



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:53 pm BST

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](mailto: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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

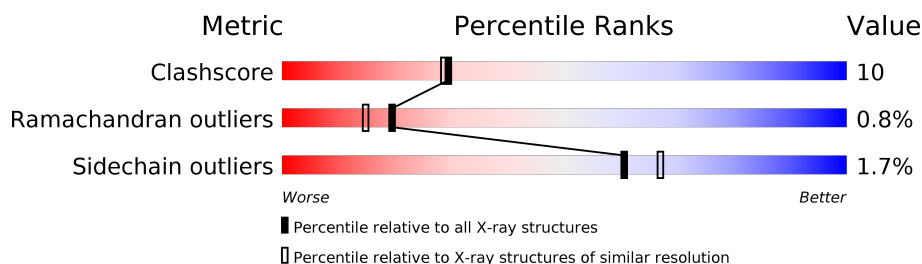
# 1 Overall quality at a glance

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

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

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	-	-	-
7	FAD	B	4006	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 [i](#)

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.

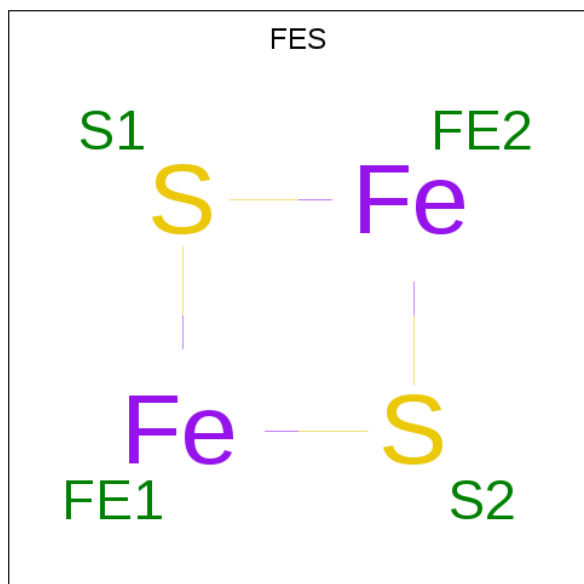
- Molecule 1 is a protein called XANTHINE DEHYDROGENASE.

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).

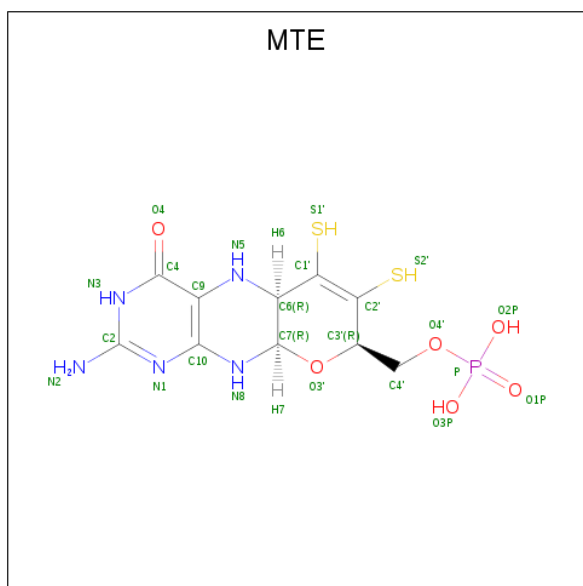
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



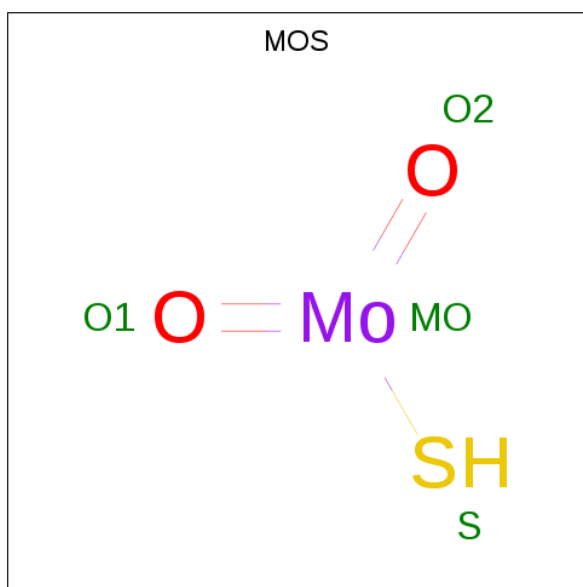
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0

- 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<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P<sub>2</sub>).



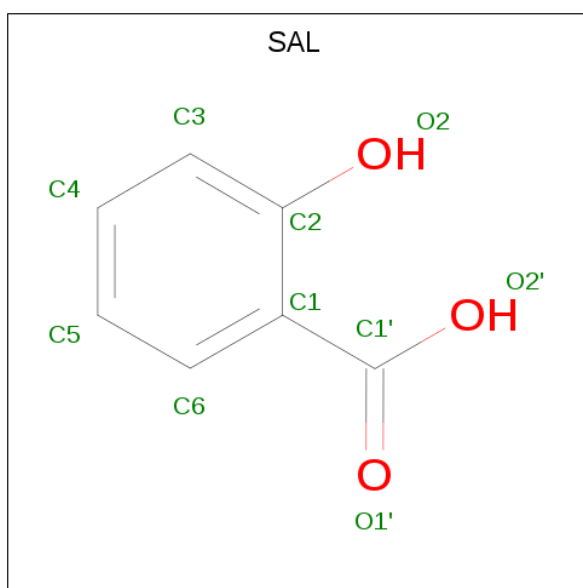
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 24 10 5 6 1 2	0	0
4	B	1	Total C N O P S 24 10 5 6 1 2	0	0

- Molecule 5 is DIOXOTHIO MOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO<sub>2</sub>S).



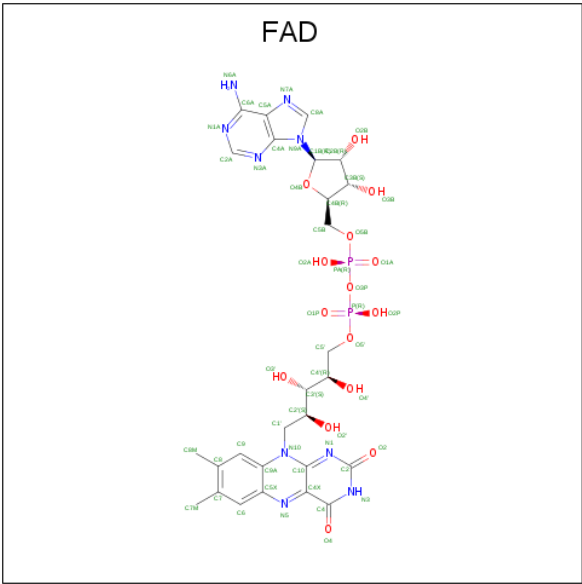
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

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



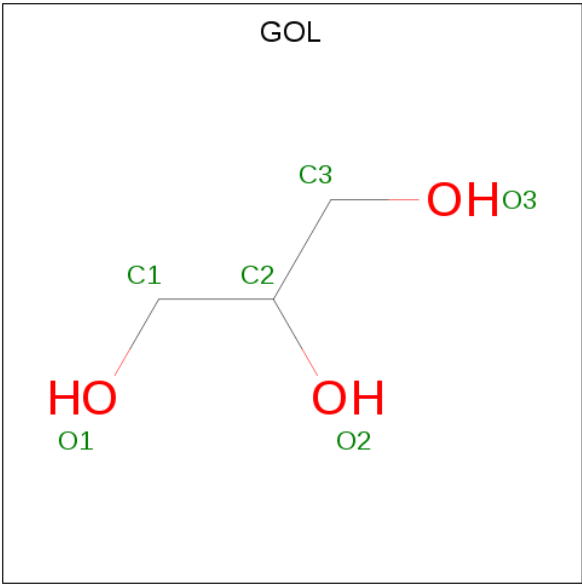
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

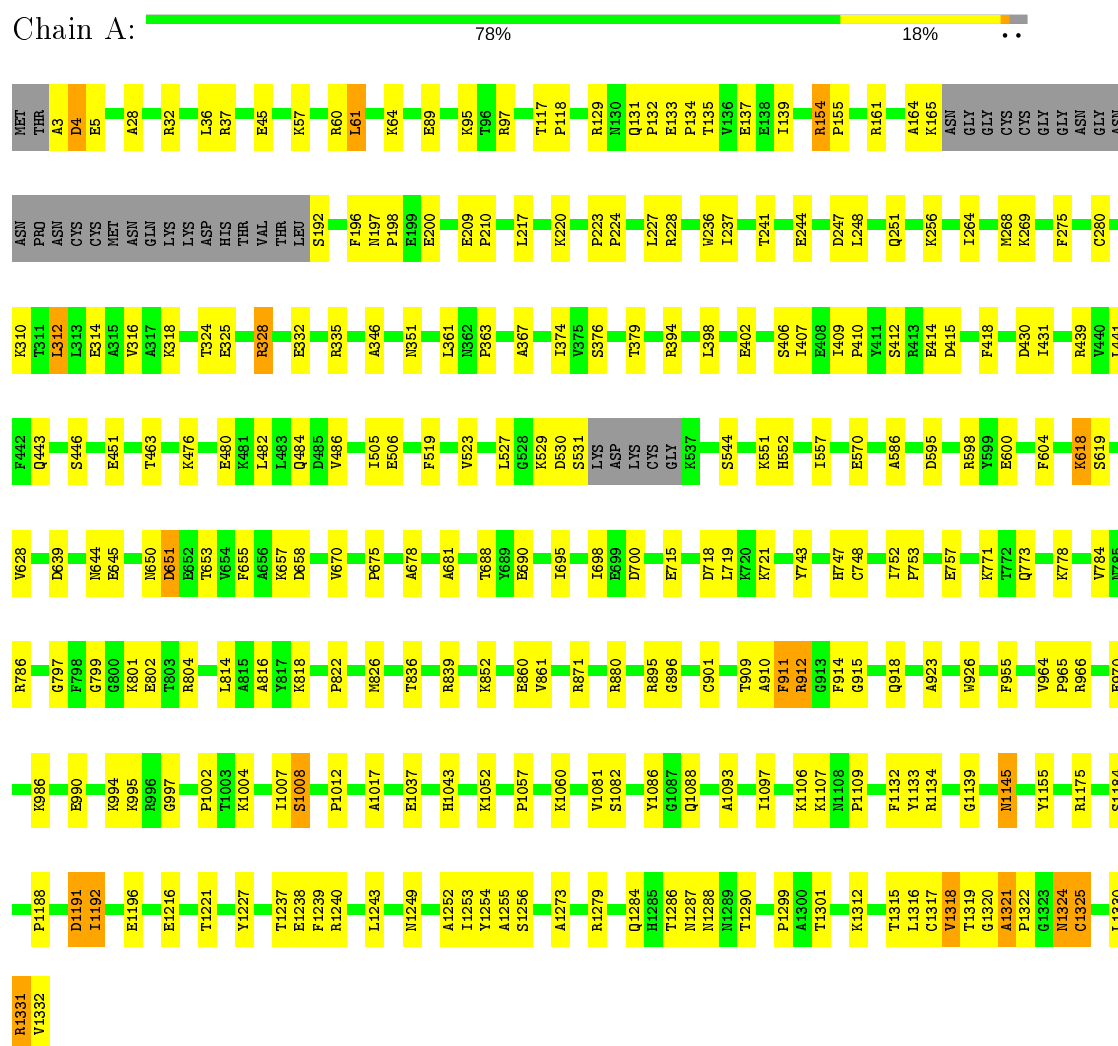


### 3 Residue-property plots

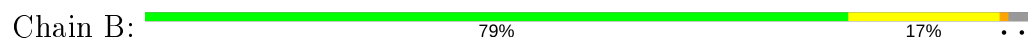
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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



#### • Molecule 1: XANTHINE DEHYDROGENASE





## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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(°)	Ideal(°)
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:1331:ARG:O	1:A:1332:VAL:O	2.05	0.74
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.87	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:839:ARG:NH1	8:A:3007:GOL:O1	2.44	0.50
1:A:60:ARG:O	1:A:61:LEU:HB2	2.09	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:1320:GLY:O	1:A:1321:ALA:C	2.52	0.48
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.11	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:117:THR:CG2	1:B:586:ALA:HA	2.44	0.48
1:B:129:ARG:HG3	1:B:129:ARG:NH1	2.29	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:557:ILE:HB	1:A:1240:ARG:HG2	1.99	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: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:223:PRO:HA	1:A:224:PRO:HD3	1.85	0.42
1:A:137:GLU:HG3	1:A:551:LYS:HZ2	1.83	0.42
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.54	0.42
1:A:237:ILE:HG21	1:A:248:LEU:HD11	2.01	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: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:A:1132:PHE:CG	1:B:1126:SER:HB2	2.55	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 [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	1293/1332 (97%)	1228 (95%)	54 (4%)	11 (1%)	17	12
1	B	1290/1332 (97%)	1236 (96%)	45 (4%)	9 (1%)	22	18
All	All	2583/2664 (97%)	2464 (95%)	99 (4%)	20 (1%)	19	15

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 [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	1101/1128 (98%)	1084 (98%)	17 (2%)	65	71
1	B	1098/1128 (97%)	1078 (98%)	20 (2%)	59	65
All	All	2199/2256 (98%)	2162 (98%)	37 (2%)	60	67

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 ⓘ

There are no RNA molecules 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 [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$
8	GOL	B	4008	-	5,5,5	4.29	3 (60%)	5,5,5	6.16	3 (60%)
3	FES	A	3001	1	0,4,4	0.00	-	-		
8	GOL	A	3008	-	5,5,5	4.37	3 (60%)	5,5,5	6.03	3 (60%)
6	SAL	A	3005	-	8,10,10	2.26	4 (50%)	9,13,13	1.18	0
8	GOL	B	4007	-	5,5,5	6.43	5 (100%)	5,5,5	6.00	3 (60%)
5	MOS	A	3004	4	0,3,3	0.00	-	-		
3	FES	A	3002	1	0,4,4	0.00	-	-		
3	FES	B	4002	1	0,4,4	0.00	-	-		
5	MOS	B	4004	4	0,3,3	0.00	-	-		
6	SAL	B	4005	-	8,10,10	2.24	4 (50%)	9,13,13	1.23	0
7	FAD	A	3006	-	51,58,58	5.18	33 (64%)	60,89,89	2.78	21 (35%)
8	GOL	A	3007	-	5,5,5	6.80	5 (100%)	5,5,5	6.09	4 (80%)
4	MTE	A	3003	5	21,26,26	7.16	17 (80%)	21,40,40	3.76	9 (42%)
7	FAD	B	4006	-	51,58,58	5.09	34 (66%)	60,89,89	2.90	22 (36%)
4	MTE	B	4003	5	21,26,26	7.10	13 (61%)	21,40,40	3.66	9 (42%)
3	FES	B	4001	1	0,4,4	0.00	-	-		

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
8	GOL	B	4008	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	3001	1	-	-	0/1/1/1
8	GOL	A	3008	-	-	2/4/4/4	-
4	MTE	B	4003	5	-	1/6/34/34	0/3/3/3
8	GOL	B	4007	-	-	2/4/4/4	-
3	FES	A	3002	1	-	-	0/1/1/1
3	FES	B	4002	1	-	-	0/1/1/1
8	GOL	A	3007	-	-	2/4/4/4	-
6	SAL	B	4005	-	-	0/0/4/4	0/1/1/1
6	SAL	A	3005	-	-	0/0/4/4	0/1/1/1
4	MTE	A	3003	5	-	1/6/34/34	0/3/3/3
7	FAD	B	4006	-	2/2/9/9	3/30/50/50	0/6/6/6
7	FAD	A	3006	-	2/2/9/9	3/30/50/50	0/6/6/6
3	FES	B	4001	1	-	-	0/1/1/1

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4003	MTE	C7-C6	23.94	1.72	1.53
4	A	3003	MTE	C7-C6	22.52	1.71	1.53
7	B	4006	FAD	C4X-C10	18.04	1.56	1.38
7	A	3006	FAD	C4X-C10	16.80	1.55	1.38
4	B	4003	MTE	C9-C10	14.64	1.69	1.41
4	A	3003	MTE	C9-C10	13.36	1.66	1.41
7	B	4006	FAD	C9A-N10	12.85	1.55	1.38
8	A	3007	GOL	C3-C2	-12.47	1.00	1.51
7	A	3006	FAD	C9A-N10	12.10	1.54	1.38
8	B	4007	GOL	C3-C2	-11.63	1.03	1.51
7	A	3006	FAD	C4A-N3A	9.83	1.49	1.35
7	A	3006	FAD	C5'-C4'	-9.44	1.38	1.51
7	B	4006	FAD	C4A-N3A	9.04	1.48	1.35
7	B	4006	FAD	C9A-C5X	8.23	1.59	1.42
7	A	3006	FAD	C2A-N3A	8.05	1.45	1.32
7	B	4006	FAD	C5'-C4'	-7.87	1.40	1.51
7	A	3006	FAD	C4-N3	7.75	1.46	1.33
4	A	3003	MTE	C6-N5	7.75	1.56	1.45
7	A	3006	FAD	C9A-C5X	7.60	1.57	1.42
4	B	4003	MTE	C6-N5	7.48	1.55	1.45
7	B	4006	FAD	C8-C7	7.43	1.59	1.40
7	B	4006	FAD	C4-N3	7.30	1.45	1.33
7	A	3006	FAD	O4B-C1B	7.27	1.51	1.41
4	A	3003	MTE	C9-N5	7.05	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4006	FAD	C2A-N1A	7.01	1.47	1.33
4	A	3003	MTE	C4'-C3'	-6.94	1.42	1.52
7	A	3006	FAD	C2A-N1A	6.91	1.46	1.33
7	A	3006	FAD	C8-C7	6.89	1.58	1.40
8	B	4008	GOL	O1-C1	6.77	1.71	1.42
8	A	3008	GOL	C3-C2	-6.65	1.24	1.51
4	A	3003	MTE	C4-N3	6.30	1.44	1.33
8	A	3008	GOL	O1-C1	6.22	1.68	1.42
7	B	4006	FAD	C8A-N7A	-6.09	1.23	1.34
7	A	3006	FAD	C4-C4X	6.05	1.51	1.41
8	B	4008	GOL	C3-C2	-5.97	1.27	1.51
4	B	4003	MTE	C9-N5	5.92	1.50	1.38
4	A	3003	MTE	P-O4'	-5.86	1.41	1.60
4	A	3003	MTE	P-O3P	-5.79	1.32	1.54
7	A	3006	FAD	C10-N1	5.73	1.40	1.33
7	A	3006	FAD	C2-N3	5.71	1.49	1.38
7	B	4006	FAD	C2A-N3A	5.67	1.41	1.32
7	A	3006	FAD	C9-C9A	5.62	1.51	1.40
4	B	4003	MTE	O3'-C3'	5.54	1.51	1.43
4	B	4003	MTE	P-O4'	-5.51	1.42	1.60
4	A	3003	MTE	C4-C9	5.34	1.48	1.41
7	A	3006	FAD	C5X-N5	5.34	1.44	1.35
4	B	4003	MTE	C4-N3	5.26	1.42	1.33
7	B	4006	FAD	C6-C5X	5.23	1.50	1.41
7	A	3006	FAD	C8A-N7A	-5.17	1.25	1.34
8	A	3007	GOL	C1-C2	-5.07	1.30	1.51
8	B	4007	GOL	O2-C2	-4.98	1.28	1.43
8	A	3007	GOL	O2-C2	-4.96	1.28	1.43
7	B	4006	FAD	C4-C4X	4.90	1.49	1.41
7	A	3006	FAD	C6A-C5A	4.84	1.61	1.43
4	B	4003	MTE	C4'-C3'	-4.80	1.45	1.52
4	A	3003	MTE	O3'-C7	4.77	1.50	1.43
7	B	4006	FAD	O5B-C5B	-4.74	1.26	1.44
7	B	4006	FAD	C4X-N5	4.73	1.40	1.33
7	B	4006	FAD	O4B-C4B	4.70	1.55	1.45
7	B	4006	FAD	C5X-N5	4.67	1.43	1.35
7	B	4006	FAD	PA-O5B	-4.65	1.40	1.59
8	A	3007	GOL	O3-C3	-4.64	1.22	1.42
7	A	3006	FAD	O3'-C3'	4.64	1.53	1.43
7	A	3006	FAD	O4B-C4B	4.59	1.55	1.45
4	A	3003	MTE	O3'-C3'	4.58	1.49	1.43
6	A	3005	SAL	C1-C1'	-4.47	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4005	SAL	C1-C1'	-4.45	1.43	1.47
7	B	4006	FAD	C6A-C5A	4.45	1.59	1.43
7	B	4006	FAD	C10-N1	4.45	1.39	1.33
7	B	4006	FAD	C9-C9A	4.41	1.49	1.40
4	B	4003	MTE	P-O3P	-4.37	1.38	1.54
7	A	3006	FAD	C4X-N5	4.30	1.39	1.33
8	B	4007	GOL	O3-C3	-4.30	1.24	1.42
7	A	3006	FAD	O5B-C5B	-4.25	1.28	1.44
7	A	3006	FAD	C5A-C4A	4.22	1.52	1.40
7	B	4006	FAD	C2-N3	3.98	1.46	1.38
4	B	4003	MTE	C4-C9	3.95	1.46	1.41
8	B	4007	GOL	O1-C1	3.92	1.59	1.42
4	A	3003	MTE	C2-N1	3.87	1.42	1.35
7	B	4006	FAD	O2B-C2B	-3.77	1.34	1.43
7	A	3006	FAD	C6-C7	3.76	1.47	1.37
7	B	4006	FAD	C5A-C4A	3.76	1.50	1.40
8	B	4007	GOL	C1-C2	-3.56	1.37	1.51
7	A	3006	FAD	PA-O2A	-3.44	1.39	1.55
7	B	4006	FAD	C2B-C1B	-3.41	1.48	1.53
7	B	4006	FAD	C6-C7	3.31	1.46	1.37
7	B	4006	FAD	O2'-C2'	3.28	1.50	1.43
7	B	4006	FAD	PA-O2A	-3.27	1.40	1.55
4	B	4003	MTE	C2-N1	3.26	1.41	1.35
7	B	4006	FAD	O3'-C3'	3.23	1.50	1.43
7	A	3006	FAD	C6A-N6A	-3.05	1.22	1.34
4	A	3003	MTE	C2-N3	3.00	1.40	1.35
7	A	3006	FAD	PA-O5B	-2.98	1.47	1.59
7	B	4006	FAD	C9-C8	2.94	1.45	1.37
7	B	4006	FAD	C5B-C4B	2.82	1.60	1.51
4	A	3003	MTE	P-O2P	-2.80	1.44	1.54
7	B	4006	FAD	C2'-C3'	-2.77	1.48	1.53
8	B	4008	GOL	O3-C3	-2.73	1.30	1.42
7	A	3006	FAD	C2B-C1B	-2.70	1.49	1.53
4	A	3003	MTE	C10-N1	2.65	1.39	1.34
7	A	3006	FAD	C5A-N7A	-2.60	1.30	1.39
6	A	3005	SAL	C5-C6	2.57	1.44	1.38
7	A	3006	FAD	O4-C4	-2.46	1.18	1.24
6	B	4005	SAL	C5-C6	2.45	1.44	1.38
6	B	4005	SAL	C6-C1	2.42	1.43	1.40
4	A	3003	MTE	O4-C4	2.40	1.30	1.24
8	A	3008	GOL	O3-C3	-2.39	1.32	1.42
4	B	4003	MTE	C2'-C1'	2.37	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4006	FAD	C5A-N7A	-2.33	1.31	1.39
4	A	3003	MTE	C2'-C1'	2.33	1.50	1.35
7	A	3006	FAD	O2'-C2'	2.32	1.48	1.43
7	A	3006	FAD	C6-C5X	2.30	1.45	1.41
7	A	3006	FAD	C2'-C3'	-2.27	1.49	1.53
6	A	3005	SAL	C3-C2	2.26	1.43	1.39
6	A	3005	SAL	C6-C1	2.25	1.43	1.40
7	B	4006	FAD	P-O2P	-2.25	1.44	1.55
7	A	3006	FAD	C1'-N10	2.20	1.50	1.48
6	B	4005	SAL	C3-C2	2.16	1.43	1.39
7	B	4006	FAD	C1'-N10	2.16	1.50	1.48
4	B	4003	MTE	O3'-C7	2.14	1.46	1.43
8	A	3007	GOL	O1-C1	2.01	1.50	1.42

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	3007	GOL	O3-C3-C2	11.67	166.16	110.20
8	B	4008	GOL	O3-C3-C2	11.50	165.33	110.20
8	B	4007	GOL	O3-C3-C2	11.44	165.04	110.20
4	A	3003	MTE	C4-C9-N5	10.93	128.29	119.12
8	A	3008	GOL	O3-C3-C2	10.91	162.50	110.20
7	B	4006	FAD	C4-N3-C2	10.29	123.83	115.14
4	B	4003	MTE	C4-C9-N5	10.13	127.62	119.12
7	A	3006	FAD	C4-N3-C2	8.10	121.98	115.14
7	B	4006	FAD	C4-C4X-C10	-7.67	114.87	119.95
7	A	3006	FAD	C4-C4X-C10	-7.52	114.98	119.95
4	B	4003	MTE	P-O4'-C4'	6.74	136.86	118.30
7	B	4006	FAD	C5'-C4'-C3'	-6.56	99.52	112.20
7	A	3006	FAD	C4X-N5-C5X	6.54	123.31	116.77
8	A	3008	GOL	O2-C2-C3	6.41	137.36	109.12
7	B	4006	FAD	C4X-N5-C5X	6.37	123.14	116.77
7	A	3006	FAD	C5'-C4'-C3'	-6.24	100.14	112.20
8	B	4008	GOL	O2-C2-C3	6.16	136.26	109.12
7	B	4006	FAD	O5B-PA-O1A	-5.87	86.14	109.07
7	A	3006	FAD	C5X-C9A-N10	-5.81	113.50	117.72
7	B	4006	FAD	C5X-C9A-N10	-5.81	113.50	117.72
8	B	4007	GOL	O2-C2-C3	5.55	133.55	109.12
8	A	3007	GOL	O2-C2-C3	5.47	133.20	109.12
4	A	3003	MTE	C2-N1-C10	5.46	126.78	114.54
4	A	3003	MTE	P-O4'-C4'	5.46	133.33	118.30
7	A	3006	FAD	O5B-PA-O1A	-5.44	87.81	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4003	MTE	C2-N1-C10	5.25	126.32	114.54
4	B	4003	MTE	C4-N3-C2	5.06	123.97	115.93
4	A	3003	MTE	C4-N3-C2	4.96	123.82	115.93
4	B	4003	MTE	O3'-C7-C6	-4.82	105.75	108.96
4	A	3003	MTE	N2-C2-N3	4.77	124.67	117.25
8	A	3008	GOL	O1-C1-C2	4.62	132.38	110.20
7	A	3006	FAD	C4-C4X-N5	4.61	123.86	118.60
4	B	4003	MTE	N2-C2-N3	4.56	124.34	117.25
4	A	3003	MTE	O3P-P-O4'	4.52	118.76	106.73
4	A	3003	MTE	N3-C2-N1	-4.47	118.41	125.42
7	B	4006	FAD	C4-C4X-N5	4.46	123.70	118.60
7	A	3006	FAD	O4B-C4B-C5B	-4.38	94.96	109.37
8	B	4008	GOL	O1-C1-C2	4.37	131.18	110.20
7	A	3006	FAD	C5A-C6A-N6A	4.36	126.98	120.35
7	B	4006	FAD	C4X-C4-N3	-4.31	117.53	123.43
7	B	4006	FAD	C5A-C6A-N6A	3.92	126.31	120.35
4	B	4003	MTE	N3-C2-N1	-3.80	119.46	125.42
8	B	4007	GOL	O1-C1-C2	3.73	128.07	110.20
7	B	4006	FAD	O4B-C4B-C5B	-3.65	97.36	109.37
7	A	3006	FAD	C4X-C4-N3	-3.58	118.53	123.43
4	A	3003	MTE	O3'-C7-C6	-3.54	106.60	108.96
7	A	3006	FAD	N3A-C2A-N1A	-3.54	123.14	128.68
8	A	3007	GOL	O1-C1-C2	3.54	127.17	110.20
7	A	3006	FAD	O3'-C3'-C2'	-3.48	100.41	108.81
7	B	4006	FAD	C4'-C3'-C2'	-3.37	106.36	113.36
7	A	3006	FAD	C2A-N1A-C6A	3.34	124.47	118.75
7	A	3006	FAD	O5B-C5B-C4B	3.26	120.21	108.99
7	B	4006	FAD	O3'-C3'-C2'	-3.23	101.01	108.81
7	B	4006	FAD	C4X-C10-N10	-3.06	117.16	120.30
7	B	4006	FAD	C8M-C8-C7	3.06	127.00	120.74
7	A	3006	FAD	C4X-C10-N10	-2.94	117.28	120.30
4	A	3003	MTE	O3'-C7-N8	-2.91	105.58	108.57
7	B	4006	FAD	O4B-C4B-C3B	-2.87	99.43	105.11
4	B	4003	MTE	O3'-C7-N8	-2.79	105.70	108.57
7	A	3006	FAD	C8M-C8-C7	2.78	126.43	120.74
7	B	4006	FAD	C2A-N1A-C6A	2.76	123.48	118.75
7	B	4006	FAD	O2P-P-O5'	2.69	120.25	107.75
7	A	3006	FAD	O2P-P-O5'	2.62	119.89	107.75
7	A	3006	FAD	C8M-C8-C9	-2.61	114.11	120.34
7	B	4006	FAD	C8M-C8-C9	-2.59	114.15	120.34
7	B	4006	FAD	O5B-C5B-C4B	2.54	117.73	108.99
7	A	3006	FAD	O4B-C4B-C3B	-2.48	100.20	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4003	MTE	O3P-P-O4'	2.47	113.32	106.73
8	A	3007	GOL	O2-C2-C1	2.35	119.45	109.12
7	B	4006	FAD	N3A-C2A-N1A	-2.35	125.01	128.68
7	B	4006	FAD	O2A-PA-O5B	2.32	118.52	107.75
7	A	3006	FAD	O2A-PA-O5B	2.27	118.29	107.75
7	A	3006	FAD	C4'-C3'-C2'	-2.23	108.72	113.36
7	B	4006	FAD	C5A-C6A-N1A	-2.21	115.34	120.35

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'

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	4008	GOL	O1-C1-C2-C3
8	B	4008	GOL	C1-C2-C3-O3
8	A	3008	GOL	O1-C1-C2-C3
8	A	3008	GOL	C1-C2-C3-O3
8	B	4007	GOL	C1-C2-C3-O3
8	A	3007	GOL	C1-C2-C3-O3
4	A	3003	MTE	C3'-C4'-O4'-P
4	B	4003	MTE	C3'-C4'-O4'-P
8	B	4007	GOL	O1-C1-C2-O2
7	A	3006	FAD	O3'-C3'-C4'-C5'
7	A	3006	FAD	O3'-C3'-C4'-O4'
8	A	3007	GOL	O1-C1-C2-O2
7	B	4006	FAD	O3'-C3'-C4'-O4'
7	B	4006	FAD	O3'-C3'-C4'-C5'
7	B	4006	FAD	O4B-C4B-C5B-O5B
7	A	3006	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	4008	GOL	4	0

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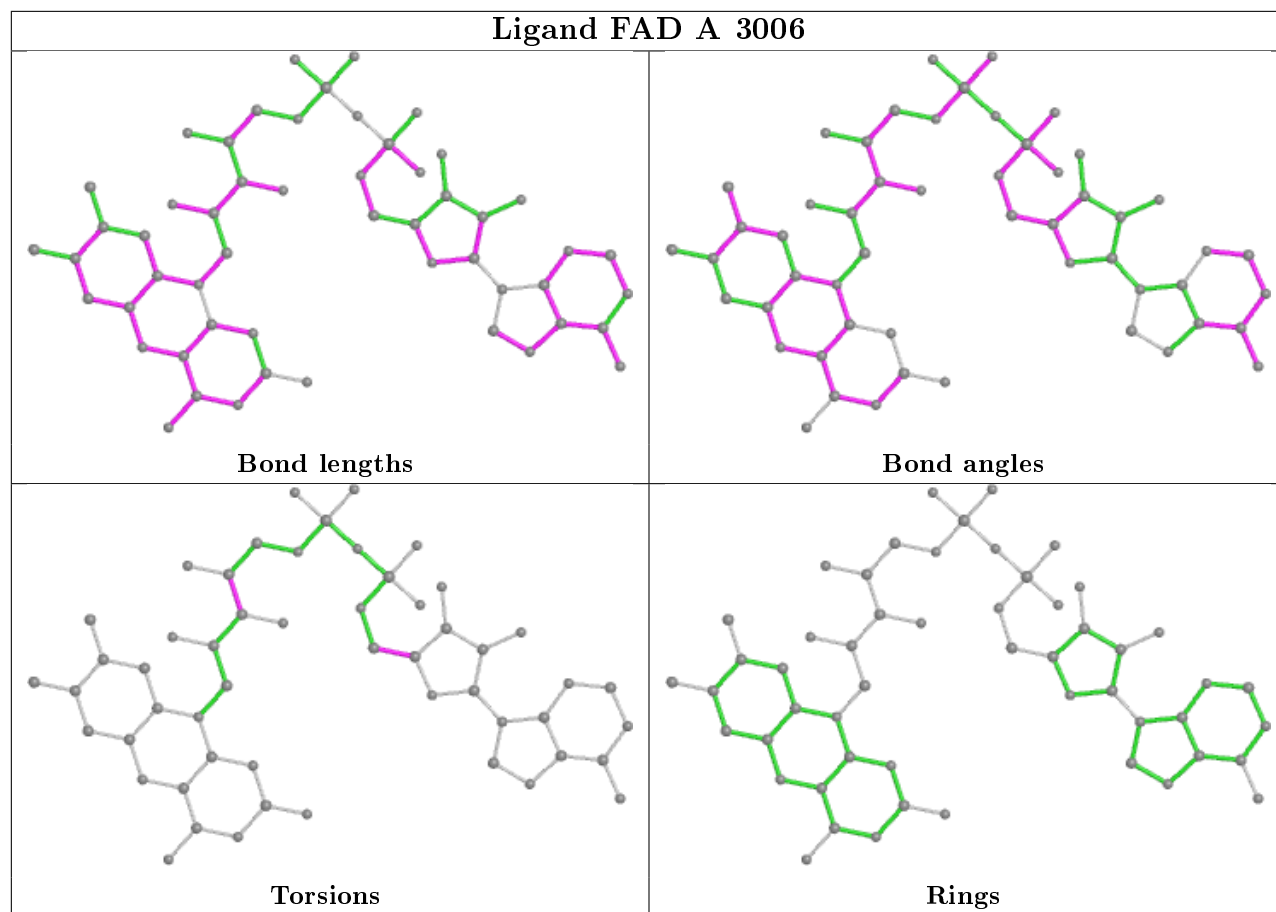


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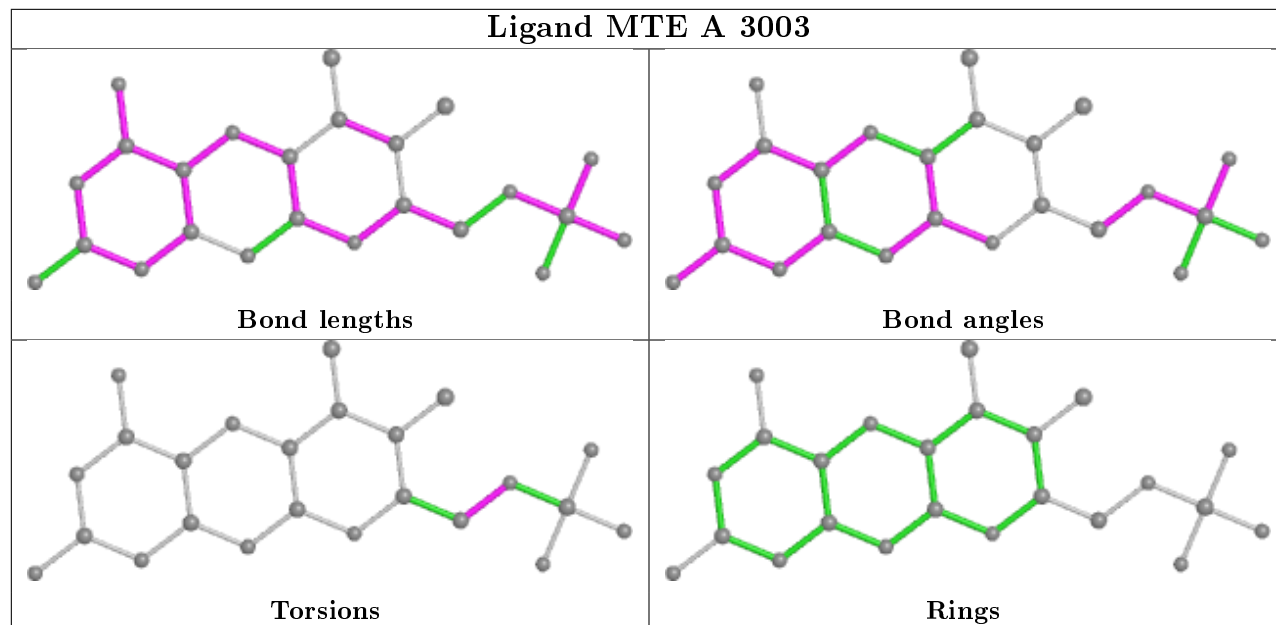
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	3008	GOL	3	0
8	B	4007	GOL	7	0
5	A	3004	MOS	2	0
5	B	4004	MOS	2	0
6	B	4005	SAL	1	0
7	A	3006	FAD	3	0
8	A	3007	GOL	4	0
4	A	3003	MTE	1	0
7	B	4006	FAD	2	0
4	B	4003	MTE	2	0

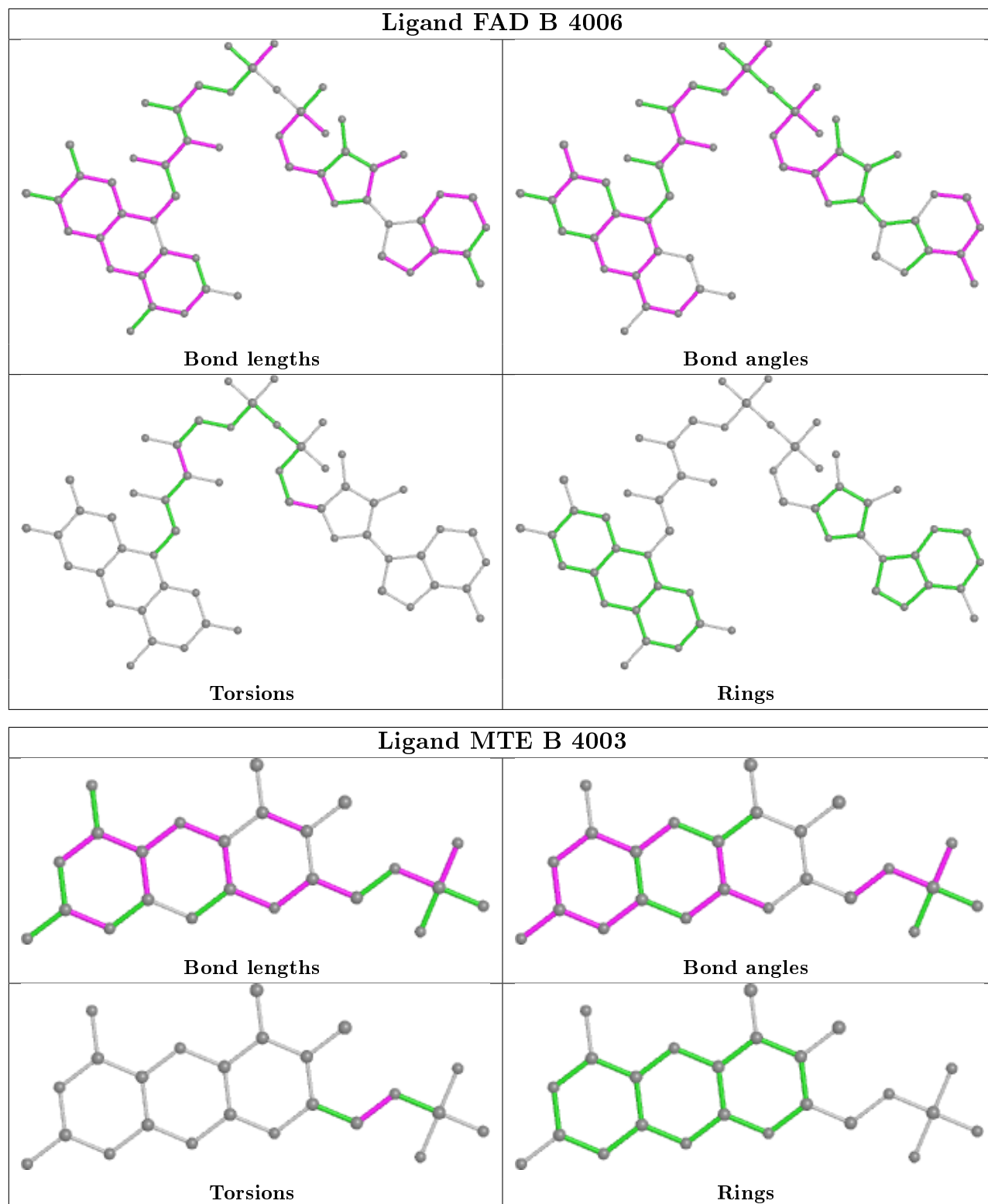
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand FAD A 3006



## Ligand MTE A 3003





## 5.7 Other polymers [i](#)

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.