LEU:HD11	1:B:895:ARG:HB2	1.57	0.85
1:B:131:GLN:HE21	1:B:133:GLU:H	1.23	0.84
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.40	0.83
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.14	0.81
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.43	0.81
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.47	0.80
1:B:1191:ASP:O	1:B:1192:ILE:HB	1.78	0.80
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.13	0.77
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.85	0.77
1:B:839:ARG:HG3	8:B:4007:GOL:H11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:ASP:O	1:A:1192:ILE:HB	1.85	0.75
1:A:131:GLN:HE21	1:A:133:GLU:H	1.34	0.75
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.87	0.74
1:A:1331:ARG:O	1:A:1332:VAL:O	2.05	0.74
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.22	0.74
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.67	0.74
1:B:376:SER:HB3	1:B:379:THR:OG1	1.86	0.74
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.52	0.74
1:B:1207:THR:O	1:B:1208:LEU:HD12	1.89	0.72
1:B:552:HIS:CE1	1:B:1172:LYS:HZ3	2.07	0.72
1:B:164:ALA:O	1:B:165:LYS:HB2	1.89	0.71
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.53	0.71
1:A:506:GLU:CG	1:A:1319:THR:HB	2.20	0.71
1:A:1330:LEU:O	1:A:1331:ARG:HG2	1.89	0.71
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.73	0.70
1:B:645:GLU:CG	1:B:650:ASN:HD22	2.01	0.70
1:B:1326:LYS:HD2	1:B:1326:LYS:N	2.06	0.70
1:B:264:ILE:HD11	7:B:4006:FAD:H3B	1.74	0.70
1:B:719:LEU:HD13	1:B:860:GLU:OE2	1.91	0.69
1:A:3:ALA:HB1	1:A:228:ARG:N	2.01	0.69
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.57	0.68
1:B:37:ARG:HD3	1:B:595:ASP:O	1.93	0.68
1:B:241:THR:OG1	1:B:243:LYS:O	2.12	0.67
1:B:918:GLN:HE22	8:B:4007:GOL:H12	1.60	0.66
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.25	0.66
1:A:598:ARG:HG2	1:B:600:GLU:OE2	1.95	0.66
1:B:1191:ASP:O	1:B:1192:ILE:CB	2.44	0.65
1:B:761:GLU:HG3	1:B:788:LEU:HD23	1.78	0.65
1:B:1318:VAL:HG23	1:B:1321:ALA:HB2	1.78	0.65
1:B:721:LYS:O	1:B:725:GLU:HG3	1.96	0.65
1:A:619:SER:HB3	1:A:688:THR:OG1	1.96	0.65
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.31	0.65
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.78	0.65
1:A:264:ILE:HD11	7:A:3006:FAD:H3B	1.78	0.65
1:A:1324:ASN:HD22	1:A:1324:ASN:C	2.00	0.65
1:A:1332:VAL:OXT	1:A:1332:VAL:HG22	1.96	0.64
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.03	0.64
1:A:600:GLU:CD	1:B:598:ARG:HG2	2.17	0.64
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.28	0.63
1:B:1017:ALA:HB2	1:B:1085:ILE:HD12	1.81	0.62
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:SER:HB3	1:A:379:THR:OG1	1.99	0.62
1:A:164:ALA:O	1:A:165:LYS:HB2	1.99	0.62
1:B:552:HIS:CE1	1:B:1172:LYS:NZ	2.68	0.61
1:B:131:GLN:HE21	1:B:133:GLU:N	1.96	0.61
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.82	0.61
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.84	0.60
1:B:980:ARG:NH1	1:B:1175:ARG:HD3	2.16	0.60
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	2.02	0.59
1:B:707:PHE:CD2	1:B:899:ARG:HG3	2.37	0.59
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.85	0.59
1:A:197:ASN:O	1:A:200:GLU:HG2	2.03	0.59
1:A:557:ILE:HD12	1:A:1240:ARG:NE	2.18	0.59
1:A:1188:PRO:O	1:A:1191:ASP:O	2.21	0.58
1:B:1188:PRO:O	1:B:1191:ASP:O	2.20	0.58
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.67	0.58
1:A:1330:LEU:HD12	1:A:1331:ARG:N	2.18	0.58
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.38	0.58
1:A:1191:ASP:O	1:A:1192:ILE:CB	2.51	0.58
1:B:1184:SER:HB3	8:B:4008:GOL:H11	1.84	0.57
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.34	0.57
1:A:618:LYS:HD2	1:A:690:GLU:OE1	2.05	0.57
1:A:1322:PRO:HG2	1:A:1324:ASN:CG	2.25	0.57
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.04	0.57
1:B:209:GLU:HG3	1:B:210:PRO:HD2	1.86	0.57
1:A:314:GLU:O	1:A:318:LYS:HD3	2.05	0.57
1:A:394:ARG:HD2	9:A:4326:HOH:O	2.05	0.57
1:A:480:GLU:O	1:A:484:GLN:HG3	2.05	0.57
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.39	0.57
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.87	0.56
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.87	0.56
1:B:217:LEU:O	1:B:220:LYS:HG2	2.05	0.56
1:B:340:LYS:HE3	9:B:4667:HOH:O	2.04	0.56
1:A:217:LEU:O	1:A:220:LYS:HG2	2.04	0.56
1:B:1325:CYS:HB2	1:B:1326:LYS:HD2	1.86	0.56
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.05	0.56
1:A:217:LEU:HD12	1:A:220:LYS:HD3	1.88	0.56
1:A:418:PHE:CD1	1:A:439:ARG:HB2	2.41	0.56
1:A:986:LYS:O	1:A:990:GLU:HG3	2.06	0.56
1:B:258:VAL:HG22	1:B:264:ILE:HG13	1.87	0.56
1:B:197:ASN:O	1:B:200:GLU:HG2	2.06	0.56
1:A:192:SER:HB2	9:A:4669:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:LYS:O	1:A:1316:LEU:HD23	2.06	0.55
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	1.87	0.55
1:A:527:LEU:C	1:A:529:LYS:H	2.08	0.55
1:B:1326:LYS:N	1:B:1326:LYS:CD	2.69	0.55
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.04	0.55
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.07	0.55
1:B:374:ILE:HD13	1:B:398:LEU:HD22	1.89	0.55
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.42	0.55
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.41	0.55
1:A:1082:SER:HB2	4:A:3003:MTE:O3P	2.07	0.55
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.42	0.55
1:A:1330:LEU:HD12	1:A:1331:ARG:H	1.70	0.55
1:A:1315:THR:O	1:A:1318:VAL:HG13	2.08	0.54
1:A:3:ALA:CB	1:A:228:ARG:H	2.06	0.54
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.09	0.54
1:B:616:LYS:HA	1:B:659:THR:HG22	1.88	0.54
1:B:1312:LYS:HE3	1:B:1313:PHE:CZ	2.42	0.54
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.89	0.54
1:A:95:LYS:HE2	9:A:4796:HOH:O	2.06	0.54
1:A:443:GLN:HB2	1:A:446:SER:OG	2.07	0.54
1:B:1185:SER:O	8:B:4008:GOL:H12	2.08	0.54
1:A:752:ILE:HD13	1:A:822:PRO:HB3	1.90	0.54
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.89	0.54
1:A:1008:SER:HA	1:A:1081:VAL:HG11	1.90	0.53
1:B:284:ILE:HB	1:B:287:LEU:HD12	1.90	0.53
1:A:799:GLY:HA2	5:A:3004:MOS:S	2.49	0.53
1:A:1093:ALA:O	1:A:1097:ILE:HG12	2.08	0.53
1:A:552:HIS:HB3	1:A:1237:THR:HG21	1.90	0.53
1:B:1294:PHE:HB2	9:B:4880:HOH:O	2.07	0.53
1:A:1012:PRO:HB2	9:A:4688:HOH:O	2.09	0.53
1:B:918:GLN:HE22	8:B:4007:GOL:C1	2.22	0.53
1:A:3:ALA:O	1:A:4:ASP:HB3	2.08	0.53
1:A:529:LYS:O	1:A:531:SER:N	2.42	0.53
1:A:406:SER:C	1:A:407:ILE:HD12	2.29	0.53
8:A:3008:GOL:C1	8:A:3008:GOL:HO1	2.12	0.53
1:A:430:ASP:OD1	1:A:431:ILE:N	2.42	0.53
1:B:802:GLU:OE1	6:B:4005:SAL:H4	2.09	0.52
1:A:316:VAL:HA	1:A:324:THR:HG21	1.92	0.52
8:B:4008:GOL:C1	8:B:4008:GOL:HO1	2.14	0.52
1:A:268:MET:HE1	9:A:4726:HOH:O	2.08	0.52
1:B:57:LYS:HE2	1:B:66:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLN:NE2	1:B:133:GLU:H	2.00	0.52
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.40	0.52
1:B:1326:LYS:HD3	1:B:1326:LYS:O	2.10	0.52
1:B:1007:ILE:O	1:B:1008:SER:CB	2.58	0.52
1:B:164:ALA:O	1:B:165:LYS:CB	2.57	0.51
1:A:1279:ARG:NH2	1:A:1290:THR:O	2.43	0.51
1:A:1332:VAL:OXT	1:A:1332:VAL:CG2	2.57	0.51
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.58	0.51
1:A:552:HIS:HB2	9:A:4617:HOH:O	2.09	0.51
1:A:137:GLU:HG3	1:A:551:LYS:NZ	2.25	0.51
1:A:966:ARG:HG3	9:A:4860:HOH:O	2.11	0.51
1:B:695:ILE:HG23	1:B:700:ASP:HB3	1.93	0.51
1:A:407:ILE:N	1:A:407:ILE:HD12	2.26	0.51
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.11	0.51
1:A:918:GLN:HE22	8:A:3007:GOL:C1	2.23	0.51
1:B:117:THR:HB	1:B:118:PRO:HD3	1.92	0.51
1:B:154:ARG:HD2	9:B:4305:HOH:O	2.11	0.50
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.41	0.50
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.93	0.50
1:A:60:ARG:O	1:A:61:LEU:HB2	2.09	0.50
1:A:839:ARG:NH1	8:A:3007:GOL:O1	2.44	0.50
1:B:1324:ASN:O	1:B:1326:LYS:N	2.44	0.50
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.92	0.50
1:A:346:ALA:HB1	7:A:3006:FAD:H4'	1.92	0.50
1:A:45:GLU:HG2	9:A:4719:HOH:O	2.12	0.50
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.77	0.50
1:A:752:ILE:HD12	1:A:822:PRO:HB3	1.93	0.50
1:B:1097:ILE:HD11	1:B:1129:THR:HG22	1.92	0.50
1:A:1322:PRO:HG2	1:A:1324:ASN:ND2	2.26	0.50
1:A:351:ASN:ND2	1:A:361:LEU:HB2	2.27	0.50
1:B:141:ASP:O	1:B:144:GLN:HG3	2.11	0.50
1:A:645:GLU:OE2	1:A:650:ASN:HB3	2.12	0.50
1:B:879:GLU:HG2	1:B:1142:PHE:CZ	2.46	0.49
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.94	0.49
1:A:994:LYS:HE3	9:A:4560:HOH:O	2.12	0.49
1:B:885:MET:SD	1:B:896:GLY:HA3	2.52	0.49
1:A:135:THR:O	1:A:139:ILE:HG13	2.12	0.49
1:A:374:ILE:HG21	1:A:398:LEU:HD22	1.94	0.49
1:A:1007:ILE:O	1:A:1008:SER:CB	2.60	0.49
1:B:336:TRP:CZ3	1:B:427:ARG:HG2	2.48	0.49
1:B:713:LYS:HG3	1:B:714:ILE:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.47	0.49
1:A:117:THR:HB	1:A:118:PRO:HD3	1.93	0.49
1:A:1184:SER:HB3	8:A:3008:GOL:H11	1.94	0.49
1:A:5:GLU:HB2	9:A:4797:HOH:O	2.12	0.49
1:B:980:ARG:HD2	9:B:4566:HOH:O	2.12	0.49
1:A:256:LYS:HG3	1:A:275:PHE:CD2	2.48	0.49
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.13	0.49
1:A:955:PHE:CA	1:A:1145:ASN:HD21	2.21	0.49
1:B:840:HIS:N	8:B:4007:GOL:O3	2.38	0.49
1:A:915:GLY:H	8:A:3007:GOL:C1	2.26	0.49
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.59	0.49
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.93	0.49
1:B:839:ARG:NH1	8:B:4007:GOL:O1	2.46	0.49
1:A:1192:ILE:HG13	1:A:1243:LEU:HD11	1.95	0.48
1:A:312:LEU:O	1:A:316:VAL:HG23	2.13	0.48
1:A:418:PHE:HD1	1:A:439:ARG:HB2	1.78	0.48
1:A:651:ASP:OD1	1:A:871:ARG:NH1	2.45	0.48
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.11	0.48
1:A:1320:GLY:O	1:A:1321:ALA:C	2.52	0.48
1:A:1320:GLY:O	1:A:1322:PRO:N	2.47	0.48
1:A:363:PRO:HG3	1:A:463:THR:HG23	1.94	0.48
1:A:600:GLU:OE2	1:B:598:ARG:HG2	2.13	0.48
1:A:367:ALA:O	1:A:439:ARG:HD3	2.14	0.48
1:A:3:ALA:HB2	1:A:227:LEU:HA	1.95	0.48
1:A:64:LYS:HE2	9:A:4653:HOH:O	2.14	0.48
1:B:129:ARG:HG3	1:B:129:ARG:NH1	2.29	0.48
1:B:117:THR:CG2	1:B:586:ALA:HA	2.44	0.48
1:A:1324:ASN:ND2	1:A:1324:ASN:C	2.68	0.47
1:A:909:THR:OG1	1:A:910:ALA:N	2.45	0.47
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.48	0.47
1:A:911:PHE:O	1:A:912:ARG:C	2.52	0.47
1:A:544:SER:HB2	1:A:994:LYS:HD2	1.95	0.47
1:B:150:CYS:SG	4:B:4003:MTE:N2	2.87	0.47
1:A:161:ARG:HD3	9:A:4840:HOH:O	2.13	0.47
1:A:719:LEU:CD1	1:A:895:ARG:HD3	2.44	0.47
1:A:325:GLU:HB2	1:A:412:SER:OG	2.14	0.47
1:A:657:LYS:O	1:A:658:ASP:HB2	2.15	0.47
1:B:739:GLN:HG2	1:B:911:PHE:CE1	2.50	0.47
1:B:473:GLN:O	1:B:476:LYS:HB2	2.14	0.47
1:B:332:GLU:CG	1:B:548:LEU:HD13	2.45	0.47
1:A:861:VAL:O	1:A:896:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLN:O	1:A:134:PRO:HD3	2.15	0.47
1:B:129:ARG:NE	1:B:209:GLU:HG2	2.30	0.47
1:B:376:SER:HB2	1:B:402:GLU:HG2	1.96	0.47
1:A:1330:LEU:O	1:A:1331:ARG:CG	2.59	0.46
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.80	0.46
1:B:911:PHE:HD2	1:B:912:ARG:N	2.13	0.46
1:A:1318:VAL:HG23	1:A:1318:VAL:O	2.16	0.46
1:B:256:LYS:HG3	1:B:275:PHE:CD2	2.51	0.46
1:A:698:ILE:HG23	1:A:901:CYS:SG	2.55	0.46
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.31	0.46
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.27	0.46
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.64	0.46
1:A:1134:ARG:HD3	1:B:1124:ARG:O	2.16	0.46
1:B:312:LEU:HB2	1:B:331:LEU:HD21	1.98	0.46
1:A:482:LEU:O	1:A:486:VAL:HG23	2.16	0.46
1:A:688:THR:HG23	9:A:4422:HOH:O	2.14	0.46
1:A:914:PHE:HA	8:A:3007:GOL:O2	2.15	0.46
1:B:1175:ARG:HG2	9:B:4751:HOH:O	2.16	0.46
1:B:1187:ASN:CG	1:B:1190:ILE:HG12	2.36	0.46
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.16	0.46
1:A:1175:ARG:HG3	1:A:1238:GLU:HB2	1.98	0.46
1:A:506:GLU:CD	1:A:506:GLU:H	2.19	0.46
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.15	0.45
1:A:747:HIS:CE1	1:A:801:LYS:HG2	2.51	0.45
1:B:915:GLY:H	8:B:4007:GOL:C1	2.29	0.45
1:A:718:ASP:HB3	1:A:721:LYS:HE3	1.97	0.45
1:B:705:ASN:HA	1:B:707:PHE:CE1	2.52	0.45
1:A:1317:CYS:O	1:A:1318:VAL:C	2.55	0.45
1:A:644:ASN:O	1:A:653:THR:HA	2.17	0.45
1:A:310:LYS:O	1:A:314:GLU:HG3	2.17	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.79	0.45
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.82	0.45
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.64	0.45
1:B:1310:VAL:HG13	9:B:4809:HOH:O	2.16	0.45
1:B:37:ARG:HG2	1:B:37:ARG:HH11	1.82	0.45
1:A:519:PHE:O	1:A:523:VAL:HG23	2.17	0.44
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.82	0.44
1:B:740:ASP:OD2	1:B:833:MET:HG2	2.16	0.44
1:A:1330:LEU:O	1:A:1331:ARG:CB	2.66	0.44
1:B:779:MET:HG3	1:B:810:VAL:CG1	2.46	0.44
1:A:695:ILE:HG23	1:A:700:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.37	0.44
1:A:37:ARG:HG2	1:A:595:ASP:HA	1.99	0.44
1:B:1299:PRO:HG2	1:B:1301:THR:HG23	1.99	0.44
1:B:346:ALA:HB1	7:B:4006:FAD:H4'	1.99	0.44
1:A:247:ASP:O	1:A:251:GLN:HG3	2.18	0.44
1:B:1108:ASN:N	1:B:1109:PRO:HD3	2.33	0.44
1:A:328:ARG:NH1	1:A:328:ARG:HG2	2.28	0.44
1:A:527:LEU:C	1:A:529:LYS:N	2.71	0.44
1:B:1192:ILE:HA	1:B:1195:VAL:HB	1.98	0.44
1:B:82:HIS:CE1	1:B:219:LEU:HD13	2.52	0.44
1:B:909:THR:OG1	1:B:910:ALA:N	2.47	0.44
1:A:1286:THR:HG22	1:A:1287:ASN:N	2.32	0.44
1:A:1320:GLY:C	1:A:1322:PRO:HD3	2.38	0.44
1:A:557:ILE:HB	1:A:1240:ARG:HG2	1.99	0.44
1:B:1323:GLY:O	1:B:1324:ASN:C	2.57	0.43
1:B:480:GLU:O	1:B:484:GLN:HG3	2.18	0.43
1:B:885:MET:HE2	1:B:894:ILE:HD11	2.00	0.43
1:A:1253:ILE:HG23	1:A:1253:ILE:O	2.18	0.43
1:B:1082:SER:HB2	4:B:4003:MTE:O2P	2.19	0.43
1:B:332:GLU:HG2	1:B:548:LEU:HD13	2.01	0.43
9:A:4946:HOH:O	1:B:95:LYS:HE2	2.18	0.43
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	2.00	0.43
1:A:1325:CYS:HA	9:A:4966:HOH:O	2.17	0.43
1:A:209:GLU:HG3	1:A:210:PRO:HD2	1.99	0.43
1:A:628:VAL:HG21	1:A:681:ALA:HA	2.00	0.43
1:B:914:PHE:HA	8:B:4007:GOL:O2	2.18	0.43
1:A:269:LYS:HE3	9:A:4958:HOH:O	2.18	0.43
1:B:606:ARG:HG2	1:B:679:GLU:HA	2.00	0.43
1:B:698:ILE:HG23	1:B:901:CYS:SG	2.58	0.43
1:B:91:ILE:O	1:B:99:HIS:HB2	2.19	0.43
1:A:715:GLU:CG	1:A:895:ARG:HG3	2.48	0.43
9:A:4908:HOH:O	1:B:1134:ARG:HD2	2.18	0.43
1:B:36:LEU:HD22	1:B:89:GLU:CG	2.44	0.43
1:B:509:ARG:HG2	1:B:509:ARG:HH11	1.84	0.43
1:B:407:ILE:HD12	1:B:407:ILE:N	2.33	0.43
1:B:1321:ALA:HB1	1:B:1322:PRO:CD	2.35	0.43
1:A:1175:ARG:NH2	1:A:1240:ARG:NH1	2.67	0.43
1:B:508:ARG:O	1:B:512:THR:HG23	2.19	0.43
1:A:505:ILE:HD12	1:A:505:ILE:N	2.35	0.42
1:A:715:GLU:HG3	1:A:895:ARG:HG3	2.01	0.42
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:THR:HG21	1:B:835:ILE:HD11	2.00	0.42
1:A:1060:LYS:HA	9:A:4504:HOH:O	2.18	0.42
1:A:1107:LYS:C	1:A:1109:PRO:HD3	2.39	0.42
1:A:1252:ALA:HB3	1:A:1256:SER:O	2.19	0.42
1:A:966:ARG:O	1:A:970:GLU:HB2	2.19	0.42
1:B:62:GLN:O	1:B:63:ASP:C	2.58	0.42
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.48	0.42
1:A:137:GLU:HG3	1:A:551:LYS:HZ2	1.83	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.85	0.42
1:A:237:ILE:HG21	1:A:248:LEU:HD11	2.01	0.42
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.54	0.42
1:B:482:LEU:O	1:B:486:VAL:HG23	2.20	0.42
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.02	0.42
1:B:1316:LEU:HD11	9:B:4974:HOH:O	2.19	0.42
1:A:236:TRP:CZ2	1:A:280:CYS:HB2	2.55	0.42
1:B:911:PHE:O	1:B:912:ARG:C	2.58	0.42
1:A:639:ASP:HB3	1:A:818:LYS:HE3	2.01	0.42
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.85	0.42
5:B:4004:MOS:O1	5:B:4004:MOS:S	2.78	0.42
1:A:719:LEU:HD12	1:A:895:ARG:HD3	2.02	0.42
1:A:748:CYS:HB2	1:A:826:MET:HG3	2.01	0.42
1:B:1054:LEU:O	1:B:1055:LYS:HB2	2.20	0.42
1:B:608:VAL:HG21	1:B:634:PHE:HE1	1.84	0.42
1:B:942:ARG:HD2	9:B:4351:HOH:O	2.20	0.42
1:A:131:GLN:HA	1:A:132:PRO:HD2	1.92	0.42
1:A:137:GLU:OE2	1:A:551:LYS:HD2	2.20	0.42
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.20	0.42
1:B:964:VAL:HB	1:B:965:PRO:HD3	2.02	0.42
1:A:1132:PHE:CG	1:B:1126:SER:HB2	2.55	0.42
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.84	0.42
1:A:154:ARG:N	1:A:155:PRO:HD2	2.34	0.42
1:B:117:THR:HG22	1:B:586:ALA:HA	2.01	0.42
1:A:196:PHE:CE1	1:A:198:PRO:HG3	2.54	0.41
1:B:1207:THR:C	1:B:1208:LEU:HD12	2.40	0.41
1:B:447:MET:HG2	1:B:527:LEU:HD13	2.02	0.41
1:A:414:GLU:O	1:A:415:ASP:HB2	2.20	0.41
1:A:771:LYS:HD3	1:A:771:LYS:HA	1.92	0.41
1:B:1321:ALA:O	1:B:1322:PRO:C	2.58	0.41
1:B:161:ARG:HD3	9:B:4822:HOH:O	2.20	0.41
1:A:117:THR:CG2	1:A:586:ALA:HA	2.50	0.41
1:B:1252:ALA:HB3	1:B:1256:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ASP:OD2	1:B:852:LYS:HG2	2.20	0.41
1:A:1106:LYS:O	1:A:1109:PRO:HD3	2.21	0.41
1:A:28:ALA:O	1:A:32:ARG:HG2	2.20	0.41
1:A:409:ILE:HA	1:A:410:PRO:HD3	1.83	0.41
1:B:22:PRO:HD2	1:B:231:GLY:HA3	2.02	0.41
1:B:257:LEU:HA	1:B:279:ILE:O	2.20	0.41
1:B:310:LYS:O	1:B:314:GLU:HG3	2.20	0.41
1:A:129:ARG:NE	1:A:209:GLU:HG2	2.35	0.41
1:A:117:THR:HG22	1:A:586:ALA:HA	2.03	0.41
1:B:109:HIS:HA	9:B:4182:HOH:O	2.19	0.41
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.21	0.41
1:B:351:ASN:ND2	1:B:361:LEU:HB2	2.36	0.41
1:B:482:LEU:HD23	1:B:482:LEU:C	2.41	0.41
1:B:670:VAL:HG11	1:B:681:ALA:HB3	2.02	0.41
1:B:1289:ASN:O	1:B:1290:THR:HB	2.20	0.41
1:B:741:HIS:CE1	1:B:838:GLY:HA2	2.56	0.41
1:A:678:ALA:HB3	9:A:4714:HOH:O	2.20	0.41
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.35	0.41
1:A:376:SER:HB2	1:A:402:GLU:HG2	2.03	0.41
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.21	0.41
1:B:394:ARG:HD2	9:B:4345:HOH:O	2.20	0.41
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.55	0.41
1:A:1004:LYS:HB2	1:A:1155:TYR:CE2	2.56	0.41
1:B:1301:THR:HB	1:B:1302:PRO:HD2	2.03	0.41
1:B:332:GLU:O	1:B:335:ARG:HB3	2.21	0.41
1:A:773:GLN:HG2	1:A:784:VAL:HG13	2.02	0.40
1:A:804:ARG:HG2	1:A:909:THR:HG21	2.02	0.40
1:B:1093:ALA:O	1:B:1097:ILE:HG12	2.20	0.40
1:B:986:LYS:O	1:B:990:GLU:HG3	2.22	0.40
1:A:332:GLU:O	1:A:335:ARG:HB3	2.22	0.40
1:A:644:ASN:HB2	9:A:4771:HOH:O	2.21	0.40
1:A:852:LYS:HE2	1:A:852:LYS:HB3	1.79	0.40
7:A:3006:FAD:HM73	9:A:4047:HOH:O	2.22	0.40
1:B:569:LYS:HE2	1:B:569:LYS:HB3	1.91	0.40
1:B:615:ALA:HB2	1:B:691:ASP:HA	2.04	0.40
1:B:987:PHE:CD2	1:B:996:ARG:HG3	2.57	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%)	1228 (95%)	54 (4%)	11 (1%)	21	15
1	B	1290/1332 (97%)	1236 (96%)	45 (4%)	9 (1%)	26	21
All	All	2583/2664 (97%)	2464 (95%)	99 (4%)	20 (1%)	24	17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	A	1331	ARG
1	B	244	GLU
1	B	1008	SER
1	B	1287	ASN
1	A	61	LEU
1	A	1192	ILE
1	A	1288	ASN
1	B	1192	ILE
1	B	1288	ASN
1	A	530	ASP
1	A	797	GLY
1	A	912	ARG
1	A	1318	VAL
1	B	912	ARG
1	B	1139	GLY
1	B	1325	CYS
1	A	1321	ALA
1	B	797	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%)	1084 (98%)	17 (2%)	72	78
1	B	1098/1128 (97%)	1078 (98%)	20 (2%)	66	72
All	All	2199/2256 (98%)	2162 (98%)	37 (2%)	68	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	57	LYS
1	A	154	ARG
1	A	312	LEU
1	A	328	ARG
1	A	476	LYS
1	A	618	LYS
1	A	651	ASP
1	A	743	TYR
1	A	802	GLU
1	A	911	PHE
1	A	1002	PRO
1	A	1145	ASN
1	A	1216	GLU
1	A	1239	PHE
1	A	1324	ASN
1	A	1325	CYS
1	B	100	PRO
1	B	129	ARG
1	B	154	ARG
1	B	328	ARG
1	B	471	GLN
1	B	476	LYS
1	B	538	LEU
1	B	565	ASN
1	B	619	SER
1	B	651	ASP
1	B	743	TYR
1	B	744	LEU
1	B	899	ARG
1	B	911	PHE

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Mol	Chain	Res	Type
1	B	1072	PRO
1	B	1239	PHE
1	B	1324	ASN
1	B	1325	CYS
1	B	1326	LYS
1	B	1330	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	351	ASN
1	A	473	GLN
1	A	626	GLN
1	A	650	ASN
1	A	683	HIS
1	A	1095	GLN
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	473	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	1145	ASN
1	B	1284	GLN
1	B	1287	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	21,26,26	7.33	16 (76%)	18,40,40	3.20	7 (38%)
5	MOS	A	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	SAL	A	3005	-	7,10,10	1.76	3 (42%)	10,13,13	1.22	0
7	FAD	A	3006	-	52,58,58	4.50	33 (63%)	52,89,89	2.94	20 (38%)
8	GOL	A	3007	-	5,5,5	7.07	4 (80%)	5,5,5	5.78	4 (80%)
8	GOL	A	3008	-	5,5,5	4.46	4 (80%)	5,5,5	5.72	3 (60%)
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	21,26,26	7.38	14 (66%)	18,40,40	3.17	7 (38%)
5	MOS	B	4004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	SAL	B	4005	-	7,10,10	1.74	3 (42%)	10,13,13	1.33	1 (10%)
7	FAD	B	4006	-	52,58,58	4.33	33 (63%)	52,89,89	3.01	19 (36%)
8	GOL	B	4007	-	5,5,5	6.66	5 (100%)	5,5,5	5.69	3 (60%)
8	GOL	B	4008	-	5,5,5	4.34	3 (60%)	5,5,5	5.84	3 (60%)

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	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	3002	1	-	0/0/4/4	0/1/1/1
4	MTE	A	3003	5	-	0/6/34/34	0/3/3/3
5	MOS	A	3004	4	-	0/0/0/0	0/0/0/0
6	SAL	A	3005	-	-	0/0/4/4	0/1/1/1
7	FAD	A	3006	-	2/2/9/9	0/30/50/50	0/6/6/6
8	GOL	A	3007	-	-	0/4/4/4	0/0/0/0
8	GOL	A	3008	-	-	0/4/4/4	0/0/0/0
3	FES	B	4001	1	-	0/0/4/4	0/1/1/1
3	FES	B	4002	1	-	0/0/4/4	0/1/1/1
4	MTE	B	4003	5	-	0/6/34/34	0/3/3/3
5	MOS	B	4004	4	-	0/0/0/0	0/0/0/0
6	SAL	B	4005	-	-	0/0/4/4	0/1/1/1
7	FAD	B	4006	-	2/2/9/9	0/30/50/50	0/6/6/6
8	GOL	B	4007	-	-	0/4/4/4	0/0/0/0
8	GOL	B	4008	-	-	0/4/4/4	0/0/0/0

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	3007	GOL	C3-C2	-13.06	1.00	1.52
8	B	4007	GOL	C3-C2	-12.20	1.03	1.52
7	A	3006	FAD	C5'-C4'	-8.84	1.38	1.51
7	B	4006	FAD	C5'-C4'	-7.37	1.40	1.51
8	A	3008	GOL	C3-C2	-7.02	1.24	1.52
4	A	3003	MTE	P-O4'	-6.55	1.41	1.59
4	A	3003	MTE	P-O3P	-6.43	1.32	1.54
8	B	4008	GOL	C3-C2	-6.32	1.27	1.52
4	B	4003	MTE	P-O4'	-6.15	1.42	1.59
7	B	4006	FAD	C8A-N7A	-5.62	1.23	1.34
8	A	3007	GOL	C1-C2	-5.38	1.30	1.52
8	B	4007	GOL	O2-C2	-5.10	1.28	1.43
8	A	3007	GOL	O2-C2	-5.08	1.28	1.43
4	B	4003	MTE	P-O3P	-4.85	1.38	1.54
7	A	3006	FAD	C8A-N7A	-4.77	1.25	1.34
7	B	4006	FAD	O5B-C5B	-4.59	1.26	1.44
8	A	3007	GOL	O3-C3	-4.52	1.22	1.42
7	B	4006	FAD	PA-O5B	-4.39	1.40	1.59
8	B	4007	GOL	O3-C3	-4.18	1.24	1.42
7	A	3006	FAD	O5B-C5B	-4.11	1.28	1.44
8	B	4007	GOL	C1-C2	-3.81	1.37	1.52
7	B	4006	FAD	O2B-C2B	-3.76	1.34	1.43
7	A	3006	FAD	PA-O2A	-3.75	1.39	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4006	FAD	PA-O2A	-3.56	1.40	1.55
7	B	4006	FAD	C2B-C1B	-3.18	1.48	1.53
4	A	3003	MTE	P-O2P	-3.10	1.44	1.54
7	A	3006	FAD	PA-O5B	-2.80	1.47	1.59
7	A	3006	FAD	C6A-N6A	-2.72	1.22	1.34
8	B	4008	GOL	O3-C3	-2.65	1.30	1.42
7	B	4006	FAD	C2'-C3'	-2.64	1.48	1.53
7	A	3006	FAD	C5A-N7A	-2.56	1.30	1.39
7	A	3006	FAD	C2B-C1B	-2.50	1.49	1.53
7	A	3006	FAD	O4-C4	-2.46	1.18	1.24
7	B	4006	FAD	P-O2P	-2.44	1.44	1.55
8	A	3008	GOL	O3-C3	-2.32	1.32	1.42
7	B	4006	FAD	C5A-N7A	-2.28	1.31	1.39
7	A	3006	FAD	C2'-C3'	-2.17	1.49	1.53
4	B	4003	MTE	P-O2P	-2.17	1.47	1.54
8	A	3008	GOL	C1-C2	-2.15	1.43	1.52
4	B	4003	MTE	C10-N8	2.08	1.41	1.35
6	B	4005	SAL	C3-C2	2.10	1.43	1.39
6	A	3005	SAL	C3-C2	2.19	1.43	1.39
7	A	3006	FAD	O2'-C2'	2.20	1.48	1.43
6	A	3005	SAL	C6-C1	2.21	1.43	1.40
4	B	4003	MTE	O3'-C7	2.22	1.46	1.43
4	A	3003	MTE	C2'-C1'	2.33	1.50	1.35
4	B	4003	MTE	C2'-C1'	2.37	1.50	1.35
4	A	3003	MTE	O4-C4	2.37	1.30	1.24
6	B	4005	SAL	C6-C1	2.38	1.43	1.40
7	A	3006	FAD	C6-C5X	2.39	1.45	1.41
6	B	4005	SAL	C5-C6	2.65	1.44	1.38
7	B	4006	FAD	C9-C8	2.67	1.45	1.37
7	B	4006	FAD	C5B-C4B	2.69	1.60	1.51
4	A	3003	MTE	C10-N1	2.78	1.39	1.34
6	A	3005	SAL	C5-C6	2.79	1.44	1.38
4	A	3003	MTE	C2-N3	2.83	1.40	1.35
7	A	3006	FAD	C10-N1	2.93	1.40	1.35
7	B	4006	FAD	C6-C7	3.00	1.46	1.37
4	B	4003	MTE	C2-N1	3.08	1.41	1.35
7	B	4006	FAD	O2'-C2'	3.10	1.50	1.43
7	B	4006	FAD	O3'-C3'	3.23	1.50	1.43
7	B	4006	FAD	C6A-C5A	3.30	1.59	1.42
7	A	3006	FAD	C6-C7	3.42	1.47	1.37
7	A	3006	FAD	C6A-C5A	3.58	1.61	1.42
7	B	4006	FAD	C10-N10	3.59	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3003	MTE	C2-N1	3.65	1.42	1.35
7	B	4006	FAD	C2-N3	3.79	1.46	1.38
8	B	4007	GOL	O1-C1	3.83	1.59	1.42
4	B	4003	MTE	C4-C9	3.84	1.46	1.41
7	A	3006	FAD	C4X-N5	4.00	1.39	1.33
7	B	4006	FAD	C9-C9A	4.03	1.49	1.40
7	B	4006	FAD	C4-C4X	4.19	1.49	1.41
4	A	3003	MTE	O3'-C3'	4.22	1.49	1.43
7	B	4006	FAD	C4X-N5	4.39	1.40	1.33
7	A	3006	FAD	O4B-C4B	4.46	1.55	1.45
7	B	4006	FAD	O4B-C4B	4.57	1.55	1.45
7	B	4006	FAD	C5A-C4A	4.60	1.50	1.40
7	A	3006	FAD	O3'-C3'	4.64	1.53	1.43
4	A	3003	MTE	O3'-C7	4.86	1.50	1.43
7	B	4006	FAD	C5X-N5	4.92	1.43	1.35
4	B	4003	MTE	C4-N3	5.07	1.42	1.33
4	B	4003	MTE	O3'-C3'	5.10	1.51	1.43
7	A	3006	FAD	C9-C9A	5.14	1.51	1.40
7	B	4006	FAD	C2A-N3A	5.14	1.41	1.32
7	A	3006	FAD	C5A-C4A	5.14	1.52	1.40
4	A	3003	MTE	C4-C9	5.15	1.48	1.41
7	A	3006	FAD	C4-C4X	5.17	1.51	1.41
7	B	4006	FAD	C6-C5X	5.37	1.50	1.41
7	A	3006	FAD	C2-N3	5.44	1.49	1.38
4	B	4003	MTE	C9-N5	5.48	1.50	1.38
7	A	3006	FAD	C5X-N5	5.62	1.44	1.35
7	A	3006	FAD	C10-N10	6.00	1.46	1.39
8	A	3008	GOL	O1-C1	6.08	1.68	1.42
4	A	3003	MTE	C4-N3	6.08	1.44	1.33
7	A	3006	FAD	C8-C7	6.38	1.58	1.41
4	A	3003	MTE	C9-N5	6.54	1.52	1.38
8	B	4008	GOL	O1-C1	6.61	1.71	1.42
7	A	3006	FAD	C2A-N1A	6.68	1.46	1.33
7	B	4006	FAD	C2A-N1A	6.78	1.47	1.33
7	B	4006	FAD	C8-C7	6.87	1.59	1.41
7	A	3006	FAD	O4B-C1B	6.99	1.51	1.41
7	B	4006	FAD	C4-N3	7.05	1.45	1.33
7	A	3006	FAD	C9A-C5X	7.19	1.57	1.42
7	A	3006	FAD	C2A-N3A	7.31	1.45	1.32
7	A	3006	FAD	C4-N3	7.48	1.46	1.33
7	B	4006	FAD	C9A-C5X	7.80	1.59	1.42
7	A	3006	FAD	C4X-C10	7.98	1.55	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4003	MTE	C6-N5	8.53	1.55	1.45
7	B	4006	FAD	C4A-N3A	8.54	1.48	1.35
7	B	4006	FAD	C4X-C10	8.65	1.56	1.40
4	A	3003	MTE	C6-N5	8.83	1.56	1.45
7	A	3006	FAD	C4A-N3A	9.28	1.49	1.35
7	A	3006	FAD	C9A-N10	11.34	1.54	1.38
7	B	4006	FAD	C9A-N10	12.06	1.55	1.38
4	A	3003	MTE	C9-C10	13.44	1.66	1.41
4	B	4003	MTE	C9-C10	14.72	1.69	1.41
4	A	3003	MTE	C7-C6	24.15	1.71	1.53
4	B	4003	MTE	C7-C6	25.67	1.72	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	4006	FAD	C4-C4X-C10	-7.92	114.87	119.94
7	A	3006	FAD	C4-C4X-C10	-7.76	114.98	119.94
7	A	3006	FAD	N3A-C2A-N1A	-7.29	123.14	128.87
7	B	4006	FAD	O5B-PA-O1A	-5.64	86.14	109.21
7	A	3006	FAD	C5X-C9A-N10	-5.44	113.50	117.58
7	B	4006	FAD	C5X-C9A-N10	-5.44	113.50	117.58
7	B	4006	FAD	N3-C2-N1	-5.35	118.68	127.69
7	A	3006	FAD	O5B-PA-O1A	-5.23	87.81	109.21
7	A	3006	FAD	N3-C2-N1	-5.08	119.14	127.69
7	B	4006	FAD	N3A-C2A-N1A	-4.91	125.01	128.87
4	B	4003	MTE	O3'-C7-C6	-4.70	105.75	108.96
7	B	4006	FAD	C4X-C10-N10	-4.63	117.16	120.52
7	B	4006	FAD	C4X-C4-N3	-4.58	117.53	123.52
7	A	3006	FAD	C4X-C10-N10	-4.46	117.28	120.52
4	A	3003	MTE	N3-C2-N1	-4.35	118.41	125.51
7	A	3006	FAD	O4B-C4B-C5B	-4.00	94.96	109.29
7	A	3006	FAD	C4X-C4-N3	-3.82	118.53	123.52
4	B	4003	MTE	N3-C2-N1	-3.70	119.46	125.51
4	A	3003	MTE	O3'-C7-C6	-3.46	106.60	108.96
7	B	4006	FAD	O4B-C4B-C5B	-3.33	97.36	109.29
7	A	3006	FAD	O3'-C3'-C2'	-3.21	100.41	108.73
7	B	4006	FAD	O3'-C3'-C2'	-2.98	101.01	108.73
7	B	4006	FAD	O4B-C4B-C3B	-2.82	99.43	105.16
7	A	3006	FAD	O4B-C4B-C3B	-2.45	100.20	105.16
7	A	3006	FAD	C8M-C8-C9	-2.20	114.11	120.33
7	B	4006	FAD	C8M-C8-C9	-2.19	114.15	120.33
7	A	3006	FAD	O2A-PA-O3P	2.01	113.89	105.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	3006	FAD	O2A-PA-O5B	2.11	118.29	108.24
7	B	4006	FAD	O2A-PA-O5B	2.16	118.52	108.24
6	B	4005	SAL	C2-C1-C1'	2.24	123.92	121.64
4	B	4003	MTE	O3P-P-O4'	2.26	113.32	106.72
8	A	3007	GOL	O2-C2-C1	2.29	119.45	108.47
7	B	4006	FAD	O5B-C5B-C4B	2.40	117.73	109.09
7	A	3006	FAD	O2P-P-O5'	2.45	119.89	108.24
7	B	4006	FAD	O2P-P-O5'	2.52	120.25	108.24
7	B	4006	FAD	C2A-N1A-C6A	2.64	123.48	118.77
7	A	3006	FAD	C8M-C8-C7	2.65	126.43	120.73
7	B	4006	FAD	C8M-C8-C7	2.92	127.00	120.73
7	A	3006	FAD	O5B-C5B-C4B	3.08	120.21	109.09
7	A	3006	FAD	C2A-N1A-C6A	3.20	124.47	118.77
8	A	3007	GOL	O1-C1-C2	3.39	127.17	109.97
8	B	4007	GOL	O1-C1-C2	3.57	128.07	109.97
7	B	4006	FAD	C4-C4X-N5	4.11	123.70	118.70
4	A	3003	MTE	O3P-P-O4'	4.12	118.76	106.72
8	B	4008	GOL	O1-C1-C2	4.18	131.18	109.97
7	A	3006	FAD	C4-C4X-N5	4.25	123.86	118.70
4	B	4003	MTE	N2-C2-N3	4.33	124.34	117.20
8	A	3008	GOL	O1-C1-C2	4.42	132.38	109.97
4	A	3003	MTE	N2-C2-N3	4.53	124.67	117.20
8	A	3007	GOL	O2-C2-C3	5.15	133.20	108.47
4	B	4003	MTE	C2-N1-C10	5.20	126.32	114.63
8	B	4007	GOL	O2-C2-C3	5.22	133.55	108.47
4	A	3003	MTE	C2-N1-C10	5.41	126.78	114.63
7	B	4006	FAD	C4X-N5-C5X	5.45	123.14	116.72
4	A	3003	MTE	N8-C10-N1	5.55	125.45	116.62
7	A	3006	FAD	C4X-N5-C5X	5.59	123.31	116.72
8	B	4008	GOL	O2-C2-C3	5.79	136.26	108.47
8	A	3008	GOL	O2-C2-C3	6.02	137.36	108.47
4	B	4003	MTE	N8-C10-N1	6.27	126.59	116.62
4	A	3003	MTE	C4-N3-C2	6.77	123.82	115.88
4	B	4003	MTE	C4-N3-C2	6.91	123.97	115.88
7	A	3006	FAD	C4-N3-C2	8.17	121.98	115.16
8	A	3008	GOL	O3-C3-C2	10.36	162.50	109.97
7	B	4006	FAD	C4-N3-C2	10.39	123.83	115.16
8	B	4007	GOL	O3-C3-C2	10.86	165.04	109.97
8	B	4008	GOL	O3-C3-C2	10.92	165.33	109.97
8	A	3007	GOL	O3-C3-C2	11.08	166.16	109.97

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	4006	FAD	C2'
7	B	4006	FAD	C3'
7	A	3006	FAD	C2'
7	A	3006	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3003	MTE	1	0
5	A	3004	MOS	2	0
7	A	3006	FAD	3	0
8	A	3007	GOL	4	0
8	A	3008	GOL	3	0
4	B	4003	MTE	2	0
5	B	4004	MOS	2	0
6	B	4005	SAL	1	0
7	B	4006	FAD	2	0
8	B	4007	GOL	7	0
8	B	4008	GOL	4	0

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.