



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:16 pm GMT

PDB ID : 1FIQ  
Title : CRYSTAL STRUCTURE OF XANTHINE OXIDASE FROM BOVINE MILK  
Authors : Enroth, C.; Eger, B.T.; Okamoto, K.; Nishino, T.; Nishino, T.; Pai, E.F.  
Deposited on : 2000-08-04  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

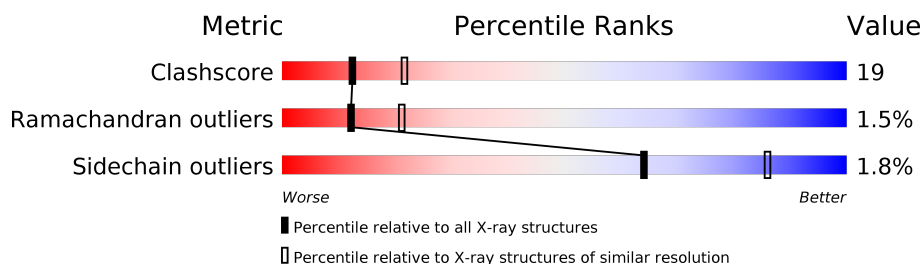
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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. 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  $\leq 5\%$ . 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	219	
2	B	350	
3	C	763	

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
6	MOS	C	1334	-	-	X	-
9	GOL	C	1336	-	X	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10106 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 OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

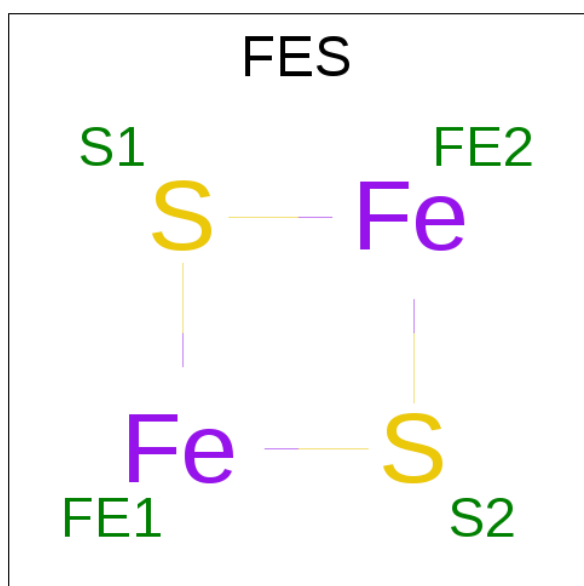
- Molecule 2 is a protein called XANTHINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

- Molecule 3 is a protein called XANTHINE OXIDASE.

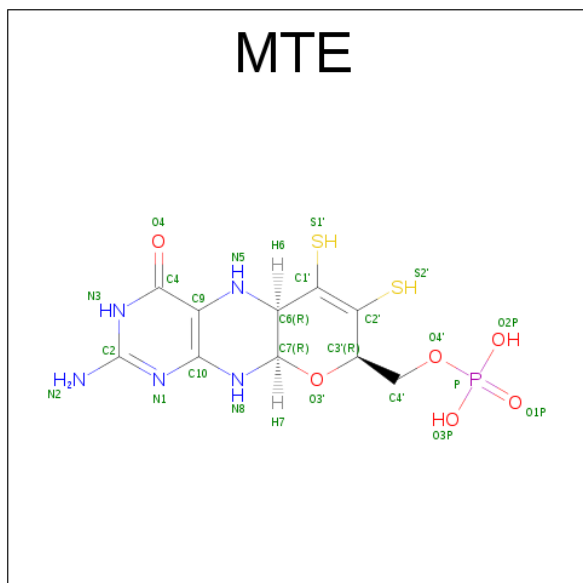
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

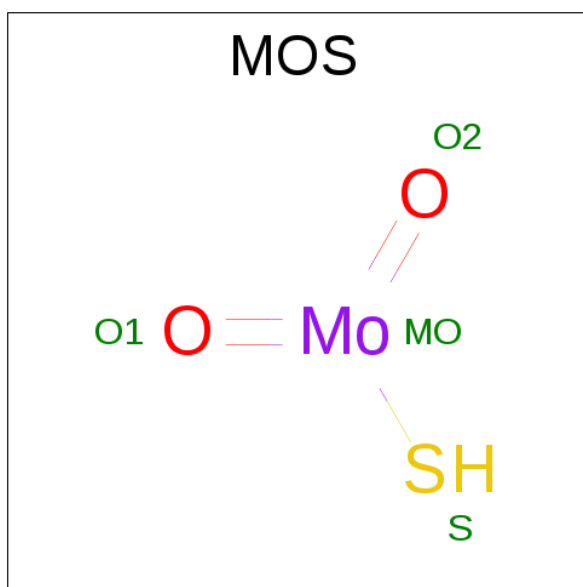
- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

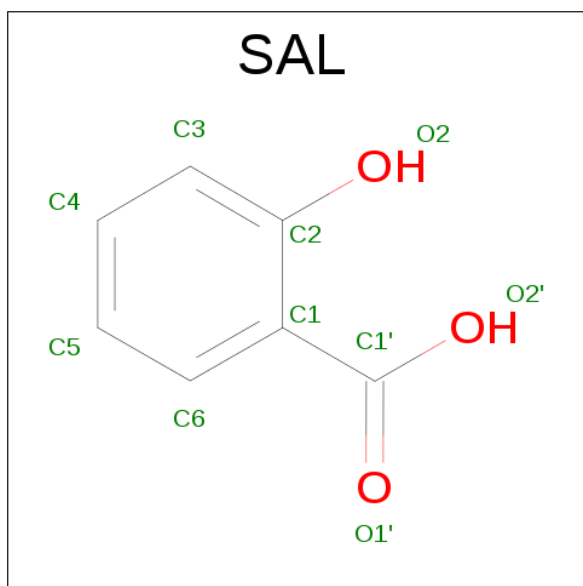
- Molecule 5 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>PS<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 7 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula:  $C_7H_6O_3$ ).



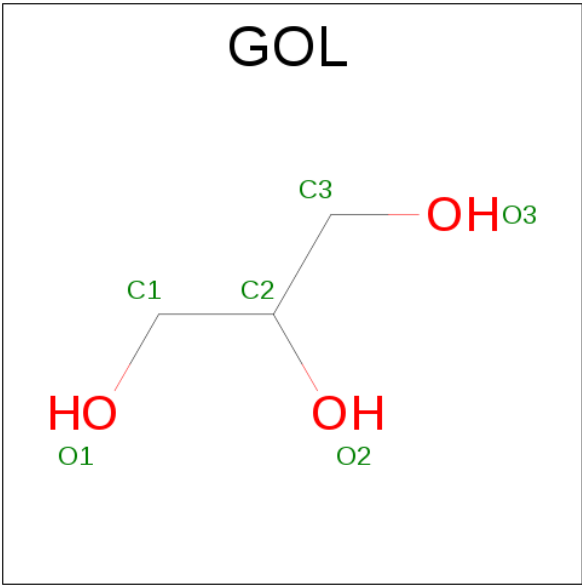
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	7	3		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 9 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
9	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

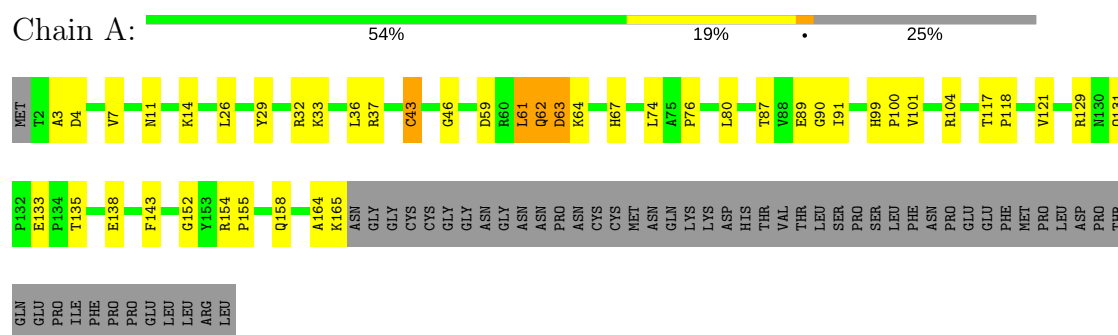
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	94	Total 94	O 94	0	0
10	B	119	Total 119	O 119	0	0
10	C	383	Total 383	O 383	0	0

### 3 Residue-property plots

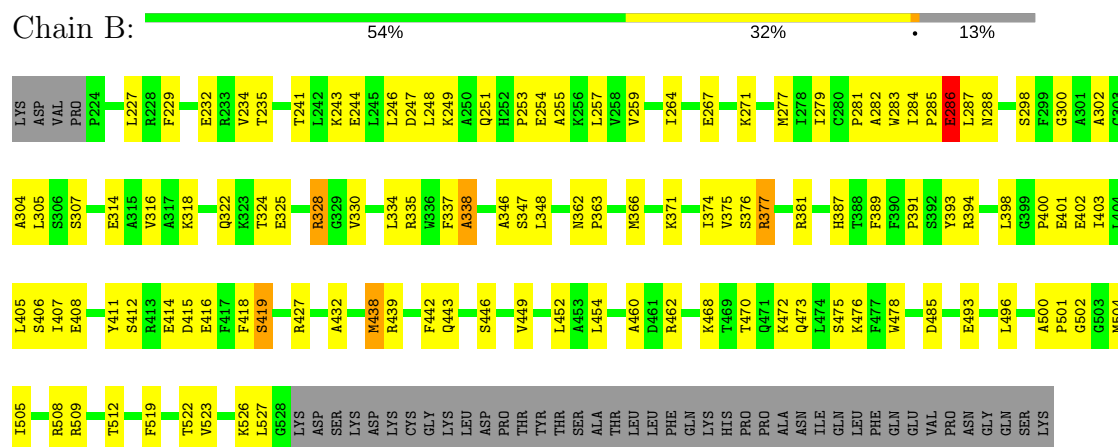
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

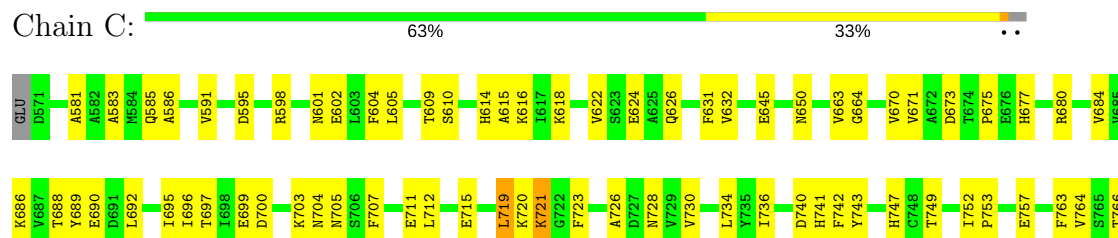
#### • Molecule 1: XANTHINE OXIDASE



#### • Molecule 2: XANTHINE OXIDASE



#### • Molecule 3: XANTHINE OXIDASE





A1300	T1221	T1083	P965	G868	Q767
E1303	R1222	D1084	W968	G869	N768
A1308	G1223	I1085	Y1086	H875	A769
C1309	T1226	G1087	K973	S876	M770
V1310	Y1227	Q1088	Q876	I877	Q773
T1315	F1232	Q1095	A979	M878	M779
LEU	I1235	K1099	R980	E879	V782
CYS	P1236	E1102	E983	R880	P783
VAL	T1237	P1103	K986	H884	V784
THR	E1238	F1104	E990	R895	N785
GLY	F1239	K1105	E990	R899	K786
ALA	R1240	K1106	E990	L900	I787
PRO	V1241	K1107	L998	L900	L788
GLY	C1247	N1108	P1002	N904	G797
ASN	P1248	G1111	T1003	S907	F798
CYS	N1249	W1116	G1006	N908	G799
LYS	K1250	V1117	I1007	T909	R804
PRO	K1251	M1118	S1008	A910	V810
TRP	A1252	Q1122	F1009	R912	A815
SER	I1253	F1132	T1010	G913	A816
LEU	Y1254	Y1133	V1011	F914	T819
ARG	A1255	E1143	P1012	G915	G820
VAL	E1261	T1144	Q1016	P917	H821
	P1262	N1145	A1017	Q918	P822
	P1263	H1151	I1021	I922	V823
	L1266	N1173	V1031	A923	R829
	G1267	L1174	S1032	E924	M833
	V1270	R1175	H1033	N925	T836
	F1271	M1180	G1034	W926	G837
	I1274	M1187	T1035	M927	G838
	I1278	D1191	E1037	V930	R839
	A1281	V1199	H1043	A931	H840
	R1282	V1200	T1044	V932	P841
	A1283	L1203	K1045	C934	F842
	Q1284	E1195	M1046	L936	L843
	H1285	E1196	V1047	P937	V848
	T1286	F1199	Q1048	A938	G849
	N1287	V1200	K1052	E939	F850
	M1288	L1208	I1058	E940	H851
	N1289	E1209	S1059	V941	K852
	T1290	L1293	N1069	R942	T853
	K1291	E1209	P1076	W943	I856
	E1292	H1212	S1082	K944	V857
	L1293	G1217		N945	A858
	F1294			D951	L859
	R1295			V964	S865
	L1296				
	D1297				

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.83Å 165.40Å 154.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.9 (8.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.212 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SAL, MOS, 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	0/1277	0.66	0/1723
2	B	0.33	0/2438	0.59	1/3290 (0.0%)
3	C	0.35	0/5888	0.62	0/7974
All	All	0.35	0/9603	0.62	1/12987 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	286	GLU	N-CA-C	-5.80	95.34	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1255	0	1265	42	0
2	B	2389	0	2459	103	0
3	C	5761	0	5685	223	1
4	A	8	0	0	1	0
5	C	24	0	10	1	0
6	C	4	0	0	3	0
7	C	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	53	0	31	1	0
9	C	6	0	3	5	0
10	A	94	0	0	3	0
10	B	119	0	0	1	0
10	C	383	0	0	6	2
All	All	10106	0	9457	357	3

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 19.

All (357) 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)
2:B:374:ILE:HD12	2:B:381:ARG:HH12	1.27	0.97
3:C:1046:MET:HE1	3:C:1087:GLY:HA2	1.47	0.97
3:C:1289:ASN:HB3	3:C:1292:GLU:HB2	1.55	0.89
3:C:618:LYS:HD3	3:C:688:THR:HG21	1.58	0.84
3:C:833:MET:HE3	3:C:1222:ARG:C	1.99	0.83
2:B:500:ALA:HB3	2:B:505:ILE:HD11	1.59	0.83
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.60	0.82
3:C:695:ILE:H	3:C:904:ASN:HD22	1.27	0.81
3:C:609:THR:CG2	3:C:664:GLY:HA2	2.13	0.79
3:C:581:ALA:O	3:C:585:GLN:HG3	1.83	0.79
2:B:241:THR:CG2	2:B:243:LYS:HG2	2.14	0.78
2:B:328:ARG:HG2	2:B:328:ARG:HH11	1.49	0.78
2:B:241:THR:HB	2:B:244:GLU:HG3	1.65	0.77
6:C:1334:MOS:S	6:C:1334:MOS:MO	1.96	0.77
3:C:726:ALA:HA	3:C:851:MET:CE	2.15	0.76
2:B:286:GLU:O	2:B:287:LEU:HB2	1.84	0.75
3:C:1021:ILE:HD12	3:C:1031:VAL:HG22	1.67	0.75
3:C:1175:ARG:HG3	3:C:1238:GLU:HB3	1.68	0.73
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.23	0.72
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.71	0.72
3:C:1108:ASN:ND2	3:C:1111:GLY:HA3	2.06	0.70
3:C:851:MET:HE3	3:C:857:VAL:HG21	1.73	0.69
3:C:1249:ASN:O	3:C:1255:ALA:HA	1.93	0.69
2:B:241:THR:HG22	2:B:243:LYS:HG2	1.74	0.68
2:B:241:THR:HG22	2:B:243:LYS:H	1.59	0.68
3:C:1102:GLU:HB3	3:C:1103:PRO:HD3	1.75	0.67
3:C:1021:ILE:CD1	3:C:1031:VAL:HG13	2.24	0.67
2:B:285:PRO:O	2:B:286:GLU:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:768:ASN:ND2	3:C:1076:PRO:HB3	2.09	0.67
2:B:325:GLU:HB2	2:B:412:SER:OG	1.93	0.66
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.41	0.66
3:C:622:VAL:HG23	3:C:626:GLN:HG3	1.77	0.66
3:C:979:ALA:O	3:C:983:GLU:HG3	1.96	0.65
3:C:779:MET:HG2	3:C:810:VAL:HG13	1.77	0.65
3:C:924:GLU:OE1	3:C:942:ARG:NH1	2.30	0.65
2:B:375:VAL:HG12	2:B:376:SER:N	2.11	0.65
2:B:246:LEU:HB3	2:B:377:ARG:HB2	1.77	0.65
3:C:833:MET:HE3	3:C:1223:GLY:N	2.11	0.65
3:C:1289:ASN:CB	3:C:1292:GLU:HB2	2.26	0.65
2:B:247:ASP:O	2:B:251:GLN:HG3	1.97	0.65
3:C:1247:CYS:N	3:C:1248:PRO:HD3	2.12	0.65
2:B:468:LYS:HB3	2:B:493:GLU:OE2	1.96	0.65
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.63	0.64
3:C:740:ASP:OD2	3:C:833:MET:HG2	1.97	0.64
1:A:152:GLY:HA2	3:C:1200:VAL:HG21	1.79	0.64
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.79	0.64
2:B:284:ILE:HG22	2:B:285:PRO:O	1.97	0.63
3:C:1021:ILE:HD11	3:C:1031:VAL:HG13	1.80	0.63
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.16	0.63
2:B:241:THR:HG21	2:B:243:LYS:HG2	1.79	0.63
3:C:618:LYS:HD3	3:C:688:THR:CG2	2.29	0.63
2:B:287:LEU:O	2:B:302:ALA:HB3	1.99	0.62
3:C:980:ARG:NH1	3:C:1175:ARG:HD3	2.14	0.62
3:C:609:THR:HG21	3:C:664:GLY:HA2	1.81	0.62
2:B:419:SER:HB2	2:B:519:PHE:CD1	2.34	0.62
3:C:695:ILE:H	3:C:904:ASN:ND2	1.97	0.62
2:B:393:TYR:CE1	2:B:394:ARG:HG2	2.33	0.62
3:C:726:ALA:HA	3:C:851:MET:HE2	1.80	0.62
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.80	0.62
3:C:1203:LEU:O	3:C:1203:LEU:HD12	1.99	0.62
2:B:407:ILE:HD12	2:B:407:ILE:N	2.15	0.62
3:C:880:ARG:HD2	3:C:914:PHE:HB3	1.80	0.62
3:C:747:HIS:CD2	3:C:836:THR:HG21	2.34	0.61
3:C:914:PHE:HA	9:C:1336:GOL:O2	2.00	0.61
1:A:59:ASP:OD2	1:A:61:LEU:HB3	2.00	0.61
1:A:99:HIS:ND1	1:A:100:PRO:HD2	2.15	0.61
2:B:375:VAL:CG1	2:B:376:SER:N	2.64	0.61
3:C:752:ILE:HD12	3:C:763:PHE:HE1	1.64	0.61
3:C:986:LYS:O	3:C:990:GLU:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:PHE:O	2:B:523:VAL:HG23	2.02	0.60
3:C:757:GLU:HB3	3:C:786:ARG:HE	1.66	0.60
2:B:314:GLU:O	2:B:318:LYS:HD3	2.01	0.60
3:C:1173:ASN:O	3:C:1236:PRO:HA	2.01	0.60
1:A:32:ARG:HD3	3:C:598:ARG:NH2	2.16	0.60
2:B:504:MET:HG2	3:C:1303:GLU:OE2	2.01	0.60
3:C:964:VAL:HB	3:C:965:PRO:HD3	1.84	0.59
3:C:1046:MET:HE1	3:C:1087:GLY:CA	2.28	0.59
2:B:366:MET:HE1	2:B:387:HIS:HA	1.84	0.59
2:B:322:GLN:HG2	2:B:414:GLU:OE2	2.03	0.59
3:C:931:ALA:HA	3:C:941:VAL:HG21	1.84	0.59
2:B:285:PRO:O	2:B:286:GLU:CB	2.51	0.59
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.50	0.59
3:C:1287:ASN:ND2	3:C:1289:ASN:HB2	2.18	0.59
3:C:1278:ILE:O	3:C:1282:ARG:HG3	2.03	0.59
2:B:418:PHE:CD1	2:B:439:ARG:HB2	2.38	0.58
3:C:1088:GLN:HG3	10:C:1622:HOH:O	2.03	0.58
2:B:376:SER:HB3	2:B:402:GLU:HG2	1.86	0.57
3:C:711:GLU:N	3:C:899:ARG:NH1	2.52	0.57
3:C:868:GLY:HA3	3:C:907:SER:HA	1.85	0.57
3:C:753:PRO:HD3	3:C:816:ALA:HB1	1.85	0.57
2:B:330:VAL:O	2:B:334:LEU:HG	2.05	0.57
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.05	0.57
3:C:610:SER:O	3:C:663:VAL:O	2.22	0.57
2:B:255:ALA:HB2	2:B:277:MET:HG2	1.87	0.57
2:B:472:LYS:O	2:B:472:LYS:HG2	2.05	0.57
3:C:715:GLU:HG3	3:C:895:ARG:HB2	1.85	0.57
2:B:286:GLU:C	2:B:288:ASN:H	2.08	0.56
1:A:61:LEU:C	1:A:63:ASP:H	2.06	0.56
3:C:740:ASP:CG	3:C:833:MET:HG2	2.25	0.56
3:C:720:LYS:O	3:C:721:LYS:CB	2.54	0.56
3:C:726:ALA:HA	3:C:851:MET:HE1	1.86	0.56
3:C:1044:THR:O	3:C:1048:GLN:HG3	2.06	0.56
3:C:1209:GLU:HB3	3:C:1227:TYR:CZ	2.40	0.56
3:C:911:PHE:O	3:C:912:ARG:C	2.44	0.56
3:C:684:VAL:O	3:C:684:VAL:HG12	2.06	0.56
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.23	0.56
6:C:1334:MOS:S	6:C:1334:MOS:O2	2.64	0.55
3:C:880:ARG:HD2	3:C:914:PHE:O	2.06	0.55
2:B:419:SER:HB2	2:B:519:PHE:HD1	1.71	0.55
1:A:152:GLY:O	3:C:1235:ILE:HG21	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HB3	1:A:155:PRO:HD3	1.87	0.55
2:B:322:GLN:O	2:B:412:SER:HB3	2.07	0.55
2:B:287:LEU:C	2:B:300:GLY:HA3	2.27	0.55
2:B:246:LEU:HD13	2:B:377:ARG:HA	1.88	0.55
3:C:848:VAL:HG22	3:C:859:LEU:CD1	2.37	0.55
3:C:711:GLU:H	3:C:899:ARG:NH1	2.05	0.54
3:C:1058:ILE:HG13	3:C:1059:SER:N	2.23	0.54
2:B:500:ALA:HB3	2:B:505:ILE:CD1	2.34	0.54
2:B:328:ARG:HG2	2:B:328:ARG:NH1	2.22	0.53
3:C:616:LYS:HB3	3:C:690:GLU:HB3	1.90	0.53
2:B:371:LYS:HD2	2:B:408:GLU:OE1	2.09	0.53
3:C:1282:ARG:NH1	3:C:1308:ALA:O	2.42	0.53
3:C:1295:ARG:HA	10:C:1422:HOH:O	2.08	0.53
3:C:1082:SER:HB2	5:C:1333:MTE:O3P	2.09	0.53
3:C:624:GLU:HB3	3:C:684:VAL:HG11	1.91	0.53
3:C:749:THR:HG23	3:C:764:VAL:HG12	1.91	0.53
3:C:770:MET:HE2	10:C:1702:HOH:O	2.08	0.53
2:B:284:ILE:O	2:B:286:GLU:O	2.27	0.52
1:A:131:GLN:HE21	1:A:133:GLU:H	1.56	0.52
1:A:117:THR:HB	1:A:118:PRO:HD3	1.91	0.52
3:C:601:ASN:O	3:C:821:HIS:HD2	1.93	0.52
3:C:909:THR:OG1	3:C:910:ALA:N	2.41	0.52
2:B:381:ARG:HH11	2:B:381:ARG:HG3	1.75	0.52
1:A:117:THR:CG2	3:C:586:ALA:HA	2.39	0.52
3:C:934:CYS:O	3:C:936:LEU:HG	2.09	0.52
3:C:799:GLY:HA2	6:C:1334:MOS:S	2.50	0.52
2:B:257:LEU:HD23	2:B:279:ILE:HB	1.90	0.52
3:C:1003:THR:HG22	3:C:1266:LEU:HD21	1.92	0.52
3:C:1095:GLN:HB3	3:C:1099:LYS:NZ	2.25	0.51
3:C:703:LYS:C	3:C:704:ASN:HD22	2.14	0.51
1:A:74:LEU:O	1:A:76:PRO:HD3	2.10	0.51
2:B:253:PRO:HG3	2:B:401:GLU:HG2	1.91	0.51
3:C:645:GLU:OE2	3:C:650:ASN:HB3	2.10	0.51
3:C:604:PHE:CD2	3:C:675:PRO:HG3	2.44	0.51
1:A:61:LEU:HG	1:A:62:GLN:NE2	2.26	0.51
3:C:1017:ALA:HB1	3:C:1086:TYR:CD2	2.45	0.51
1:A:4:ASP:HB3	2:B:227:LEU:HD22	1.93	0.51
2:B:328:ARG:HH11	2:B:328:ARG:CG	2.21	0.51
3:C:1052:LYS:HD3	3:C:1254:TYR:CZ	2.46	0.51
1:A:3:ALA:HB1	10:A:687:HOH:O	2.11	0.51
2:B:418:PHE:HD1	2:B:439:ARG:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.93	0.50
3:C:875:HIS:CD2	3:C:879:GLU:OE2	2.64	0.50
3:C:1118:MET:O	3:C:1122:GLN:HG2	2.11	0.50
1:A:99:HIS:CE1	1:A:100:PRO:HD2	2.46	0.50
1:A:3:ALA:HB2	10:B:643:HOH:O	2.12	0.50
3:C:1144:THR:O	3:C:1145:ASN:C	2.50	0.50
3:C:1199:PHE:CE1	3:C:1267:GLY:HA2	2.47	0.50
2:B:473:GLN:O	2:B:476:LYS:HB2	2.11	0.50
2:B:496:LEU:H	2:B:509:ARG:NH2	2.09	0.50
3:C:764:VAL:HG23	3:C:766:THR:CG2	2.36	0.50
3:C:918:GLN:O	3:C:922:ILE:HG13	2.12	0.50
3:C:632:VAL:HB	3:C:671:VAL:O	2.12	0.49
3:C:712:LEU:HD21	3:C:875:HIS:CE1	2.46	0.49
3:C:1143:GLU:O	3:C:1144:THR:HG23	2.12	0.49
2:B:376:SER:O	2:B:377:ARG:C	2.50	0.49
3:C:1016:GLN:HE21	3:C:1132:PHE:HZ	1.61	0.49
1:A:37:ARG:HG2	3:C:595:ASP:HA	1.94	0.49
3:C:856:ILE:HD13	3:C:945:ASN:CG	2.32	0.49
1:A:152:GLY:CA	3:C:1200:VAL:HG21	2.41	0.49
3:C:1281:ALA:O	3:C:1284:GLN:HB3	2.11	0.49
3:C:730:VAL:HG23	3:C:850:PHE:CE2	2.47	0.49
2:B:267:GLU:O	2:B:271:LYS:HB3	2.13	0.49
3:C:741:HIS:CE1	3:C:838:GLY:HA2	2.48	0.49
3:C:1286:THR:CG2	3:C:1310:VAL:HB	2.43	0.49
2:B:249:LYS:NZ	2:B:400:PRO:O	2.46	0.49
3:C:1007:ILE:O	3:C:1008:SER:CB	2.60	0.49
2:B:243:LYS:N	2:B:243:LYS:HD3	2.27	0.49
3:C:1209:GLU:HB3	3:C:1227:TYR:OH	2.13	0.49
2:B:452:LEU:HD23	2:B:470:THR:HG22	1.95	0.48
2:B:374:ILE:HD13	2:B:398:LEU:HD23	1.95	0.48
3:C:728:ASN:HD21	3:C:852:LYS:HG2	1.77	0.48
3:C:857:VAL:O	3:C:857:VAL:HG12	2.13	0.48
3:C:696:ILE:HD13	3:C:1217:GLY:CA	2.43	0.48
2:B:375:VAL:CG1	2:B:376:SER:H	2.27	0.48
2:B:449:VAL:O	2:B:475:SER:N	2.44	0.48
3:C:1143:GLU:C	3:C:1144:THR:HG23	2.34	0.48
1:A:91:ILE:O	1:A:99:HIS:HB2	2.14	0.48
3:C:622:VAL:O	3:C:622:VAL:HG23	2.14	0.48
2:B:406:SER:C	2:B:407:ILE:HD12	2.34	0.48
2:B:257:LEU:HA	2:B:279:ILE:O	2.14	0.47
3:C:615:ALA:HA	3:C:692:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:LEU:HG	2:B:405:LEU:HD12	1.97	0.47
2:B:414:GLU:O	2:B:415:ASP:HB2	2.14	0.47
8:B:606:FAD:H8A	8:B:606:FAD:H51A	1.96	0.47
3:C:1271:PHE:CE1	3:C:1300:ALA:HB2	2.48	0.47
3:C:842:PHE:CE2	3:C:865:SER:HB3	2.50	0.47
3:C:926:TRP:O	3:C:930:VAL:HG23	2.14	0.47
2:B:389:PHE:O	2:B:391:PRO:HD3	2.13	0.47
3:C:1292:GLU:O	3:C:1293:LEU:HD23	2.15	0.47
3:C:1270:VAL:O	3:C:1274:ILE:HG13	2.15	0.47
3:C:968:TRP:HZ3	3:C:1002:PRO:HD3	1.79	0.47
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.43	0.47
2:B:285:PRO:C	2:B:286:GLU:O	2.53	0.47
3:C:1284:GLN:HG3	3:C:1285:HIS:N	2.30	0.47
2:B:316:VAL:HA	2:B:324:THR:HG21	1.96	0.47
1:A:117:THR:HG22	3:C:586:ALA:HA	1.98	0.46
3:C:923:ALA:HA	3:C:926:TRP:NE1	2.30	0.46
2:B:286:GLU:C	2:B:288:ASN:N	2.69	0.46
3:C:915:GLY:H	9:C:1336:GOL:HO1	1.61	0.46
3:C:1310:VAL:HG13	10:C:1695:HOH:O	2.16	0.46
1:A:11:ASN:OD1	1:A:90:GLY:HA3	2.15	0.46
1:A:61:LEU:C	1:A:63:ASP:N	2.68	0.46
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.78	0.46
3:C:591:VAL:HG13	3:C:595:ASP:HB2	1.97	0.46
3:C:605:LEU:C	3:C:605:LEU:HD23	2.36	0.46
3:C:815:ALA:O	3:C:819:THR:HG23	2.15	0.46
3:C:1191:ASP:O	3:C:1195:VAL:HG23	2.16	0.46
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.50	0.46
3:C:699:GLU:OE2	3:C:843:LEU:HD22	2.14	0.46
3:C:927:MET:HE3	3:C:945:ASN:HB2	1.98	0.46
3:C:1203:LEU:HD12	3:C:1203:LEU:C	2.36	0.46
2:B:232:GLU:OE1	3:C:677:HIS:HE1	1.99	0.46
3:C:1286:THR:HG22	3:C:1310:VAL:HB	1.98	0.46
3:C:1196:GLU:O	3:C:1200:VAL:HG23	2.16	0.45
3:C:1247:CYS:N	3:C:1248:PRO:CD	2.79	0.45
3:C:720:LYS:O	3:C:721:LYS:HB2	2.15	0.45
2:B:244:GLU:O	2:B:248:LEU:HG	2.17	0.45
2:B:389:PHE:C	2:B:391:PRO:HD3	2.35	0.45
3:C:911:PHE:HD2	3:C:912:ARG:N	2.14	0.45
3:C:782:VAL:HG13	3:C:783:PRO:HD2	1.98	0.45
3:C:839:ARG:HG3	9:C:1336:GOL:H12	1.98	0.45
3:C:925:ASN:O	3:C:929:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HB3	2:B:377:ARG:CB	2.46	0.45
2:B:432:ALA:HB2	2:B:502:GLY:HA3	1.98	0.45
2:B:281:PRO:O	2:B:283:TRP:N	2.50	0.45
3:C:911:PHE:O	9:C:1336:GOL:H11	2.17	0.45
3:C:695:ILE:N	3:C:904:ASN:HD22	2.05	0.45
3:C:976:GLN:O	3:C:980:ARG:HG3	2.15	0.45
2:B:318:LYS:HD2	2:B:318:LYS:N	2.30	0.45
3:C:937:PRO:HB2	3:C:940:GLU:HB2	1.99	0.45
3:C:734:LEU:HD12	3:C:1297:ASP:OD1	2.16	0.45
1:A:29:TYR:CZ	1:A:33:LYS:HD2	2.52	0.45
2:B:259:VAL:HG11	2:B:347:SER:HB3	1.99	0.45
1:A:61:LEU:O	1:A:63:ASP:N	2.49	0.44
2:B:438:MET:CE	2:B:454:LEU:HD22	2.47	0.44
3:C:616:LYS:O	3:C:689:TYR:HA	2.16	0.44
1:A:101:VAL:HG12	1:A:121:VAL:HG22	2.00	0.44
2:B:427:ARG:O	2:B:427:ARG:HG2	2.16	0.44
2:B:443:GLN:HB2	2:B:446:SER:OG	2.18	0.44
1:A:143:PHE:HB3	3:C:1232:PHE:CE1	2.52	0.44
3:C:840:HIS:CE1	3:C:908:ASN:HB2	2.53	0.44
1:A:26:LEU:HD22	1:A:80:LEU:HD11	2.00	0.44
3:C:1292:GLU:HG2	3:C:1293:LEU:N	2.33	0.44
3:C:684:VAL:HG13	3:C:686:LYS:HZ2	1.82	0.44
3:C:821:HIS:O	3:C:823:VAL:HG23	2.18	0.44
3:C:980:ARG:NH2	3:C:998:LEU:HD11	2.33	0.44
1:A:46:GLY:HA2	4:A:602:FES:S1	2.58	0.44
3:C:933:THR:O	3:C:1291:LYS:HD3	2.18	0.44
2:B:393:TYR:CD1	2:B:394:ARG:HG2	2.53	0.43
3:C:1103:PRO:O	3:C:1107:LYS:HG3	2.19	0.43
3:C:614:HIS:CE1	3:C:692:LEU:HD12	2.53	0.43
1:A:67:HIS:NE2	1:A:129:ARG:NH1	2.65	0.43
3:C:749:THR:OG1	3:C:764:VAL:HG12	2.17	0.43
2:B:460:ALA:C	2:B:462:ARG:H	2.21	0.43
3:C:1084:ASP:OD1	3:C:1252:ALA:HB1	2.19	0.43
3:C:1180:MET:CE	3:C:1263:PRO:HG3	2.48	0.43
3:C:712:LEU:HA	10:C:1573:HOH:O	2.17	0.43
3:C:839:ARG:NH2	3:C:917:PRO:HG2	2.34	0.43
3:C:736:ILE:CG2	3:C:842:PHE:HB2	2.48	0.43
3:C:719:LEU:HD11	3:C:895:ARG:HD3	2.00	0.43
3:C:913:GLY:HA3	3:C:917:PRO:HG2	2.01	0.43
2:B:234:VAL:HG12	2:B:235:THR:N	2.34	0.43
3:C:1287:ASN:HD21	3:C:1289:ASN:HB2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:697:THR:H	3:C:700:ASP:HB2	1.82	0.43
3:C:840:HIS:HB2	9:C:1336:GOL:O3	2.19	0.43
3:C:851:MET:HE3	3:C:857:VAL:CG2	2.45	0.43
1:A:7:VAL:HG11	1:A:14:LYS:HE3	2.01	0.43
2:B:298:SER:HA	2:B:408:GLU:HA	2.00	0.43
3:C:1175:ARG:HG3	3:C:1238:GLU:CB	2.44	0.43
3:C:609:THR:HG23	3:C:664:GLY:CA	2.46	0.43
3:C:707:PHE:HB3	3:C:900:LEU:O	2.19	0.43
3:C:773:GLN:HG2	3:C:784:VAL:HG13	2.01	0.43
3:C:1095:GLN:HB3	3:C:1099:LYS:HZ3	1.83	0.43
3:C:704:ASN:N	3:C:704:ASN:HD22	2.16	0.42
3:C:856:ILE:N	3:C:856:ILE:HD12	2.33	0.42
2:B:286:GLU:HB3	2:B:405:LEU:HD11	2.00	0.42
3:C:1108:ASN:HD21	3:C:1111:GLY:HA3	1.83	0.42
3:C:610:SER:HB3	3:C:663:VAL:O	2.18	0.42
10:A:687:HOH:O	2:B:229:PHE:HA	2.19	0.42
3:C:696:ILE:HD13	3:C:1217:GLY:N	2.34	0.42
3:C:1282:ARG:O	3:C:1286:THR:OG1	2.35	0.42
3:C:680:ARG:O	3:C:684:VAL:HG23	2.19	0.42
1:A:62:GLN:O	1:A:63:ASP:HB3	2.19	0.42
2:B:337:PHE:O	2:B:338:ALA:C	2.57	0.42
3:C:1196:GLU:HG2	3:C:1241:VAL:HG21	2.01	0.42
1:A:104:ARG:HD2	1:A:104:ARG:HA	1.69	0.42
2:B:381:ARG:NH1	2:B:381:ARG:HG3	2.34	0.42
2:B:403:ILE:O	2:B:403:ILE:HD12	2.20	0.42
2:B:508:ARG:O	2:B:512:THR:HG23	2.20	0.42
3:C:583:ALA:HB3	10:C:1444:HOH:O	2.19	0.42
3:C:631:PHE:CE1	3:C:670:VAL:HG13	2.55	0.42
3:C:609:THR:CG2	3:C:610:SER:N	2.82	0.42
3:C:848:VAL:HG22	3:C:859:LEU:HD12	2.00	0.42
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.18	0.42
2:B:438:MET:HE2	2:B:454:LEU:HD22	2.02	0.42
3:C:602:GLU:HA	3:C:822:PRO:HG2	2.01	0.42
3:C:788:LEU:HD13	3:C:1069:ASN:HB3	2.01	0.42
2:B:304:ALA:O	2:B:307:SER:HB2	2.20	0.41
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.85	0.41
2:B:328:ARG:CG	2:B:328:ARG:NH1	2.79	0.41
2:B:500:ALA:HA	2:B:501:PRO:HD3	1.92	0.41
3:C:1151:HIS:CE1	3:C:1251:LYS:HD2	2.55	0.41
3:C:840:HIS:HD2	3:C:877:ILE:HD13	1.84	0.41
2:B:305:LEU:HG	2:B:346:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:PHE:HE2	2:B:478:TRP:HB2	1.84	0.41
3:C:1143:GLU:O	3:C:1144:THR:CB	2.69	0.41
1:A:158:GLN:HG3	10:A:649:HOH:O	2.20	0.41
3:C:736:ILE:HG23	3:C:736:ILE:O	2.20	0.41
1:A:43:CYS:HA	3:C:829:ARG:HB2	2.01	0.41
2:B:362:ASN:N	2:B:363:PRO:CD	2.83	0.41
3:C:1286:THR:HG22	3:C:1310:VAL:O	2.19	0.41
3:C:853:THR:HG22	3:C:944:LYS:HZ2	1.85	0.41
2:B:374:ILE:CD1	2:B:381:ARG:HH12	2.14	0.41
2:B:452:LEU:HD23	2:B:470:THR:HA	2.03	0.41
3:C:684:VAL:CG1	3:C:686:LYS:NZ	2.83	0.41
2:B:264:ILE:HD13	2:B:267:GLU:OE2	2.20	0.41
3:C:609:THR:HG22	3:C:610:SER:O	2.21	0.41
3:C:730:VAL:HG23	3:C:850:PHE:HE2	1.85	0.41
3:C:1105:LYS:HG3	3:C:1116:TRP:CH2	2.55	0.41
3:C:1221:THR:HA	3:C:1226:THR:OG1	2.21	0.41
3:C:705:ASN:HA	3:C:707:PHE:CE1	2.56	0.41
3:C:911:PHE:C	3:C:911:PHE:CD2	2.94	0.41
3:C:877:ILE:HG13	3:C:914:PHE:CZ	2.55	0.41
1:A:135:THR:OG1	1:A:138:GLU:HG3	2.21	0.41
1:A:154:ARG:C	1:A:154:ARG:HD2	2.41	0.41
3:C:1010:THR:O	3:C:1012:PRO:HD3	2.20	0.41
3:C:1033:HIS:CE1	3:C:1046:MET:HG3	2.56	0.41
3:C:624:GLU:HB2	3:C:684:VAL:HG12	2.03	0.41
3:C:1037:GLU:HB2	3:C:1043:HIS:CD2	2.55	0.41
3:C:850:PHE:CD2	3:C:850:PHE:N	2.88	0.41
3:C:911:PHE:HD2	3:C:911:PHE:C	2.24	0.41
1:A:117:THR:HG21	3:C:586:ALA:HA	2.03	0.40
1:A:164:ALA:O	1:A:165:LYS:HB2	2.20	0.40
2:B:254:GLU:OE1	2:B:254:GLU:N	2.51	0.40
2:B:522:THR:HG22	2:B:526:LYS:HE3	2.03	0.40
3:C:742:PHE:CZ	3:C:829:ARG:HD3	2.56	0.40
2:B:374:ILE:HD13	2:B:398:LEU:CD2	2.50	0.40
2:B:442:PHE:CE1	2:B:527:LEU:HD21	2.57	0.40
3:C:618:LYS:HB3	3:C:688:THR:HG22	2.04	0.40
3:C:853:THR:HG22	3:C:853:THR:O	2.22	0.40
2:B:416:GLU:OE1	2:B:439:ARG:NE	2.49	0.40
3:C:880:ARG:O	3:C:884:HIS:HD2	2.05	0.40
3:C:804:ARG:N	3:C:804:ARG:HD2	2.36	0.40
1:A:61:LEU:HG	1:A:62:GLN:N	2.37	0.40
2:B:271:LYS:O	2:B:271:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:ARG:HD3	3:C:1212:HIS:CG	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1509:HOH:O	10:C:1509:HOH:O[3_556]	1.82	0.38
3:C:973:LYS:NZ	3:C:973:LYS:NZ[4_556]	1.86	0.34
10:C:1598:HOH:O	10:C:1598:HOH:O[3_556]	1.99	0.21

## 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	162/219 (74%)	152 (94%)	5 (3%)	5 (3%)	5	6
2	B	303/350 (87%)	274 (90%)	25 (8%)	4 (1%)	14	25
3	C	743/763 (97%)	687 (92%)	47 (6%)	9 (1%)	15	27
All	All	1208/1332 (91%)	1113 (92%)	77 (6%)	18 (2%)	12	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	64	LYS
3	C	1008	SER
3	C	1287	ASN
2	B	282	ALA
3	C	719	LEU
3	C	721	LYS
3	C	912	ARG
3	C	1284	GLN

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Mol	Chain	Res	Type
1	A	62	GLN
3	C	798	PHE
1	A	43	CYS
1	A	63	ASP
2	B	335	ARG
2	B	338	ALA
2	B	377	ARG
3	C	797	GLY
3	C	1253	ILE

### 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	137/187 (73%)	137 (100%)	0	100	100
2	B	261/302 (86%)	254 (97%)	7 (3%)	50	77
3	C	624/639 (98%)	613 (98%)	11 (2%)	64	86
All	All	1022/1128 (91%)	1004 (98%)	18 (2%)	64	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	286	GLU
2	B	328	ARG
2	B	348	LEU
2	B	411	TYR
2	B	419	SER
2	B	438	MET
2	B	485	ASP
3	C	723	PHE
3	C	743	TYR
3	C	829	ARG
3	C	911	PHE
3	C	939	GLU
3	C	951	ASP

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Mol	Chain	Res	Type
3	C	1002	PRO
3	C	1016	GLN
3	C	1203	LEU
3	C	1208	LEU
3	C	1239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	71	ASN
1	A	82	HIS
1	A	131	GLN
1	A	146	ASN
2	B	272	ASN
2	B	351	ASN
2	B	471	GLN
2	B	473	GLN
3	C	585	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	683	HIS
3	C	704	ASN
3	C	728	ASN
3	C	821	HIS
3	C	840	HIS
3	C	875	HIS
3	C	884	HIS
3	C	904	ASN
3	C	991	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1108	ASN
3	C	1284	GLN
3	C	1287	ASN

### 5.3.3 RNA ⓘ

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](#)

7 ligands are modelled in this entry.

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$
4	FES	A	601	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	A	602	1	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	B	606	-	51,58,58	5.13	37 (72%)	54,89,89	2.76	19 (35%)
5	MTE	C	1333	6	21,26,26	7.22	14 (66%)	19,40,40	4.51	10 (52%)
6	MOS	C	1334	5	0,3,3	0.00	-	0,3,3	0.00	-
7	SAL	C	1335	-	7,10,10	1.63	2 (28%)	9,13,13	1.24	0
9	GOL	C	1336	-	5,5,5	6.90	5 (100%)	5,5,5	5.41	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
4	FES	A	601	1	-	0/0/4/4	0/1/1/1
4	FES	A	602	1	-	0/0/4/4	0/1/1/1
8	FAD	B	606	-	-	0/28/50/50	0/6/6/6
5	MTE	C	1333	6	-	1/6/34/34	0/3/3/3
6	MOS	C	1334	5	-	0/0/0/0	0/0/0/0
7	SAL	C	1335	-	-	0/0/4/4	0/1/1/1
9	GOL	C	1336	-	-	0/4/4/4	0/0/0/0



All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1336	GOL	C3-C2	-12.30	1.06	1.52
5	C	1333	MTE	P-O4'	-7.00	1.37	1.60
5	C	1333	MTE	C4'-C3'	-6.70	1.42	1.52
9	C	1336	GOL	O2-C2	-5.94	1.25	1.43
5	C	1333	MTE	P-O3P	-5.87	1.30	1.54
8	B	606	FAD	C8A-N7A	-5.52	1.24	1.34
8	B	606	FAD	O4-C4	-5.52	1.10	1.24
9	C	1336	GOL	C1-C2	-4.76	1.34	1.52
9	C	1336	GOL	O3-C3	-4.60	1.23	1.42
8	B	606	FAD	P-O5'	-3.67	1.43	1.59
8	B	606	FAD	PA-O2A	-3.59	1.37	1.55
8	B	606	FAD	C1'-N10	-3.16	1.45	1.48
8	B	606	FAD	P-O2P	-2.99	1.40	1.55
5	C	1333	MTE	P-O2P	-2.29	1.45	1.54
8	B	606	FAD	O5B-C5B	-2.15	1.36	1.44
8	B	606	FAD	O2B-C2B	-2.14	1.38	1.43
8	B	606	FAD	C5A-N7A	-2.12	1.32	1.39
7	C	1335	SAL	C6-C1	2.16	1.43	1.39
8	B	606	FAD	O5'-C5'	2.21	1.53	1.44
8	B	606	FAD	C3B-C4B	2.27	1.58	1.53
8	B	606	FAD	C2B-C3B	2.33	1.59	1.53
8	B	606	FAD	C2'-C3'	2.41	1.58	1.53
5	C	1333	MTE	C2'-C1'	2.44	1.51	1.35
7	C	1335	SAL	C5-C6	2.47	1.43	1.38
8	B	606	FAD	O3'-C3'	2.54	1.48	1.43
9	C	1336	GOL	O1-C1	2.76	1.54	1.42
8	B	606	FAD	O4'-C4'	2.83	1.49	1.43
8	B	606	FAD	C9-C8	2.93	1.45	1.37
5	C	1333	MTE	O3'-C7	3.03	1.48	1.43
8	B	606	FAD	C5B-C4B	3.10	1.61	1.51
5	C	1333	MTE	O3'-C3'	3.25	1.48	1.43
8	B	606	FAD	C6A-C5A	3.75	1.62	1.42
5	C	1333	MTE	C2-N1	4.23	1.43	1.35
5	C	1333	MTE	C4-N3	4.53	1.41	1.33
8	B	606	FAD	C9-C9A	4.61	1.50	1.40
8	B	606	FAD	C4-C4X	4.71	1.50	1.41
8	B	606	FAD	C4X-N5	4.83	1.40	1.33
8	B	606	FAD	C6-C7	5.01	1.51	1.37
8	B	606	FAD	O4B-C4B	5.24	1.56	1.45
8	B	606	FAD	C2-N3	5.56	1.49	1.38
8	B	606	FAD	C5A-C4A	5.60	1.53	1.40
8	B	606	FAD	C5X-N5	5.71	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	606	FAD	C2A-N3A	6.03	1.42	1.32
8	B	606	FAD	C9A-C5X	6.06	1.55	1.42
8	B	606	FAD	C8-C7	6.64	1.57	1.41
8	B	606	FAD	C4-N3	6.70	1.45	1.33
8	B	606	FAD	C4X-C10	7.14	1.53	1.41
5	C	1333	MTE	C9-N5	7.22	1.53	1.37
8	B	606	FAD	C2A-N1A	7.36	1.47	1.33
5	C	1333	MTE	C4-C9	7.62	1.50	1.41
8	B	606	FAD	C6-C5X	7.78	1.53	1.41
8	B	606	FAD	O4B-C1B	7.93	1.52	1.41
5	C	1333	MTE	C6-N5	9.06	1.57	1.45
8	B	606	FAD	C10-N1	9.48	1.46	1.33
8	B	606	FAD	C4A-N3A	11.78	1.52	1.35
5	C	1333	MTE	C9-C10	13.26	1.66	1.41
8	B	606	FAD	C9A-N10	17.50	1.61	1.38
5	C	1333	MTE	C7-C6	22.88	1.70	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	606	FAD	C5X-C9A-N10	-6.89	112.54	117.66
8	B	606	FAD	C4-C4X-C10	-6.30	114.87	119.96
5	C	1333	MTE	O4'-P-O1P	-5.93	89.85	106.47
8	B	606	FAD	O5B-PA-O1A	-5.64	86.47	109.25
8	B	606	FAD	C4X-C10-N10	-5.41	116.76	120.52
5	C	1333	MTE	O3'-C7-C6	-4.43	106.01	108.96
5	C	1333	MTE	N3-C2-N1	-4.34	118.42	125.45
8	B	606	FAD	O4B-C4B-C3B	-3.34	98.53	105.17
8	B	606	FAD	O4B-C4B-C5B	-3.15	98.78	109.40
8	B	606	FAD	N3A-C2A-N1A	-2.92	126.32	128.86
8	B	606	FAD	O3'-C3'-C2'	-2.49	102.65	108.82
8	B	606	FAD	O5'-C5'-C4'	-2.28	103.28	109.36
8	B	606	FAD	C4X-C4-N3	-2.20	120.35	123.48
8	B	606	FAD	O2'-C2'-C1'	-2.13	104.87	109.79
8	B	606	FAD	C8M-C8-C7	2.22	125.39	120.72
8	B	606	FAD	O2'-C2'-C3'	2.47	115.21	109.09
8	B	606	FAD	C5A-C6A-N6A	3.06	126.71	120.47
8	B	606	FAD	C2A-N1A-C6A	3.39	124.69	118.77
8	B	606	FAD	O5B-C5B-C4B	3.69	122.10	109.00
9	C	1336	GOL	O1-C1-C2	3.77	129.06	110.07
5	C	1333	MTE	N2-C2-N3	4.15	123.88	117.24
8	B	606	FAD	C4-C4X-N5	4.38	123.48	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1333	MTE	O3P-P-O4'	4.56	118.87	106.73
5	C	1333	MTE	N8-C10-N1	4.76	126.12	116.90
5	C	1333	MTE	C4-N3-C2	5.62	124.14	116.06
5	C	1333	MTE	C2-N1-C10	5.93	127.87	114.51
5	C	1333	MTE	O2P-P-O4'	6.30	123.50	106.73
9	C	1336	GOL	O2-C2-C3	6.43	139.23	108.84
8	B	606	FAD	C4-N3-C2	7.32	121.56	115.16
8	B	606	FAD	C4X-N5-C5X	7.39	124.56	116.76
9	C	1336	GOL	O3-C3-C2	9.53	158.08	110.07
5	C	1333	MTE	P-O4'-C4'	11.80	150.81	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1333	MTE	P-O4'-C4'-C3'

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	FES	1	0
8	B	606	FAD	1	0
5	C	1333	MTE	1	0
6	C	1334	MOS	3	0
9	C	1336	GOL	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.