Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 07:09 PM EDT

PDB ID	:	1N5X
Title	:	Xanthine Dehydrogenase from Bovine Milk with Inhibitor TEI-6720 Bound
Authors	:	Okamoto, K.; Eger, B.T.; Nishino, T.; Kondo, S.; Pai, E.F.; Nishino, T.
Deposited on	:	2002-11-07
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

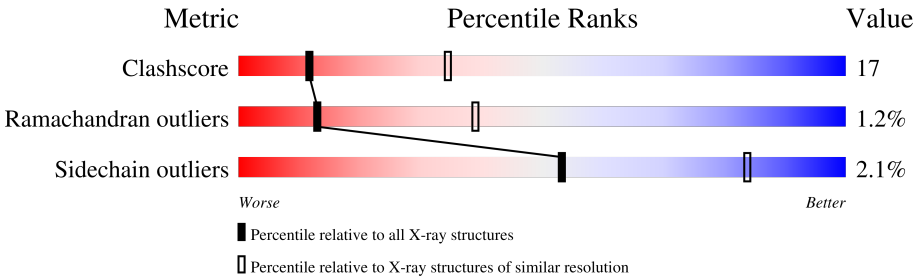
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1331	64% 31%
1	B	1331	64% 31%

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
4	MOS	A	3004	-	-	X	-
4	MOS	B	4004	-	-	X	-

2 Entry composition

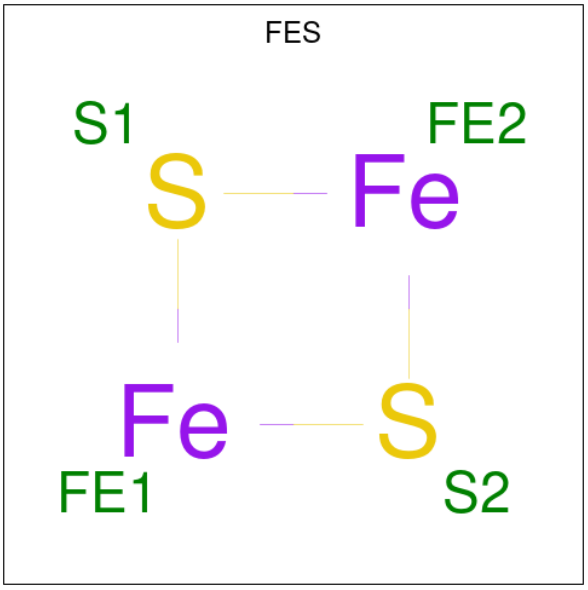
There are 6 unique types of molecules in this entry. The entry contains 20268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

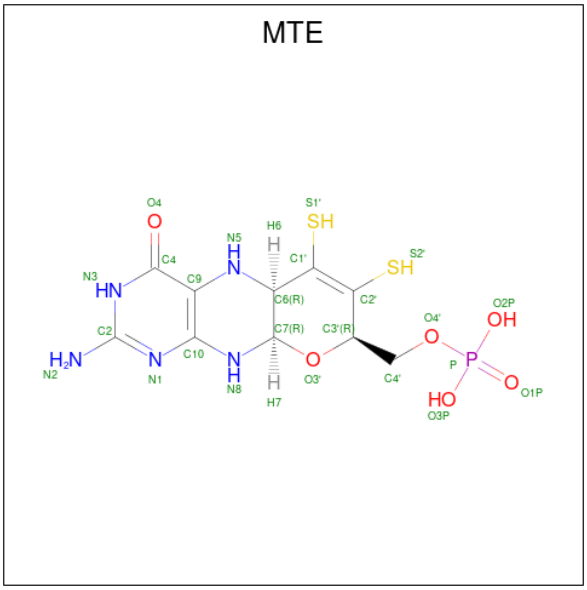
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			
1	B	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



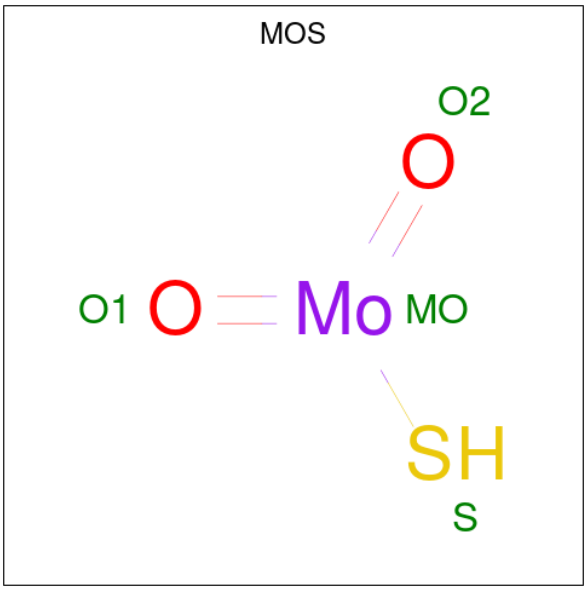
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Fe	S		0	0
			4	2	2			
2	A	1	Total	Fe	S		0	0
			4	2	2			
2	B	1	Total	Fe	S		0	0
			4	2	2			
2	B	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 3 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: $C_{10}H_{14}N_5O_6PS_2$).



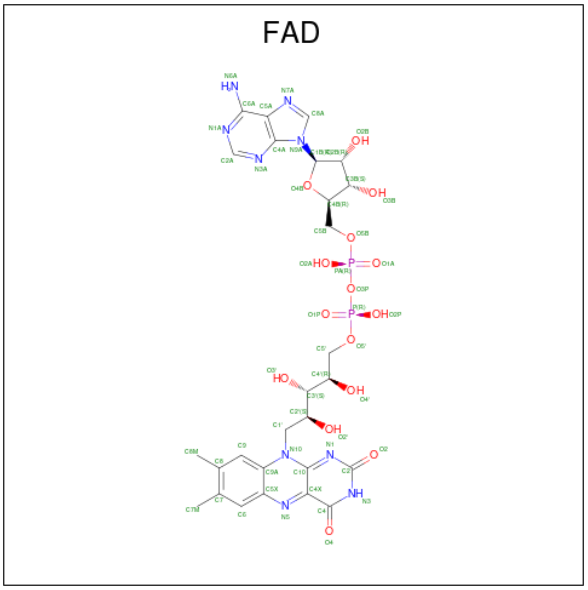
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



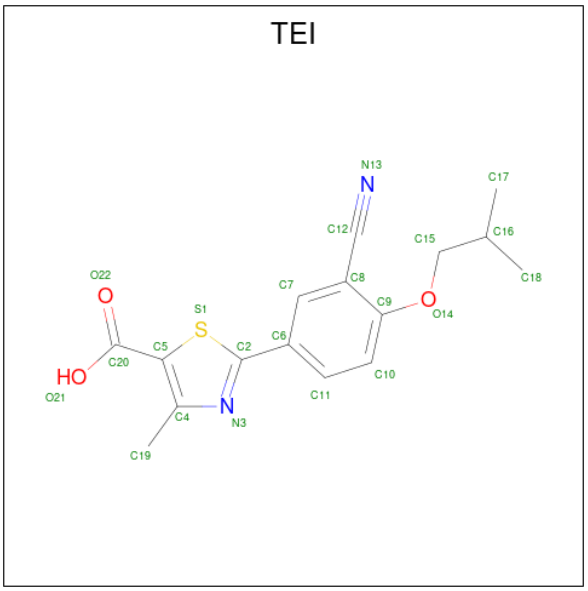
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is 2-(3-CYANO-4-ISOBUTOXY-PHENYL)-4-METHYL-5-THIAZOLE-CARB OXYLIC ACID (three-letter code: TEI) (formula: $C_{16}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			22	16	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			22	16	2	3	1		

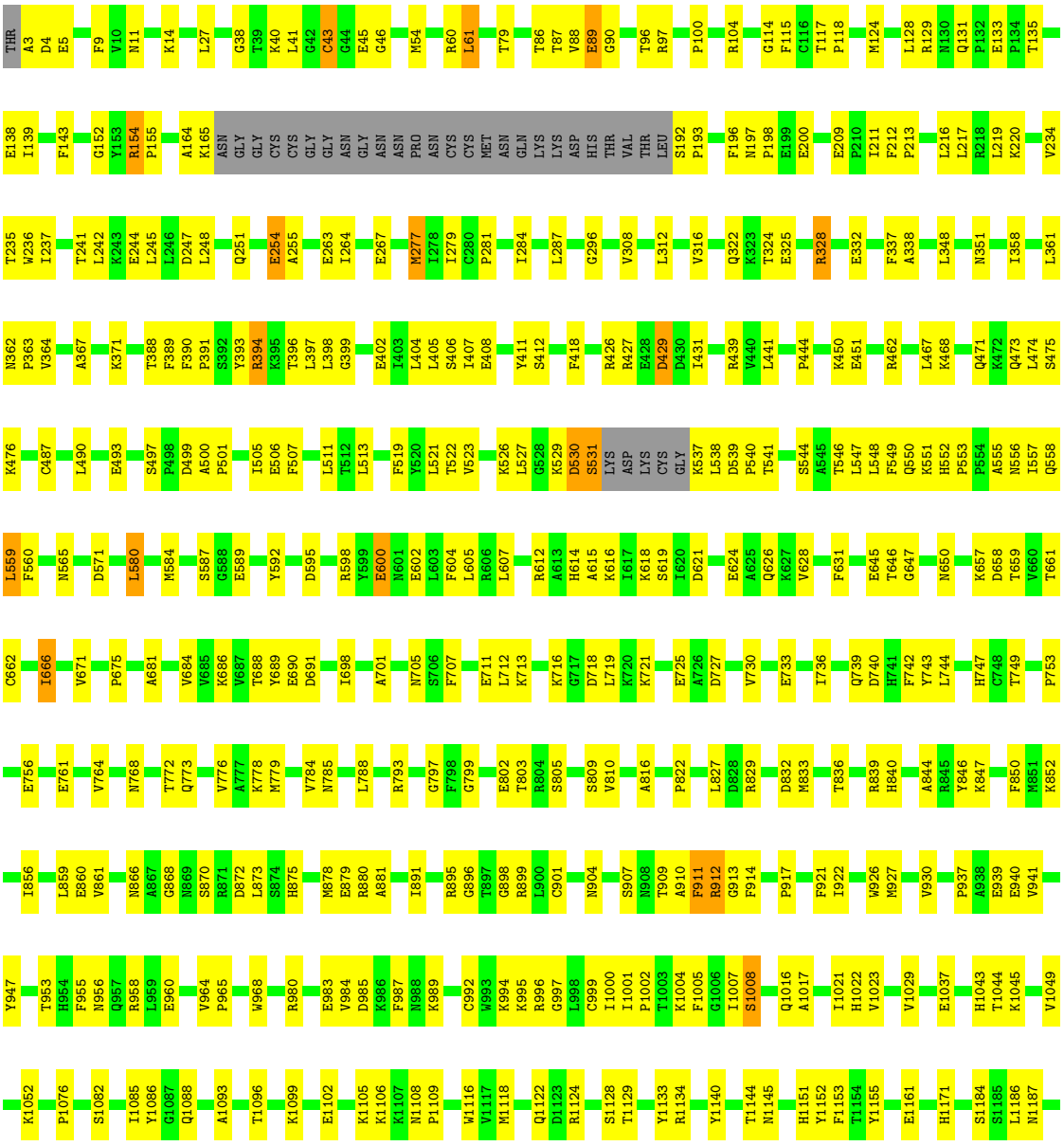
3 Residue-property plots (i)

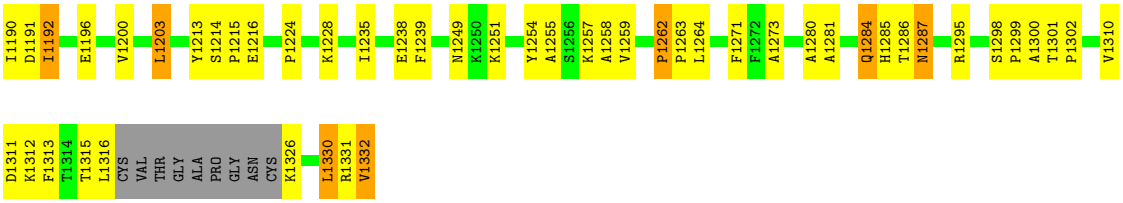
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

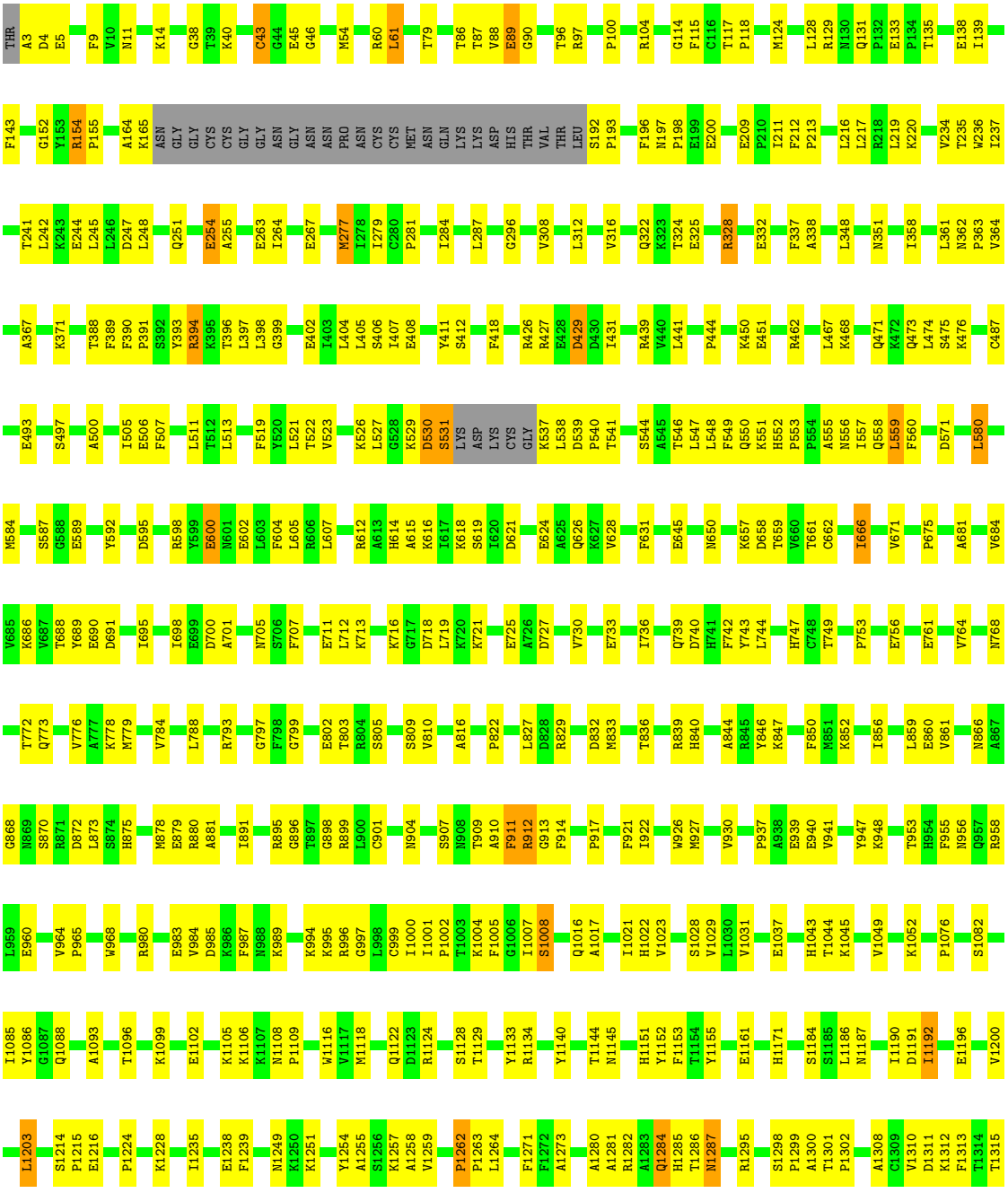
Chain A:





• Molecule 1: Xanthine Dehydrogenase

Chain B:




L1316
CYS
VAL
THR
GLY
ALA
PRO
GLY
ASN
CYS
K1326
P1327
W1328
S1329
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	168.27Å 124.66Å 147.32Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	93.7 (20.00-2.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.244 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20268	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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: MTE, FES, TEI, FAD, MOS

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	0.43	0/10242	0.66	0/13860
1	B	0.43	0/10242	0.66	0/13860
All	All	0.43	0/20484	0.66	0/27720

There are no bond length outliers.

There are no bond angle outliers.

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	10023	0	10026	349	5
1	B	10023	0	10026	348	4
2	A	8	0	0	2	0
2	B	8	0	0	2	0
3	A	24	0	10	4	0
3	B	24	0	10	4	0
4	A	4	0	0	8	0
4	B	4	0	0	8	0
5	A	53	0	29	2	0
5	B	53	0	29	2	0
6	A	22	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	0	15	0	0
All	All	20268	0	20160	706	5

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 17.

All (706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1330:LEU:HD22	1:A:1331:ARG:N	1.62	1.14
1:B:1330:LEU:HD22	1:B:1331:ARG:N	1.62	1.13
1:A:537:LYS:HG3	1:A:538:LEU:H	1.18	1.07
1:A:1286:THR:HG22	1:A:1287:ASN:H	1.19	1.07
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.19	1.04
1:B:537:LYS:HG3	1:B:538:LEU:H	1.18	1.02
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.20	1.01
1:A:666:ILE:HD12	1:A:666:ILE:H	1.27	0.99
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.20	0.99
1:B:666:ILE:H	1:B:666:ILE:HD12	1.27	0.98
1:B:131:GLN:HE21	1:B:133:GLU:H	1.01	0.95
1:A:131:GLN:HE21	1:A:133:GLU:H	1.01	0.93
1:B:1330:LEU:HD22	1:B:1331:ARG:H	1.34	0.92
4:B:4004:MOS:S	4:B:4004:MOS:MO	1.81	0.91
1:A:1330:LEU:HD22	1:A:1331:ARG:H	1.34	0.90
4:A:3004:MOS:S	4:A:3004:MOS:MO	1.81	0.90
1:A:1330:LEU:HD13	1:A:1332:VAL:N	1.90	0.87
1:B:1330:LEU:HD13	1:B:1332:VAL:N	1.90	0.86
1:B:1330:LEU:CD2	1:B:1331:ARG:H	1.90	0.84
4:B:4004:MOS:S	4:B:4004:MOS:O1	2.36	0.84
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.43	0.83
4:A:3004:MOS:S	4:A:3004:MOS:O1	2.36	0.83
1:A:1330:LEU:CD2	1:A:1331:ARG:H	1.90	0.83
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.43	0.83
1:A:1330:LEU:CD2	1:A:1331:ARG:N	2.42	0.82
1:A:1286:THR:HG22	1:A:1287:ASN:N	1.95	0.81
1:B:1286:THR:HG22	1:B:1287:ASN:N	1.95	0.81
1:A:322:GLN:O	1:A:412:SER:HB3	1.82	0.80
1:B:322:GLN:O	1:B:412:SER:HB3	1.82	0.80
1:B:404:LEU:HD21	1:B:407:ILE:HD11	1.64	0.80
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.64	0.80
1:B:1330:LEU:CD2	1:B:1331:ARG:N	2.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1330:LEU:HD13	1:B:1331:ARG:H	1.48	0.78
1:B:1106:LYS:O	1:B:1109:PRO:HD3	1.84	0.77
1:A:1330:LEU:HD13	1:A:1331:ARG:H	1.48	0.76
1:A:868:GLY:HA3	1:A:907:SER:HA	1.67	0.76
1:A:1106:LYS:O	1:A:1109:PRO:HD3	1.84	0.76
1:B:868:GLY:HA3	1:B:907:SER:HA	1.67	0.76
1:B:1330:LEU:CG	1:B:1331:ARG:H	1.97	0.76
4:B:4004:MOS:MO	4:B:4004:MOS:O2	1.57	0.76
1:B:537:LYS:HG3	1:B:538:LEU:N	2.00	0.75
1:A:1330:LEU:CD1	1:A:1331:ARG:H	2.00	0.74
1:A:1330:LEU:CG	1:A:1331:ARG:H	1.97	0.74
4:A:3004:MOS:MO	4:A:3004:MOS:O2	1.57	0.74
1:A:247:ASP:O	1:A:251:GLN:HG3	1.87	0.74
1:B:1330:LEU:CD1	1:B:1331:ARG:H	2.00	0.74
1:A:955:PHE:HA	1:A:1145:ASN:ND2	2.01	0.74
1:B:247:ASP:O	1:B:251:GLN:HG3	1.87	0.74
1:B:870:SER:HB3	1:B:907:SER:HB2	1.70	0.73
1:A:721:LYS:O	1:A:725:GLU:HG3	1.89	0.73
1:A:537:LYS:HG3	1:A:538:LEU:N	2.00	0.73
1:B:721:LYS:O	1:B:725:GLU:HG3	1.89	0.73
1:B:666:ILE:HD12	1:B:666:ILE:N	2.03	0.72
1:A:467:LEU:O	1:A:471:GLN:HG2	1.90	0.72
1:A:756:GLU:HB3	1:B:584:MET:SD	2.29	0.72
1:A:870:SER:HB3	1:A:907:SER:HB2	1.70	0.72
1:A:955:PHE:CA	1:A:1145:ASN:HD21	1.99	0.72
1:A:584:MET:SD	1:B:756:GLU:HB3	2.30	0.71
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.01	0.71
1:B:467:LEU:O	1:B:471:GLN:HG2	1.90	0.71
1:B:955:PHE:CA	1:B:1145:ASN:HD21	1.99	0.71
1:A:600:GLU:HG2	1:B:598:ARG:O	1.90	0.70
1:A:718:ASP:HB3	1:A:721:LYS:HB3	1.74	0.70
1:B:389:PHE:O	1:B:391:PRO:HD3	1.91	0.70
1:B:718:ASP:HB3	1:B:721:LYS:HB3	1.74	0.70
1:A:666:ILE:HD12	1:A:666:ILE:N	2.03	0.70
1:A:1331:ARG:O	1:A:1332:VAL:HG12	1.91	0.70
1:B:519:PHE:O	1:B:523:VAL:HG23	1.91	0.70
1:B:1331:ARG:O	1:B:1332:VAL:HG12	1.91	0.70
1:A:519:PHE:O	1:A:523:VAL:HG23	1.91	0.69
1:B:131:GLN:HE21	1:B:133:GLU:N	1.84	0.69
1:A:389:PHE:O	1:A:391:PRO:HD3	1.91	0.69
1:A:9:PHE:CE2	1:A:14:LYS:HB2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LYS:O	1:A:530:ASP:HB2	1.92	0.69
1:B:529:LYS:O	1:B:530:ASP:HB2	1.92	0.69
1:A:131:GLN:HE21	1:A:133:GLU:N	1.84	0.68
1:B:9:PHE:CE2	1:B:14:LYS:HB2	2.28	0.68
1:A:406:SER:C	1:A:407:ILE:HD12	2.14	0.68
1:B:1005:PHE:HB3	1:B:1262:PRO:HG3	1.75	0.68
1:B:325:GLU:HB2	1:B:412:SER:OG	1.94	0.67
1:A:1005:PHE:HB3	1:A:1262:PRO:HG3	1.75	0.67
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.95	0.67
1:A:325:GLU:HB2	1:A:412:SER:OG	1.93	0.67
1:A:287:LEU:HD23	1:A:405:LEU:HD12	1.77	0.67
1:A:612:ARG:NH1	1:A:689:TYR:HB2	2.10	0.67
1:B:406:SER:C	1:B:407:ILE:HD12	2.14	0.67
1:B:612:ARG:NH1	1:B:689:TYR:HB2	2.10	0.67
1:A:598:ARG:O	1:B:600:GLU:HG2	1.95	0.67
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.95	0.66
1:B:241:THR:OG1	1:B:244:GLU:HG3	1.96	0.66
1:B:287:LEU:HD23	1:B:405:LEU:HD12	1.77	0.66
1:A:666:ILE:H	1:A:666:ILE:CD1	2.05	0.66
1:A:241:THR:OG1	1:A:244:GLU:HG3	1.96	0.65
1:B:544:SER:HA	1:B:547:LEU:HD12	1.77	0.65
1:A:544:SER:HA	1:A:547:LEU:HD12	1.77	0.65
1:A:1301:THR:HB	1:A:1302:PRO:HD2	1.77	0.64
1:B:1301:THR:HB	1:B:1302:PRO:HD2	1.78	0.64
1:A:1187:ASN:CG	1:A:1190:ILE:HG12	2.19	0.63
1:B:367:ALA:O	1:B:439:ARG:HD3	1.99	0.63
1:B:537:LYS:CG	1:B:538:LEU:H	2.00	0.62
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.00	0.62
1:A:487:CYS:HA	1:A:513:LEU:HD22	1.80	0.62
1:B:60:ARG:O	1:B:61:LEU:CB	2.48	0.62
4:B:4004:MOS:MO	4:B:4004:MOS:O1	1.70	0.62
1:A:60:ARG:O	1:A:61:LEU:CB	2.48	0.62
1:A:135:THR:OG1	1:A:138:GLU:HG3	2.00	0.62
1:B:487:CYS:HA	1:B:513:LEU:HD22	1.80	0.62
1:B:1187:ASN:CG	1:B:1190:ILE:HG12	2.19	0.62
1:A:296:GLY:HA2	1:A:411:TYR:CD1	2.34	0.61
1:A:367:ALA:O	1:A:439:ARG:HD3	1.99	0.61
1:B:802:GLU:HG2	1:B:803:THR:HG23	1.82	0.61
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.66	0.61
1:B:296:GLY:HA2	1:B:411:TYR:CD1	2.34	0.61
1:B:870:SER:HB3	1:B:907:SER:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:VAL:HG21	1:A:681:ALA:HA	1.83	0.61
1:A:870:SER:HB3	1:A:907:SER:CB	2.30	0.61
1:A:980:ARG:O	1:A:984:VAL:HG23	2.01	0.61
4:A:3004:MOS:MO	4:A:3004:MOS:O1	1.70	0.61
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.66	0.61
1:B:1203:LEU:C	1:B:1203:LEU:HD12	2.21	0.60
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.83	0.60
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.84	0.60
1:A:468:LYS:HB2	1:A:493:GLU:OE2	2.01	0.60
1:A:196:PHE:HE1	1:A:198:PRO:HG3	1.66	0.60
1:A:1203:LEU:C	1:A:1203:LEU:HD12	2.21	0.60
1:B:468:LYS:HB2	1:B:493:GLU:OE2	2.01	0.60
1:B:730:VAL:O	1:B:847:LYS:HA	2.02	0.60
1:A:730:VAL:O	1:A:847:LYS:HA	2.02	0.60
4:A:3004:MOS:S	4:A:3004:MOS:O2	2.60	0.60
1:B:358:ILE:HD13	1:B:431:ILE:HG23	1.84	0.60
1:B:1330:LEU:HD13	1:B:1332:VAL:H	1.67	0.60
1:B:980:ARG:O	1:B:984:VAL:HG23	2.01	0.60
1:A:1118:MET:O	1:A:1122:GLN:HG2	2.01	0.60
1:A:749:THR:HG21	1:A:809:SER:HA	1.84	0.59
1:A:802:GLU:HG2	1:A:803:THR:HG23	1.82	0.59
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.84	0.59
1:B:749:THR:HG21	1:B:809:SER:HA	1.84	0.59
4:B:4004:MOS:S	4:B:4004:MOS:O2	2.60	0.59
1:B:1118:MET:O	1:B:1122:GLN:HG2	2.01	0.59
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.33	0.59
1:B:196:PHE:HE1	1:B:198:PRO:HG3	1.66	0.59
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.84	0.59
1:A:281:PRO:HB2	1:A:287:LEU:CD1	2.33	0.59
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.15	0.59
1:A:358:ILE:HD13	1:A:431:ILE:HG23	1.84	0.58
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.15	0.58
1:B:761:GLU:HG3	1:B:788:LEU:HD23	1.85	0.58
1:A:539:ASP:OD1	1:A:541:THR:N	2.37	0.58
1:B:393:TYR:CZ	1:B:394:ARG:HD2	2.39	0.58
1:B:937:PRO:O	1:B:941:VAL:HG23	2.03	0.58
1:A:937:PRO:O	1:A:941:VAL:HG23	2.03	0.58
1:B:1191:ASP:OD1	1:B:1259:VAL:HG11	2.04	0.58
1:B:255:ALA:HB2	1:B:277:MET:HG2	1.86	0.58
1:A:761:GLU:HG3	1:A:788:LEU:HD23	1.85	0.58
1:B:131:GLN:NE2	1:B:133:GLU:H	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:HB2	1:A:277:MET:HG2	1.86	0.58
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.58
1:B:1330:LEU:HD13	1:B:1331:ARG:N	2.19	0.58
1:A:196:PHE:CE1	1:A:198:PRO:HG3	2.39	0.57
1:B:539:ASP:OD1	1:B:541:THR:N	2.37	0.57
1:B:544:SER:OG	1:B:994:LYS:HD2	2.04	0.57
1:A:544:SER:OG	1:A:994:LYS:HD2	2.04	0.57
1:B:666:ILE:H	1:B:666:ILE:CD1	2.05	0.57
1:A:1191:ASP:OD1	1:A:1259:VAL:HG11	2.04	0.57
1:A:393:TYR:CZ	1:A:394:ARG:HD2	2.39	0.57
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.39	0.57
1:B:1052:LYS:HD3	1:B:1254:TYR:CZ	2.39	0.57
1:A:242:LEU:HA	1:A:284:ILE:HD13	1.87	0.57
1:A:96:THR:OG1	1:A:97:ARG:N	2.38	0.57
1:B:552:HIS:CG	1:B:553:PRO:HD2	2.40	0.57
1:B:450:LYS:O	1:B:474:LEU:HD22	2.05	0.57
1:A:192:SER:HB3	1:A:193:PRO:HD2	1.86	0.57
1:A:1191:ASP:O	1:A:1192:ILE:HG13	2.05	0.57
1:B:602:GLU:HG3	1:B:822:PRO:HG2	1.85	0.57
1:B:1191:ASP:O	1:B:1192:ILE:HG13	2.05	0.56
1:A:602:GLU:HG3	1:A:822:PRO:HG2	1.85	0.56
1:B:192:SER:HB3	1:B:193:PRO:HD2	1.86	0.56
1:B:196:PHE:CE1	1:B:198:PRO:HG3	2.39	0.56
1:A:450:LYS:O	1:A:474:LEU:HD22	2.05	0.56
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.41	0.56
1:A:1326:LYS:O	1:A:1326:LYS:HG2	2.06	0.56
1:A:1330:LEU:HD22	1:A:1330:LEU:C	2.22	0.56
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.40	0.56
1:A:911:PHE:HD2	1:A:912:ARG:N	2.03	0.56
1:B:96:THR:OG1	1:B:97:ARG:N	2.38	0.56
1:A:744:LEU:HD23	2:A:3001:FES:S2	2.46	0.56
1:A:999:CYS:SG	1:A:1001:ILE:HD11	2.46	0.56
1:B:744:LEU:HD23	2:B:4001:FES:S2	2.46	0.56
1:A:587:SER:OG	1:A:589:GLU:HG3	2.06	0.56
1:B:587:SER:OG	1:B:589:GLU:HG3	2.06	0.56
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.41	0.56
1:B:1330:LEU:HD22	1:B:1330:LEU:C	2.22	0.56
1:A:1330:LEU:HD13	1:A:1332:VAL:H	1.67	0.56
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.05	0.55
1:B:1326:LYS:O	1:B:1326:LYS:HG2	2.06	0.55
1:A:506:GLU:CD	1:A:506:GLU:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:CYS:SG	1:B:1001:ILE:HD11	2.46	0.55
1:A:131:GLN:NE2	1:A:133:GLU:H	1.86	0.55
1:B:242:LEU:HA	1:B:284:ILE:HD13	1.87	0.55
1:B:3:ALA:O	1:B:5:GLU:N	2.38	0.55
1:A:844:ALA:HB2	1:A:922:ILE:HD13	1.89	0.55
5:A:3005:FAD:H8A	5:A:3005:FAD:H51A	1.89	0.55
1:B:911:PHE:HD2	1:B:912:ARG:N	2.03	0.55
1:B:1105:LYS:HG3	1:B:1116:TRP:CZ2	2.42	0.55
1:B:1215:PRO:HD2	1:B:1216:GLU:OE2	2.07	0.55
1:B:284:ILE:HB	1:B:287:LEU:HD12	1.88	0.55
1:B:740:ASP:OD2	1:B:833:MET:HG2	2.07	0.55
1:B:1007:ILE:HD12	1:B:1258:ALA:HB3	1.89	0.55
1:B:506:GLU:CD	1:B:506:GLU:H	2.09	0.55
1:B:556:ASN:C	1:B:557:ILE:HD12	2.27	0.55
1:B:997:GLY:HA3	1:B:1273:ALA:O	2.05	0.55
1:B:1330:LEU:CG	1:B:1331:ARG:N	2.68	0.55
1:A:1215:PRO:HD2	1:A:1216:GLU:OE2	2.07	0.55
1:B:555:ALA:HB3	1:B:1238:GLU:HG2	1.89	0.55
1:B:287:LEU:CD2	1:B:405:LEU:HD12	2.37	0.54
1:B:521:LEU:HD22	1:B:538:LEU:HD11	1.89	0.54
1:B:939:GLU:HG2	1:B:940:GLU:N	2.22	0.54
1:A:556:ASN:C	1:A:557:ILE:HD12	2.27	0.54
1:B:1271:PHE:CE1	1:B:1300:ALA:HB2	2.43	0.54
1:A:856:ILE:HD12	1:A:856:ILE:N	2.23	0.54
1:A:555:ALA:HB3	1:A:1238:GLU:HG2	1.89	0.54
1:A:521:LEU:HD22	1:A:538:LEU:HD11	1.89	0.54
1:A:832:ASP:O	1:A:836:THR:HG23	2.08	0.54
1:A:396:THR:OG1	1:A:398:LEU:HD23	2.08	0.54
1:A:619:SER:HB3	1:A:688:THR:OG1	2.07	0.54
1:B:618:LYS:HD2	1:B:690:GLU:OE1	2.08	0.54
1:B:619:SER:HB3	1:B:688:THR:OG1	2.07	0.54
1:B:832:ASP:O	1:B:836:THR:HG23	2.08	0.54
5:B:4005:FAD:H8A	5:B:4005:FAD:H51A	1.89	0.54
1:A:618:LYS:HD2	1:A:690:GLU:OE1	2.08	0.54
1:A:939:GLU:HG2	1:A:940:GLU:N	2.22	0.54
1:B:404:LEU:CD2	1:B:407:ILE:HD11	2.37	0.54
1:A:287:LEU:CD2	1:A:405:LEU:HD12	2.37	0.54
1:A:284:ILE:HB	1:A:287:LEU:HD12	1.88	0.54
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.37	0.54
1:A:740:ASP:OD2	1:A:833:MET:HG2	2.07	0.54
1:A:1105:LYS:HG3	1:A:1116:TRP:CZ2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PRO:O	1:B:104:ARG:HG3	2.08	0.53
1:B:844:ALA:HB2	1:B:922:ILE:HD13	1.89	0.53
1:A:3:ALA:O	1:A:5:GLU:N	2.38	0.53
1:A:100:PRO:O	1:A:104:ARG:HG3	2.09	0.53
1:A:1007:ILE:HD12	1:A:1258:ALA:HB3	1.89	0.53
1:B:1017:ALA:HB2	1:B:1085:ILE:HD12	1.91	0.53
1:B:396:THR:OG1	1:B:398:LEU:HD23	2.08	0.53
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.09	0.53
1:A:1271:PHE:CE1	1:A:1300:ALA:HB2	2.43	0.53
1:B:727:ASP:OD2	1:B:852:LYS:HG3	2.09	0.53
1:B:773:GLN:HG2	1:B:784:VAL:HG13	1.90	0.53
1:B:736:ILE:HG12	1:B:921:PHE:CD2	2.44	0.53
1:A:736:ILE:HG12	1:A:921:PHE:CD2	2.44	0.53
1:A:1017:ALA:HB2	1:A:1085:ILE:HD12	1.91	0.53
1:B:856:ILE:N	1:B:856:ILE:HD12	2.23	0.53
1:A:727:ASP:OD2	1:A:852:LYS:HG3	2.09	0.53
1:A:1315:THR:HG22	1:A:1316:LEU:N	2.23	0.53
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.09	0.53
1:A:1330:LEU:HD13	1:A:1331:ARG:N	2.19	0.53
1:B:552:HIS:ND1	1:B:553:PRO:HD2	2.24	0.53
1:B:1315:THR:HG22	1:B:1316:LEU:N	2.23	0.53
1:B:61:LEU:O	1:B:61:LEU:HD23	2.09	0.52
1:A:474:LEU:O	1:A:475:SER:HB3	2.09	0.52
1:B:474:LEU:O	1:B:475:SER:HB3	2.09	0.52
1:B:650:ASN:ND2	1:B:778:LYS:HE3	2.24	0.52
1:A:559:LEU:HD23	1:A:559:LEU:N	2.25	0.52
1:A:61:LEU:HD23	1:A:61:LEU:O	2.09	0.52
1:A:1005:PHE:CB	1:A:1262:PRO:HG3	2.39	0.52
1:B:559:LEU:N	1:B:559:LEU:HD23	2.25	0.52
1:A:552:HIS:ND1	1:A:553:PRO:HD2	2.24	0.52
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.91	0.52
1:A:985:ASP:O	1:A:989:LYS:HG3	2.10	0.52
1:B:985:ASP:O	1:B:989:LYS:HG3	2.10	0.52
3:A:3003:MTE:S2'	4:A:3004:MOS:O1	2.69	0.51
1:A:650:ASN:ND2	1:A:778:LYS:HE3	2.24	0.51
1:A:264:ILE:HD11	5:A:3005:FAD:H3B	1.91	0.51
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.91	0.51
1:A:773:GLN:HG2	1:A:784:VAL:HG13	1.90	0.51
1:B:880:ARG:HD2	1:B:914:PHE:O	2.11	0.51
1:A:1021:ILE:HD12	1:A:1093:ALA:HB3	1.91	0.51
1:B:124:MET:HE3	1:B:128:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1140:TYR:HE1	1:B:1145:ASN:HD22	1.57	0.51
1:B:1005:PHE:CB	1:B:1262:PRO:HG3	2.39	0.51
1:A:1186:LEU:HD21	1:A:1254:TYR:HB2	1.93	0.51
1:B:560:PHE:CD2	1:B:560:PHE:N	2.79	0.51
1:B:1021:ILE:HD12	1:B:1093:ALA:HB3	1.91	0.51
1:A:880:ARG:HD2	1:A:914:PHE:O	2.11	0.51
1:B:264:ILE:HD11	5:B:4005:FAD:H3B	1.91	0.51
1:B:164:ALA:O	1:B:165:LYS:HB3	2.11	0.51
1:B:263:GLU:O	1:B:267:GLU:HG3	2.11	0.51
1:B:522:THR:HG22	1:B:526:LYS:HE3	1.93	0.51
1:A:507:PHE:CZ	1:A:511:LEU:HD11	2.47	0.50
1:A:1124:ARG:O	1:B:1134:ARG:HD3	2.11	0.50
3:B:4003:MTE:S2'	4:B:4004:MOS:O1	2.69	0.50
1:A:263:GLU:O	1:A:267:GLU:HG3	2.11	0.50
1:A:605:LEU:HD23	1:A:605:LEU:C	2.32	0.50
1:A:164:ALA:O	1:A:165:LYS:HB3	2.11	0.50
1:B:1186:LEU:HD21	1:B:1254:TYR:HB2	1.93	0.50
1:A:912:ARG:O	1:A:1264:LEU:HD13	2.11	0.50
1:A:1000:ILE:HG23	1:A:1000:ILE:O	2.11	0.50
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	1.94	0.50
1:B:1299:PRO:HG2	1:B:1301:THR:HG23	1.94	0.50
1:B:245:LEU:HD22	1:B:284:ILE:HD12	1.93	0.50
1:B:909:THR:OG1	1:B:910:ALA:N	2.44	0.50
1:B:1286:THR:CG2	1:B:1287:ASN:N	2.64	0.50
1:A:522:THR:HG22	1:A:526:LYS:HE3	1.93	0.50
1:A:560:PHE:N	1:A:560:PHE:CD2	2.79	0.50
1:A:779:MET:HG3	1:A:810:VAL:CG1	2.42	0.50
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.21	0.50
1:A:364:VAL:HG13	1:A:418:PHE:CE2	2.46	0.50
1:B:364:VAL:HG13	1:B:418:PHE:CE2	2.46	0.50
1:B:793:ARG:HG2	1:B:793:ARG:HH11	1.77	0.50
1:B:1000:ILE:HG23	1:B:1000:ILE:O	2.11	0.50
1:A:592:TYR:O	1:A:595:ASP:HB2	2.12	0.49
1:B:507:PHE:CZ	1:B:511:LEU:HD11	2.46	0.49
1:B:1315:THR:HG22	1:B:1316:LEU:HD22	1.94	0.49
1:A:615:ALA:HB2	1:A:691:ASP:HA	1.93	0.49
1:A:1140:TYR:HE1	1:A:1145:ASN:HD22	1.57	0.49
1:B:237:ILE:HD12	1:B:277:MET:CE	2.42	0.49
1:B:605:LEU:C	1:B:605:LEU:HD23	2.32	0.49
1:B:719:LEU:HD13	1:B:860:GLU:OE2	2.12	0.49
1:B:739:GLN:HG2	1:B:911:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HD12	1:A:277:MET:CE	2.42	0.49
1:A:245:LEU:HD22	1:A:284:ILE:HD12	1.93	0.49
1:A:793:ARG:HG2	1:A:793:ARG:HH11	1.77	0.49
1:A:1281:ALA:O	1:A:1284:GLN:HB3	2.12	0.49
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.12	0.49
1:A:332:GLU:OE2	1:A:548:LEU:HD13	2.13	0.49
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.42	0.49
1:B:779:MET:HG3	1:B:810:VAL:CG1	2.42	0.49
1:B:332:GLU:OE2	1:B:548:LEU:HD13	2.13	0.49
1:B:592:TYR:O	1:B:595:ASP:HB2	2.12	0.49
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.12	0.49
1:A:909:THR:OG1	1:A:910:ALA:N	2.44	0.49
1:A:54:MET:HB3	1:A:86:THR:HB	1.94	0.49
1:A:987:PHE:CE2	1:A:996:ARG:HG3	2.47	0.49
1:A:1330:LEU:CG	1:A:1331:ARG:N	2.68	0.49
1:B:912:ARG:O	1:B:1264:LEU:HD13	2.11	0.49
1:B:980:ARG:NH1	1:B:1161:GLU:OE1	2.46	0.49
1:A:351:ASN:ND2	1:A:361:LEU:HB2	2.28	0.49
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.47	0.49
1:A:1330:LEU:CD1	1:A:1332:VAL:N	2.70	0.49
1:B:661:THR:O	1:B:662:CYS:HB3	2.13	0.49
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.42	0.49
1:A:661:THR:O	1:A:662:CYS:HB3	2.13	0.49
1:B:399:GLY:N	1:B:402:GLU:OE1	2.45	0.49
1:B:471:GLN:OE1	1:B:471:GLN:HA	2.13	0.49
1:B:749:THR:OG1	1:B:764:VAL:HG13	2.13	0.49
1:B:1096:THR:HB	1:B:1129:THR:HG21	1.95	0.49
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.78	0.49
1:A:712:LEU:CD2	1:A:879:GLU:HG2	2.43	0.49
1:A:1192:ILE:O	1:A:1196:GLU:HG3	2.13	0.49
1:B:88:VAL:HG13	1:B:89:GLU:N	2.28	0.49
1:B:987:PHE:CE2	1:B:996:ARG:HG3	2.47	0.49
1:B:1022:HIS:CE1	1:B:1128:SER:HG	2.30	0.49
1:B:1192:ILE:O	1:B:1196:GLU:HG3	2.13	0.49
1:B:54:MET:HB3	1:B:86:THR:HB	1.94	0.48
1:A:61:LEU:HD23	1:A:61:LEU:C	2.34	0.48
1:A:749:THR:OG1	1:A:764:VAL:HG13	2.13	0.48
1:A:980:ARG:NH1	1:A:1161:GLU:OE1	2.46	0.48
1:A:1315:THR:HG22	1:A:1316:LEU:HD22	1.94	0.48
1:B:351:ASN:ND2	1:B:361:LEU:HB2	2.28	0.48
1:B:615:ALA:HB2	1:B:691:ASP:HA	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASN:HB2	1:A:363:PRO:HD3	1.95	0.48
1:A:615:ALA:CB	1:A:691:ASP:HA	2.43	0.48
1:A:616:LYS:HA	1:A:659:THR:HG22	1.96	0.48
1:B:61:LEU:HD23	1:B:61:LEU:C	2.34	0.48
1:B:114:GLY:HA2	1:B:117:THR:OG1	2.13	0.48
1:B:615:ALA:CB	1:B:691:ASP:HA	2.43	0.48
1:A:607:LEU:HD22	1:A:666:ILE:HG21	1.96	0.48
1:A:698:ILE:O	1:A:701:ALA:HB3	2.14	0.48
1:B:154:ARG:NH1	1:B:1196:GLU:OE1	2.47	0.48
1:B:362:ASN:HB2	1:B:363:PRO:HD3	1.95	0.48
1:B:607:LEU:HD22	1:B:666:ILE:HG21	1.96	0.48
1:A:114:GLY:HA2	1:A:117:THR:OG1	2.13	0.48
1:A:213:PRO:HB2	1:A:216:LEU:HB3	1.96	0.48
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.78	0.48
1:B:698:ILE:O	1:B:701:ALA:HB3	2.14	0.48
1:A:46:GLY:HA2	2:A:3002:FES:S1	2.54	0.48
1:A:245:LEU:HB2	1:A:284:ILE:HD11	1.96	0.48
1:A:308:VAL:HG21	1:A:348:LEU:HD12	1.96	0.48
1:B:213:PRO:HB2	1:B:216:LEU:HB3	1.96	0.48
1:B:245:LEU:HB2	1:B:284:ILE:HD11	1.96	0.48
1:B:1262:PRO:HB2	1:B:1263:PRO:HD3	1.95	0.48
1:A:529:LYS:O	1:A:530:ASP:CB	2.62	0.48
1:B:712:LEU:CD2	1:B:879:GLU:HG2	2.43	0.48
1:A:154:ARG:NH1	1:A:1196:GLU:OE1	2.47	0.48
1:A:388:THR:O	1:A:397:LEU:HD11	2.14	0.48
1:A:399:GLY:N	1:A:402:GLU:OE1	2.45	0.48
1:A:1262:PRO:HB2	1:A:1263:PRO:HD3	1.95	0.48
1:B:46:GLY:HA2	2:B:4002:FES:S1	2.54	0.48
1:B:418:PHE:CD1	1:B:439:ARG:HB2	2.49	0.48
1:A:471:GLN:HA	1:A:471:GLN:OE1	2.13	0.47
1:B:129:ARG:NE	1:B:209:GLU:HG2	2.29	0.47
1:B:154:ARG:N	1:B:155:PRO:HD2	2.29	0.47
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.21	0.47
1:A:698:ILE:HG23	1:A:901:CYS:SG	2.55	0.47
1:B:698:ILE:HG23	1:B:901:CYS:SG	2.54	0.47
1:A:88:VAL:HG13	1:A:89:GLU:N	2.28	0.47
1:B:747:HIS:ND1	1:B:805:SER:HA	2.29	0.47
1:B:1152:TYR:HE1	1:B:1257:LYS:HB3	1.79	0.47
1:A:1022:HIS:CE1	1:A:1128:SER:HG	2.32	0.47
1:B:616:LYS:HA	1:B:659:THR:HG22	1.95	0.47
1:A:736:ILE:CD1	1:A:921:PHE:HD2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:MET:CE	1:B:128:LEU:HG	2.45	0.47
1:A:129:ARG:NE	1:A:209:GLU:HG2	2.29	0.47
1:A:154:ARG:N	1:A:155:PRO:HD2	2.29	0.47
1:A:544:SER:HA	1:A:547:LEU:CD1	2.44	0.47
1:A:772:THR:O	1:A:776:VAL:HG23	2.15	0.47
1:A:1096:THR:HB	1:A:1129:THR:HG21	1.95	0.47
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.96	0.47
1:A:124:MET:CE	1:A:128:LEU:HG	2.45	0.47
1:A:418:PHE:CD1	1:A:439:ARG:HB2	2.49	0.47
1:A:747:HIS:ND1	1:A:805:SER:HA	2.29	0.47
1:A:872:ASP:OD1	1:A:873:LEU:N	2.47	0.47
1:A:1007:ILE:O	1:A:1008:SER:CB	2.62	0.47
1:A:1330:LEU:CD1	1:A:1332:VAL:H	2.28	0.47
3:A:3003:MTE:S1'	4:A:3004:MOS:O2	2.73	0.47
1:B:947:TYR:OH	1:B:953:THR:HA	2.14	0.47
1:B:1007:ILE:O	1:B:1008:SER:CB	2.62	0.47
1:B:1082:SER:HB2	3:B:4003:MTE:O1P	2.14	0.47
1:B:1330:LEU:CD1	1:B:1332:VAL:H	2.28	0.47
3:B:4003:MTE:S1'	4:B:4004:MOS:O2	2.73	0.47
1:A:747:HIS:HD2	1:A:832:ASP:OD1	1.97	0.47
1:B:388:THR:O	1:B:397:LEU:HD11	2.14	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.47
1:A:712:LEU:HD11	1:A:875:HIS:CE1	2.50	0.47
1:B:308:VAL:HG21	1:B:348:LEU:HD12	1.96	0.47
1:B:439:ARG:NH2	1:B:451:GLU:OE1	2.46	0.47
1:B:712:LEU:HD11	1:B:875:HIS:CE1	2.50	0.47
1:A:43:CYS:HA	1:A:829:ARG:HB2	1.97	0.46
1:A:1082:SER:HB2	3:A:3003:MTE:O1P	2.14	0.46
1:B:43:CYS:HA	1:B:829:ARG:HB2	1.97	0.46
1:B:197:ASN:O	1:B:200:GLU:HG2	2.15	0.46
1:A:197:ASN:O	1:A:200:GLU:HG2	2.15	0.46
1:A:45:GLU:OE1	1:A:1224:PRO:HD2	2.15	0.46
1:A:947:TYR:OH	1:A:953:THR:HA	2.14	0.46
1:A:1134:ARG:HD3	1:B:1124:ARG:O	2.15	0.46
1:B:772:THR:O	1:B:776:VAL:HG23	2.15	0.46
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.50	0.46
1:B:1102:GLU:OE1	1:B:1106:LYS:HE3	2.16	0.46
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.15	0.46
1:A:537:LYS:CG	1:A:538:LEU:H	2.00	0.46
1:B:747:HIS:HD2	1:B:832:ASP:OD1	1.97	0.46
1:B:768:ASN:ND2	1:B:1076:PRO:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:VAL:N	1:A:965:PRO:CD	2.79	0.46
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.50	0.46
1:A:1152:TYR:HE1	1:A:1257:LYS:HB3	1.80	0.46
1:B:87:THR:OG1	1:B:89:GLU:HG2	2.15	0.46
1:B:736:ILE:CD1	1:B:921:PHE:HD2	2.27	0.46
1:A:657:LYS:O	1:A:658:ASP:HB2	2.16	0.46
1:A:711:GLU:HA	1:A:899:ARG:HD2	1.96	0.46
1:A:911:PHE:O	1:A:912:ARG:C	2.53	0.46
1:B:657:LYS:O	1:B:658:ASP:HB2	2.16	0.46
1:A:234:VAL:HG12	1:A:235:THR:N	2.31	0.46
1:B:60:ARG:O	1:B:61:LEU:HB3	2.16	0.46
1:A:468:LYS:HB2	1:A:493:GLU:CD	2.37	0.45
1:B:45:GLU:OE1	1:B:1224:PRO:HD2	2.15	0.45
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.51	0.45
1:B:234:VAL:HG12	1:B:235:THR:N	2.31	0.45
1:B:872:ASP:OD1	1:B:873:LEU:N	2.47	0.45
1:B:964:VAL:N	1:B:965:PRO:CD	2.79	0.45
1:A:624:GLU:HB3	1:A:684:VAL:CG2	2.46	0.45
1:B:281:PRO:HB2	1:B:287:LEU:HD13	1.97	0.45
1:B:1099:LYS:HD2	1:B:1099:LYS:HA	1.76	0.45
1:A:768:ASN:ND2	1:A:1076:PRO:HB3	2.31	0.45
1:A:1102:GLU:OE1	1:A:1106:LYS:HE3	2.16	0.45
1:A:1152:TYR:OH	1:A:1257:LYS:HA	2.17	0.45
1:B:427:ARG:NE	1:B:549:PHE:CE1	2.85	0.45
1:B:473:GLN:HA	1:B:473:GLN:NE2	2.32	0.45
1:B:544:SER:HA	1:B:547:LEU:CD1	2.44	0.45
1:B:846:TYR:HA	1:B:860:GLU:O	2.17	0.45
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.52	0.45
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.51	0.45
1:A:60:ARG:O	1:A:61:LEU:HB3	2.16	0.45
1:A:426:ARG:CZ	1:A:1228:LYS:HE3	2.47	0.45
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.98	0.45
1:A:1184:SER:HB2	1:A:1255:ALA:HB3	1.98	0.45
1:B:254:GLU:CD	1:B:254:GLU:H	2.19	0.45
1:B:468:LYS:HB2	1:B:493:GLU:CD	2.37	0.45
1:B:624:GLU:HB3	1:B:684:VAL:CG2	2.46	0.45
1:A:296:GLY:HA2	1:A:411:TYR:CE1	2.52	0.45
1:A:719:LEU:HD13	1:A:860:GLU:HG3	1.99	0.45
1:A:926:TRP:CE3	1:A:927:MET:N	2.85	0.45
1:A:219:LEU:N	1:A:219:LEU:HD23	2.32	0.45
1:A:427:ARG:NE	1:A:549:PHE:CE1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:CD1	1:B:220:LYS:HD3	2.46	0.45
1:B:926:TRP:CE3	1:B:927:MET:N	2.85	0.45
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.98	0.45
1:B:1191:ASP:O	1:B:1192:ILE:CB	2.65	0.45
1:B:1330:LEU:CD1	1:B:1332:VAL:N	2.70	0.45
1:A:254:GLU:H	1:A:254:GLU:CD	2.19	0.45
1:A:736:ILE:HG23	1:A:1298:SER:HB3	1.99	0.45
1:A:1286:THR:CG2	1:A:1287:ASN:N	2.64	0.45
1:B:79:THR:HG22	1:B:236:TRP:CZ2	2.52	0.45
1:B:296:GLY:HA2	1:B:411:TYR:CE1	2.52	0.45
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.77	0.45
1:A:557:ILE:HD12	1:A:557:ILE:N	2.33	0.44
1:A:1191:ASP:O	1:A:1192:ILE:CB	2.65	0.44
1:B:219:LEU:HD23	1:B:219:LEU:N	2.32	0.44
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.53	0.44
1:B:705:ASN:HA	1:B:707:PHE:HE1	1.82	0.44
1:B:733:GLU:HG2	1:B:1295:ARG:NH1	2.32	0.44
1:B:733:GLU:O	1:B:1295:ARG:HD2	2.18	0.44
1:A:152:GLY:O	1:A:1235:ILE:HG21	2.18	0.44
1:A:217:LEU:CD1	1:A:220:LYS:HD3	2.46	0.44
1:B:557:ILE:HD12	1:B:557:ILE:N	2.32	0.44
1:B:604:PHE:O	1:B:671:VAL:HA	2.18	0.44
1:B:747:HIS:HB2	1:B:827:LEU:HD12	1.99	0.44
1:A:79:THR:HG22	1:A:236:TRP:CZ2	2.52	0.44
1:A:281:PRO:HB2	1:A:287:LEU:HD13	1.97	0.44
1:A:604:PHE:O	1:A:671:VAL:HA	2.18	0.44
1:A:846:TYR:HA	1:A:860:GLU:O	2.17	0.44
1:A:1016:GLN:HA	1:A:1133:TYR:O	2.18	0.44
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.52	0.44
1:A:87:THR:HG1	1:A:89:GLU:HG2	1.82	0.44
1:A:705:ASN:HA	1:A:707:PHE:HE1	1.82	0.44
1:B:1184:SER:HB2	1:B:1255:ALA:HB3	1.98	0.44
1:A:612:ARG:HG3	1:A:612:ARG:HH11	1.83	0.44
1:B:571:ASP:OD2	1:B:1052:LYS:NZ	2.47	0.44
1:B:612:ARG:HG3	1:B:612:ARG:HH11	1.82	0.44
1:A:328:ARG:CG	1:A:328:ARG:NH1	2.77	0.44
1:A:733:GLU:HG2	1:A:1295:ARG:NH1	2.32	0.44
1:A:859:LEU:HD22	1:A:891:ILE:HD13	2.00	0.44
1:A:1264:LEU:C	1:A:1264:LEU:HD23	2.38	0.44
1:B:719:LEU:HD13	1:B:860:GLU:HG3	1.99	0.44
1:B:1016:GLN:HA	1:B:1133:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:VAL:O	1:B:896:GLY:HA2	2.18	0.44
1:B:1259:VAL:HG22	1:B:1259:VAL:O	2.18	0.44
1:A:139:ILE:CD1	1:A:164:ALA:HB2	2.48	0.44
1:A:165:LYS:O	1:A:165:LYS:HG2	2.18	0.44
1:A:212:PHE:CD1	1:A:213:PRO:HD2	2.53	0.44
1:A:371:LYS:HB2	1:A:408:GLU:HB3	1.99	0.44
1:A:733:GLU:O	1:A:1295:ARG:HD2	2.18	0.44
1:B:152:GLY:O	1:B:1235:ILE:HG21	2.18	0.44
1:B:212:PHE:CD1	1:B:213:PRO:HD2	2.53	0.44
1:B:426:ARG:CZ	1:B:1228:LYS:HE3	2.47	0.44
1:B:705:ASN:HA	1:B:707:PHE:CE1	2.53	0.44
1:B:733:GLU:HG2	1:B:1295:ARG:HH12	1.83	0.44
1:B:736:ILE:HG23	1:B:1298:SER:HB3	1.99	0.44
1:B:878:MET:O	1:B:881:ALA:HB3	2.18	0.44
1:B:839:ARG:HG2	1:B:840:HIS:N	2.32	0.43
1:B:1286:THR:O	1:B:1287:ASN:O	2.36	0.43
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.53	0.43
1:A:711:GLU:HA	1:A:899:ARG:CD	2.48	0.43
1:A:747:HIS:HB2	1:A:827:LEU:HD12	1.99	0.43
1:A:839:ARG:HG2	1:A:840:HIS:N	2.32	0.43
1:B:60:ARG:O	1:B:61:LEU:HB2	2.18	0.43
1:B:165:LYS:O	1:B:165:LYS:HG2	2.18	0.43
1:B:389:PHE:C	1:B:391:PRO:HD3	2.38	0.43
1:B:497:SER:O	1:B:500:ALA:N	2.51	0.43
1:B:712:LEU:HD23	1:B:879:GLU:HG2	2.00	0.43
1:B:1152:TYR:OH	1:B:1257:LYS:HA	2.17	0.43
1:A:497:SER:O	1:A:500:ALA:N	2.51	0.43
1:A:861:VAL:O	1:A:896:GLY:HA2	2.17	0.43
1:B:115:PHE:HD2	1:B:744:LEU:HB3	1.84	0.43
1:B:898:GLY:O	1:B:899:ARG:HD2	2.18	0.43
1:B:1264:LEU:C	1:B:1264:LEU:HD23	2.38	0.43
1:A:712:LEU:HD23	1:A:879:GLU:HG2	2.00	0.43
1:A:898:GLY:O	1:A:899:ARG:HD2	2.18	0.43
1:B:371:LYS:HB2	1:B:408:GLU:HB3	1.99	0.43
1:B:1023:VAL:HG13	1:B:1029:VAL:HG22	2.00	0.43
1:A:124:MET:HE3	1:A:128:LEU:HG	1.99	0.43
1:A:733:GLU:HG2	1:A:1295:ARG:HH12	1.83	0.43
1:B:521:LEU:CD2	1:B:538:LEU:HD11	2.48	0.43
1:A:390:PHE:O	1:A:462:ARG:HD2	2.19	0.43
1:B:139:ILE:CD1	1:B:164:ALA:HB2	2.48	0.43
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1312:LYS:O	1:B:1316:LEU:HB2	2.19	0.43
1:A:115:PHE:HD2	1:A:744:LEU:HB3	1.84	0.43
1:A:521:LEU:CD2	1:A:538:LEU:HD11	2.48	0.43
1:A:850:PHE:CD1	1:A:930:VAL:HG13	2.53	0.43
1:A:878:MET:O	1:A:881:ALA:HB3	2.18	0.43
1:A:1085:ILE:HG13	1:A:1086:TYR:N	2.34	0.43
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.18	0.43
1:A:60:ARG:O	1:A:61:LEU:HB2	2.18	0.43
1:A:1023:VAL:HG13	1:A:1029:VAL:HG22	2.00	0.43
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.18	0.43
1:B:1082:SER:HB2	3:B:4003:MTE:P	2.59	0.43
1:B:1284:GLN:HG2	1:B:1285:HIS:CE1	2.54	0.43
1:A:705:ASN:HA	1:A:707:PHE:CE1	2.53	0.43
1:A:1286:THR:O	1:A:1287:ASN:O	2.36	0.43
1:A:1311:ASP:OD1	1:A:1313:PHE:HB2	2.19	0.43
1:B:117:THR:HB	1:B:118:PRO:HD3	2.01	0.43
1:A:571:ASP:OD2	1:A:1052:LYS:NZ	2.47	0.43
1:A:439:ARG:NH2	1:A:451:GLU:OE1	2.46	0.42
1:A:557:ILE:HG22	1:A:559:LEU:HD22	2.01	0.42
1:A:742:PHE:CE1	1:A:829:ARG:HD3	2.54	0.42
1:B:850:PHE:CD1	1:B:930:VAL:HG13	2.53	0.42
1:B:913:GLY:HA3	1:B:917:PRO:HG2	2.00	0.42
1:B:1085:ILE:HG13	1:B:1086:TYR:N	2.34	0.42
1:A:968:TRP:CH2	1:A:1000:ILE:HG23	2.54	0.42
1:A:1099:LYS:HA	1:A:1099:LYS:HD2	1.76	0.42
1:A:1284:GLN:HG2	1:A:1285:HIS:CE1	2.54	0.42
1:B:742:PHE:CE1	1:B:829:ARG:HD3	2.54	0.42
1:A:473:GLN:HA	1:A:473:GLN:NE2	2.32	0.42
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.85	0.42
1:B:711:GLU:HA	1:B:899:ARG:CD	2.48	0.42
1:B:1004:LYS:HB2	1:B:1155:TYR:CE2	2.54	0.42
1:B:1311:ASP:OD1	1:B:1313:PHE:HB2	2.19	0.42
1:A:128:LEU:HA	1:A:131:GLN:O	2.20	0.42
1:A:612:ARG:HH12	1:A:689:TYR:HB2	1.84	0.42
1:A:995:LYS:HD2	1:A:1280:ALA:HB1	2.02	0.42
1:A:1082:SER:HB2	3:A:3003:MTE:P	2.59	0.42
1:B:539:ASP:OD2	1:B:540:PRO:HD2	2.20	0.42
1:B:859:LEU:HD22	1:B:891:ILE:HD13	2.00	0.42
1:A:211:ILE:HG12	1:A:212:PHE:N	2.35	0.42
1:A:580:LEU:HG	1:A:1044:THR:HG23	2.01	0.42
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ILE:HD12	1:B:277:MET:HE1	2.01	0.42
1:B:721:LYS:HB2	1:B:721:LYS:HE3	1.89	0.42
1:A:427:ARG:NH2	1:A:1171:HIS:O	2.53	0.42
1:A:753:PRO:HD3	1:A:816:ALA:HB1	2.02	0.42
1:A:1312:LYS:O	1:A:1316:LEU:HB2	2.19	0.42
1:B:580:LEU:HG	1:B:1044:THR:HG23	2.00	0.42
1:B:799:GLY:HA2	4:B:4004:MOS:S	2.60	0.42
1:B:968:TRP:CH2	1:B:1000:ILE:HG23	2.54	0.42
1:A:621:ASP:HB3	1:A:686:LYS:HB3	2.00	0.42
1:A:1214:SER:OG	1:A:1216:GLU:HG2	2.19	0.42
1:B:38:GLY:O	1:B:40:LYS:HE2	2.20	0.42
1:B:753:PRO:HD3	1:B:816:ALA:HB1	2.02	0.42
1:A:389:PHE:C	1:A:391:PRO:HD3	2.38	0.42
1:A:614:HIS:HB2	1:A:904:ASN:ND2	2.35	0.42
1:A:799:GLY:HA2	4:A:3004:MOS:S	2.60	0.42
1:B:598:ARG:HG3	1:B:602:GLU:HB3	2.02	0.42
1:A:713:LYS:HD2	1:A:895:ARG:NH1	2.35	0.42
1:B:128:LEU:HA	1:B:131:GLN:O	2.20	0.42
1:B:529:LYS:O	1:B:530:ASP:CB	2.62	0.42
1:B:621:ASP:HB3	1:B:686:LYS:HB3	2.00	0.42
1:B:995:LYS:HD2	1:B:1280:ALA:HB1	2.02	0.42
1:A:541:THR:O	1:A:992:CYS:HB3	2.20	0.41
1:A:744:LEU:HD13	1:A:744:LEU:HA	1.78	0.41
1:B:390:PHE:O	1:B:462:ARG:HD2	2.19	0.41
1:B:427:ARG:NH2	1:B:1171:HIS:O	2.53	0.41
1:B:1144:THR:O	1:B:1145:ASN:C	2.58	0.41
1:A:539:ASP:OD2	1:A:540:PRO:HD2	2.20	0.41
1:A:913:GLY:HA3	1:A:917:PRO:HG2	2.00	0.41
1:A:11:ASN:OD1	1:A:90:GLY:HA3	2.21	0.41
1:A:117:THR:HB	1:A:118:PRO:HD3	2.01	0.41
1:A:124:MET:HB2	1:A:143:PHE:HZ	1.86	0.41
1:A:248:LEU:HB3	1:A:279:ILE:HD13	2.02	0.41
1:A:500:ALA:HB3	1:A:505:ILE:HD11	2.02	0.41
1:A:626:GLN:HA	1:A:631:PHE:CD2	2.55	0.41
1:B:124:MET:HB2	1:B:143:PHE:HZ	1.86	0.41
1:B:1286:THR:CG2	1:B:1287:ASN:H	1.94	0.41
1:A:38:GLY:O	1:A:40:LYS:HE2	2.20	0.41
1:A:237:ILE:HD12	1:A:277:MET:HE3	2.02	0.41
1:A:523:VAL:O	1:A:527:LEU:N	2.54	0.41
1:A:646:THR:OG1	1:A:647:GLY:N	2.53	0.41
1:B:500:ALA:HB3	1:B:505:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ASP:O	1:B:531:SER:CB	2.69	0.41
1:B:718:ASP:CB	1:B:721:LYS:HB3	2.48	0.41
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	2.02	0.41
1:A:707:PHE:CD2	1:A:899:ARG:HB3	2.56	0.41
1:B:248:LEU:HB3	1:B:279:ILE:HD13	2.03	0.41
1:B:612:ARG:HH12	1:B:689:TYR:HB2	1.84	0.41
1:B:958:ARG:HH21	1:B:960:GLU:HG2	1.85	0.41
1:B:1049:VAL:HG13	1:B:1254:TYR:HE1	1.85	0.41
1:A:598:ARG:HG3	1:A:602:GLU:HB3	2.02	0.41
1:A:1004:LYS:HB2	1:A:1155:TYR:CE2	2.54	0.41
1:A:1049:VAL:HG13	1:A:1254:TYR:HE1	1.85	0.41
1:B:948:LYS:HE2	1:B:948:LYS:HB3	1.92	0.41
1:A:721:LYS:HB2	1:A:721:LYS:HE3	1.89	0.41
1:A:1105:LYS:HG3	1:A:1116:TRP:CH2	2.56	0.41
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	2.03	0.41
1:B:211:ILE:HG12	1:B:212:PHE:N	2.35	0.41
1:B:557:ILE:HG22	1:B:559:LEU:HD22	2.01	0.41
1:B:614:HIS:HB2	1:B:904:ASN:ND2	2.35	0.41
1:B:626:GLN:HA	1:B:631:PHE:CD2	2.55	0.41
1:B:744:LEU:HD13	1:B:744:LEU:HA	1.78	0.41
1:B:1214:SER:OG	1:B:1216:GLU:HG2	2.20	0.41
1:A:958:ARG:HH21	1:A:960:GLU:HG2	1.85	0.41
1:A:1151:HIS:NE2	1:A:1251:LYS:HE3	2.36	0.41
1:B:135:THR:O	1:B:139:ILE:HG13	2.21	0.41
1:B:713:LYS:HD2	1:B:895:ARG:NH1	2.35	0.41
1:A:135:THR:O	1:A:139:ILE:HG13	2.21	0.41
1:A:612:ARG:NH1	1:A:612:ARG:HG3	2.36	0.41
1:A:785:ASN:ND2	1:B:1028:SER:HB2	2.36	0.41
1:B:11:ASN:OD1	1:B:90:GLY:HA3	2.21	0.41
1:B:312:LEU:O	1:B:316:VAL:HG23	2.20	0.41
1:B:506:GLU:CD	1:B:506:GLU:N	2.74	0.41
1:B:695:ILE:HG23	1:B:700:ASP:HB2	2.02	0.41
1:B:707:PHE:CD2	1:B:899:ARG:HB3	2.56	0.41
1:B:1105:LYS:HG3	1:B:1116:TRP:CH2	2.56	0.41
1:B:1282:ARG:NH1	1:B:1308:ALA:O	2.51	0.41
1:A:154:ARG:HD2	1:A:558:GLN:NE2	2.36	0.40
1:A:530:ASP:O	1:A:531:SER:CB	2.69	0.40
1:A:705:ASN:ND2	1:A:707:PHE:HE1	2.20	0.40
1:A:716:LYS:HE3	1:A:956:ASN:OD1	2.22	0.40
1:B:316:VAL:HA	1:B:324:THR:HG21	2.04	0.40
1:B:549:PHE:HE2	1:B:551:LYS:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1151:HIS:NE2	1:B:1251:LYS:HE3	2.36	0.40
1:A:490:LEU:HB2	1:A:513:LEU:CD2	2.51	0.40
1:A:522:THR:CG2	1:A:526:LYS:HE3	2.51	0.40
1:A:548:LEU:O	1:A:550:GLN:HG2	2.21	0.40
1:A:1045:LYS:O	1:A:1049:VAL:HG23	2.21	0.40
1:A:1249:ASN:HD22	1:A:1257:LYS:HG2	1.85	0.40
1:B:548:LEU:O	1:B:550:GLN:HG2	2.21	0.40
1:A:312:LEU:O	1:A:316:VAL:HG23	2.20	0.40
1:A:549:PHE:HE2	1:A:551:LYS:HG3	1.86	0.40
1:A:1144:THR:O	1:A:1145:ASN:C	2.58	0.40
1:B:154:ARG:HD2	1:B:558:GLN:NE2	2.36	0.40
1:B:716:LYS:HE3	1:B:956:ASN:OD1	2.22	0.40
1:B:1021:ILE:HG12	1:B:1031:VAL:HG13	2.03	0.40
1:B:1045:LYS:O	1:B:1049:VAL:HG23	2.21	0.40
1:B:1249:ASN:HD22	1:B:1257:LYS:HG2	1.85	0.40
1:B:523:VAL:O	1:B:527:LEU:N	2.54	0.40
1:A:27:LEU:HD21	1:A:41:LEU:HB2	2.03	0.40
1:A:316:VAL:HA	1:A:324:THR:HG21	2.04	0.40

All (5) 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)
1:A:499:ASP:OD2	1:B:1326:LYS:O[1_545]	1.88	0.32
1:A:501:PRO:CA	1:B:1328:TRP:CB[1_545]	1.96	0.24
1:A:1213:TYR:CB	1:B:1332:VAL:CG1[1_545]	2.09	0.11
1:A:565:ASN:CB	1:A:565:ASN:CB[2_655]	2.17	0.03
1:A:501:PRO:CB	1:B:1328:TRP:CG[1_545]	2.19	0.01

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	1282/1331 (96%)	1173 (92%)	94 (7%)	15 (1%)	13	39
1	B	1282/1331 (96%)	1172 (91%)	95 (7%)	15 (1%)	13	39
All	All	2564/2662 (96%)	2345 (92%)	189 (7%)	30 (1%)	13	39

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	530	ASP
1	A	1008	SER
1	A	1192	ILE
1	A	1287	ASN
1	B	4	ASP
1	B	530	ASP
1	B	1008	SER
1	B	1192	ILE
1	B	1287	ASN
1	A	61	LEU
1	A	429	ASP
1	B	61	LEU
1	B	429	ASP
1	A	580	LEU
1	A	912	ARG
1	B	580	LEU
1	B	912	ARG
1	A	43	CYS
1	A	394	ARG
1	B	43	CYS
1	B	394	ARG
1	A	444	PRO
1	A	1002	PRO
1	B	444	PRO
1	B	1002	PRO
1	A	797	GLY
1	B	797	GLY
1	A	1262	PRO
1	B	1262	PRO

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	1095/1127 (97%)	1072 (98%)	23 (2%)	53	84
1	B	1095/1127 (97%)	1072 (98%)	23 (2%)	53	84
All	All	2190/2254 (97%)	2144 (98%)	46 (2%)	53	84

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	154	ARG
1	A	254	GLU
1	A	277	MET
1	A	328	ARG
1	A	337	PHE
1	A	476	LYS
1	A	531	SER
1	A	546	THR
1	A	559	LEU
1	A	600	GLU
1	A	666	ILE
1	A	743	TYR
1	A	866	ASN
1	A	911	PHE
1	A	983	GLU
1	A	1108	ASN
1	A	1203	LEU
1	A	1239	PHE
1	A	1284	GLN
1	A	1310	VAL
1	A	1330	LEU
1	A	1332	VAL
1	B	89	GLU
1	B	154	ARG
1	B	254	GLU
1	B	277	MET
1	B	328	ARG
1	B	337	PHE
1	B	476	LYS
1	B	531	SER

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Mol	Chain	Res	Type
1	B	546	THR
1	B	559	LEU
1	B	600	GLU
1	B	666	ILE
1	B	743	TYR
1	B	866	ASN
1	B	911	PHE
1	B	983	GLU
1	B	1108	ASN
1	B	1203	LEU
1	B	1239	PHE
1	B	1284	GLN
1	B	1310	VAL
1	B	1330	LEU
1	B	1332	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	131	GLN
1	A	208	GLN
1	A	292	HIS
1	A	351	ASN
1	A	473	GLN
1	A	585	GLN
1	A	626	GLN
1	A	650	ASN
1	A	705	ASN
1	A	747	HIS
1	A	866	ASN
1	A	875	HIS
1	A	1108	ASN
1	A	1145	ASN
1	A	1284	GLN
1	A	1287	ASN
1	B	71	ASN
1	B	131	GLN
1	B	208	GLN
1	B	292	HIS
1	B	351	ASN
1	B	473	GLN

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Mol	Chain	Res	Type
1	B	585	GLN
1	B	626	GLN
1	B	650	ASN
1	B	705	ASN
1	B	866	ASN
1	B	875	HIS
1	B	1108	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
2	FES	A	3002	1	0,4,4	-	-	-		
6	TEI	A	3006	-	16,23,23	3.55	6 (37%)	19,32,32	1.46	4 (21%)
3	MTE	A	3003	4	21,26,26	6.04	12 (57%)	21,40,40	3.27	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FES	B	4001	1	0,4,4	-	-	-		
4	MOS	A	3004	3	0,3,3	-	-	-		
4	MOS	B	4004	3	0,3,3	-	-	-		
5	FAD	A	3005	-	53,58,58	4.62	38 (71%)	68,89,89	2.49	27 (39%)
5	FAD	B	4005	-	53,58,58	4.62	38 (71%)	68,89,89	2.49	27 (39%)
3	MTE	B	4003	4	21,26,26	6.04	12 (57%)	21,40,40	3.27	8 (38%)
2	FES	B	4002	1	0,4,4	-	-	-		
2	FES	A	3001	1	0,4,4	-	-	-		
6	TEI	B	4006	-	16,23,23	3.55	6 (37%)	19,32,32	1.46	4 (21%)

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
2	FES	A	3002	1	-	-	0/1/1/1
6	TEI	A	3006	-	-	0/9/15/15	0/2/2/2
3	MTE	A	3003	4	-	0/6/34/34	0/3/3/3
2	FES	B	4001	1	-	-	0/1/1/1
5	FAD	A	3005	-	-	7/30/50/50	0/6/6/6
5	FAD	B	4005	-	-	7/30/50/50	0/6/6/6
3	MTE	B	4003	4	-	0/6/34/34	0/3/3/3
2	FES	B	4002	1	-	-	0/1/1/1
2	FES	A	3001	1	-	-	0/1/1/1
6	TEI	B	4006	-	-	0/9/15/15	0/2/2/2

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3003	MTE	C7-C6	17.21	1.67	1.53
3	B	4003	MTE	C7-C6	17.21	1.67	1.53
3	B	4003	MTE	C9-C10	11.64	1.63	1.41
3	A	3003	MTE	C9-C10	11.63	1.63	1.41
5	A	3005	FAD	C5'-C4'	-10.31	1.37	1.51
5	B	4005	FAD	C5'-C4'	-10.27	1.37	1.51
5	A	3005	FAD	C9A-C5X	10.12	1.58	1.41
5	B	4005	FAD	C9A-C5X	10.08	1.58	1.41
5	B	4005	FAD	C9A-N10	9.94	1.58	1.41
5	A	3005	FAD	C9A-N10	9.89	1.58	1.41
5	B	4005	FAD	C2A-N3A	9.29	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	FAD	C2A-N3A	9.28	1.47	1.32
3	A	3003	MTE	C6-N5	8.90	1.57	1.45
3	B	4003	MTE	C6-N5	8.89	1.57	1.45
5	A	3005	FAD	C2A-N1A	8.81	1.50	1.33
5	B	4005	FAD	C2A-N1A	8.80	1.50	1.33
6	B	4006	TEI	C11-C6	8.62	1.62	1.41
6	A	3006	TEI	C11-C6	8.61	1.62	1.41
6	B	4006	TEI	C10-C9	8.36	1.57	1.39
6	A	3006	TEI	C10-C9	8.34	1.57	1.39
3	B	4003	MTE	C4'-C3'	-8.13	1.41	1.52
3	A	3003	MTE	C4'-C3'	-8.12	1.41	1.52
5	A	3005	FAD	C4A-N3A	7.97	1.46	1.35
5	B	4005	FAD	C4A-N3A	7.92	1.46	1.35
3	A	3003	MTE	P-O4'	-7.69	1.35	1.60
3	B	4003	MTE	P-O4'	-7.68	1.35	1.60
5	B	4005	FAD	C8-C7	6.90	1.58	1.40
5	A	3005	FAD	C8-C7	6.88	1.58	1.40
3	A	3003	MTE	C9-N5	6.73	1.51	1.38
3	B	4003	MTE	C9-N5	6.70	1.51	1.38
5	B	4005	FAD	C4'-C3'	6.24	1.65	1.53
5	A	3005	FAD	C4'-C3'	6.22	1.65	1.53
6	A	3006	TEI	C8-C12	5.90	1.53	1.44
6	B	4006	TEI	C8-C12	5.87	1.53	1.44
5	B	4005	FAD	O3'-C3'	5.85	1.56	1.43
5	A	3005	FAD	O3'-C3'	5.84	1.56	1.43
5	B	4005	FAD	C2B-C1B	-5.49	1.45	1.53
5	A	3005	FAD	C2B-C1B	-5.48	1.45	1.53
5	A	3005	FAD	C9-C9A	5.36	1.48	1.39
5	B	4005	FAD	C6-C5X	5.36	1.48	1.40
5	B	4005	FAD	C9-C9A	5.33	1.48	1.39
5	A	3005	FAD	C6-C5X	5.32	1.48	1.40
5	A	3005	FAD	C5A-C4A	5.31	1.55	1.40
5	B	4005	FAD	C5A-C4A	5.30	1.55	1.40
3	B	4003	MTE	P-O3P	-5.25	1.34	1.54
3	A	3003	MTE	P-O3P	-5.24	1.34	1.54
5	A	3005	FAD	C4X-N5	5.23	1.40	1.30
5	B	4005	FAD	C4X-N5	5.19	1.40	1.30
5	A	3005	FAD	O2-C2	-5.02	1.15	1.24
5	B	4005	FAD	O2-C2	-4.99	1.15	1.24
5	A	3005	FAD	C7M-C7	-4.88	1.41	1.51
5	B	4005	FAD	C7M-C7	-4.88	1.41	1.51
5	A	3005	FAD	O2B-C2B	-4.83	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4005	FAD	O2B-C2B	-4.80	1.31	1.43
5	B	4005	FAD	C2'-C3'	-4.72	1.44	1.53
5	A	3005	FAD	C2'-C3'	-4.72	1.44	1.53
5	B	4005	FAD	PA-O2A	-4.36	1.34	1.55
5	A	3005	FAD	PA-O2A	-4.35	1.34	1.55
3	B	4003	MTE	C9-C4	4.31	1.47	1.41
3	A	3003	MTE	C9-C4	4.30	1.47	1.41
5	A	3005	FAD	C2-N3	4.18	1.48	1.39
5	B	4005	FAD	C2-N3	4.17	1.48	1.39
5	A	3005	FAD	C4-N3	4.02	1.46	1.38
5	B	4005	FAD	C4-N3	4.00	1.46	1.38
3	B	4003	MTE	C4-N3	3.91	1.39	1.33
3	A	3003	MTE	C4-N3	3.90	1.39	1.33
5	B	4005	FAD	O2'-C2'	-3.88	1.35	1.43
5	A	3005	FAD	O2'-C2'	-3.87	1.35	1.43
5	B	4005	FAD	O5'-C5'	3.75	1.59	1.44
5	A	3005	FAD	O5'-C5'	3.74	1.59	1.44
5	B	4005	FAD	O4B-C1B	3.61	1.46	1.41
5	A	3005	FAD	O4B-C1B	3.60	1.46	1.41
5	A	3005	FAD	C6-C7	3.42	1.44	1.39
5	B	4005	FAD	C6-C7	3.38	1.44	1.39
5	B	4005	FAD	C6A-C5A	3.34	1.55	1.43
5	A	3005	FAD	C6A-C5A	3.34	1.55	1.43
5	A	3005	FAD	P-O2P	-3.24	1.40	1.55
5	B	4005	FAD	P-O2P	-3.22	1.40	1.55
5	B	4005	FAD	P-O5'	-3.13	1.46	1.59
5	A	3005	FAD	P-O5'	-3.12	1.46	1.59
5	A	3005	FAD	C9-C8	3.11	1.44	1.39
5	B	4005	FAD	C9-C8	3.10	1.44	1.39
5	A	3005	FAD	C5A-N7A	-3.10	1.28	1.39
5	B	4005	FAD	C5A-N7A	-3.08	1.28	1.39
5	A	3005	FAD	C8A-N7A	-3.07	1.29	1.34
5	B	4005	FAD	C8A-N7A	-3.06	1.29	1.34
6	A	3006	TEI	O14-C9	3.01	1.43	1.37
6	B	4006	TEI	O14-C9	2.98	1.43	1.37
5	B	4005	FAD	C8M-C8	-2.97	1.45	1.51
5	A	3005	FAD	C8M-C8	-2.95	1.45	1.51
5	A	3005	FAD	O4-C4	2.95	1.29	1.23
5	B	4005	FAD	O4-C4	2.94	1.29	1.23
5	A	3005	FAD	C4X-C4	2.93	1.55	1.44
5	B	4005	FAD	C4X-C4	2.93	1.55	1.44
5	B	4005	FAD	C10-N10	2.64	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	FAD	C10-N10	2.63	1.43	1.37
5	B	4005	FAD	P-O1P	-2.57	1.41	1.50
5	A	3005	FAD	P-O1P	-2.57	1.41	1.50
5	B	4005	FAD	PA-O5B	-2.54	1.49	1.59
5	A	3005	FAD	PA-O5B	-2.54	1.49	1.59
5	B	4005	FAD	C4X-C10	2.45	1.51	1.44
5	A	3005	FAD	C4X-C10	2.44	1.51	1.44
3	B	4003	MTE	O4-C4	2.43	1.30	1.24
3	A	3003	MTE	O4-C4	2.43	1.30	1.24
3	B	4003	MTE	C2-N1	2.41	1.39	1.35
3	A	3003	MTE	C2-N1	2.38	1.39	1.35
3	B	4003	MTE	O3'-C3'	2.17	1.46	1.43
3	A	3003	MTE	O3'-C3'	2.15	1.46	1.43
6	B	4006	TEI	O21-C20	-2.14	1.24	1.30
6	A	3006	TEI	O21-C20	-2.13	1.24	1.30
6	B	4006	TEI	C8-C9	2.02	1.44	1.40
6	A	3006	TEI	C8-C9	2.01	1.44	1.40

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3003	MTE	C4-C9-N5	10.14	127.63	119.12
3	B	4003	MTE	C4-C9-N5	10.12	127.62	119.12
3	A	3003	MTE	C2-N1-C10	5.90	127.76	114.54
3	B	4003	MTE	C2-N1-C10	5.90	127.76	114.54
5	B	4005	FAD	O4'-C4'-C5'	-5.69	97.12	109.92
5	A	3005	FAD	O4'-C4'-C5'	-5.69	97.13	109.92
5	A	3005	FAD	C9-C9A-N10	5.37	129.09	121.84
5	B	4005	FAD	C9-C9A-N10	5.35	129.07	121.84
5	B	4005	FAD	C5X-C9A-N10	-5.22	112.57	117.95
5	A	3005	FAD	C5X-C9A-N10	-5.20	112.58	117.95
5	A	3005	FAD	O3'-C3'-C2'	5.15	121.25	108.81
5	B	4005	FAD	O3'-C3'-C2'	5.15	121.25	108.81
5	A	3005	FAD	O3'-C3'-C4'	4.92	120.70	108.81
5	B	4005	FAD	O3'-C3'-C4'	4.92	120.69	108.81
5	A	3005	FAD	O5B-PA-O1A	-4.80	90.33	109.07
5	B	4005	FAD	O5B-PA-O1A	-4.79	90.34	109.07
5	B	4005	FAD	C8M-C8-C9	-4.60	110.99	119.49
5	A	3005	FAD	C8M-C8-C9	-4.59	111.00	119.49
3	B	4003	MTE	N2-C2-N3	4.57	124.36	117.25
3	A	3003	MTE	N2-C2-N3	4.55	124.33	117.25
3	B	4003	MTE	C2-N3-C4	4.51	123.09	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3003	MTE	C2-N3-C4	4.49	123.07	115.93
5	B	4005	FAD	C8M-C8-C7	4.27	129.50	120.74
5	A	3005	FAD	C8M-C8-C7	4.26	129.47	120.74
5	B	4005	FAD	C10-N1-C2	4.06	125.03	116.90
5	A	3005	FAD	C10-N1-C2	4.06	125.02	116.90
5	A	3005	FAD	C7M-C7-C6	-4.05	112.00	119.49
5	B	4005	FAD	C7M-C7-C6	-4.05	112.01	119.49
5	B	4005	FAD	C4'-C3'-C2'	-3.88	105.29	113.36
5	A	3005	FAD	C4'-C3'-C2'	-3.88	105.30	113.36
5	B	4005	FAD	O4B-C4B-C5B	-3.85	96.71	109.37
5	A	3005	FAD	O4B-C4B-C5B	-3.84	96.75	109.37
3	B	4003	MTE	N1-C2-N3	-3.81	119.44	125.42
3	A	3003	MTE	N1-C2-N3	-3.79	119.47	125.42
6	B	4006	TEI	C7-C6-C11	3.40	122.38	118.15
6	A	3006	TEI	C7-C6-C11	3.38	122.36	118.15
5	A	3005	FAD	C7M-C7-C8	3.31	127.52	120.74
5	B	4005	FAD	C7M-C7-C8	3.30	127.49	120.74
5	A	3005	FAD	O5B-C5B-C4B	3.20	119.99	108.99
5	B	4005	FAD	O5B-C5B-C4B	3.19	119.98	108.99
5	B	4005	FAD	P-O3P-PA	3.17	143.69	132.83
5	A	3005	FAD	P-O3P-PA	3.16	143.69	132.83
5	A	3005	FAD	C5X-N5-C4X	3.10	123.23	118.07
5	B	4005	FAD	C5X-N5-C4X	3.10	123.22	118.07
5	B	4005	FAD	C5A-C6A-N6A	3.09	125.05	120.35
5	A	3005	FAD	C5A-C6A-N6A	3.06	125.00	120.35
5	B	4005	FAD	O5'-P-O1P	-2.88	97.80	109.07
5	A	3005	FAD	O5'-P-O1P	-2.88	97.80	109.07
5	A	3005	FAD	O2'-C2'-C1'	2.81	116.59	109.80
5	B	4005	FAD	O2'-C2'-C1'	2.81	116.58	109.80
3	B	4003	MTE	O3'-C7-N8	-2.77	105.72	108.57
3	A	3003	MTE	O3'-C7-N8	-2.72	105.77	108.57
5	B	4005	FAD	C4-C4X-N5	2.72	122.10	118.23
5	A	3005	FAD	C4-C4X-N5	2.70	122.08	118.23
5	A	3005	FAD	C4-N3-C2	-2.67	120.70	125.64
3	A	3003	MTE	C9-C10-N8	2.67	120.57	118.13
5	B	4005	FAD	C4-N3-C2	-2.67	120.71	125.64
3	B	4003	MTE	C9-C10-N8	2.61	120.52	118.13
6	B	4006	TEI	C10-C11-C6	-2.59	116.81	120.82
6	A	3006	TEI	C10-C11-C6	-2.57	116.84	120.82
3	A	3003	MTE	O2P-P-O4'	2.44	113.23	106.73
3	B	4003	MTE	O2P-P-O4'	2.43	113.20	106.73
5	B	4005	FAD	N3A-C2A-N1A	-2.39	124.94	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3005	FAD	N3A-C2A-N1A	-2.36	124.99	128.68
6	A	3006	TEI	O21-C20-C5	2.33	121.90	114.43
6	B	4006	TEI	O21-C20-C5	2.33	121.90	114.43
5	B	4005	FAD	C2A-N1A-C6A	2.26	122.63	118.75
5	B	4005	FAD	O3B-C3B-C2B	2.26	119.12	111.82
5	A	3005	FAD	C2A-N1A-C6A	2.25	122.60	118.75
5	A	3005	FAD	O3B-C3B-C2B	2.25	119.09	111.82
6	A	3006	TEI	C4-C5-C20	-2.22	127.52	131.25
6	B	4006	TEI	C4-C5-C20	-2.22	127.52	131.25
5	B	4005	FAD	O2'-C2'-C3'	2.16	114.34	109.10
5	A	3005	FAD	O2'-C2'-C3'	2.15	114.34	109.10
5	B	4005	FAD	C5B-C4B-C3B	2.11	123.09	115.18
5	A	3005	FAD	C5B-C4B-C3B	2.11	123.09	115.18
5	A	3005	FAD	O4'-C4'-C3'	-2.04	104.13	109.10
5	B	4005	FAD	O4'-C4'-C3'	-2.04	104.13	109.10

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3005	FAD	N10-C1'-C2'-O2'
5	A	3005	FAD	C2'-C3'-C4'-O4'
5	A	3005	FAD	O3'-C3'-C4'-O4'
5	A	3005	FAD	O3'-C3'-C4'-C5'
5	B	4005	FAD	N10-C1'-C2'-O2'
5	B	4005	FAD	C2'-C3'-C4'-O4'
5	B	4005	FAD	O3'-C3'-C4'-O4'
5	B	4005	FAD	O3'-C3'-C4'-C5'
5	A	3005	FAD	C4'-C5'-O5'-P
5	B	4005	FAD	C4'-C5'-O5'-P
5	A	3005	FAD	O4B-C4B-C5B-O5B
5	B	4005	FAD	O4B-C4B-C5B-O5B
5	A	3005	FAD	C1'-C2'-C3'-O3'
5	B	4005	FAD	C1'-C2'-C3'-O3'

There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	FES	1	0
3	A	3003	MTE	4	0

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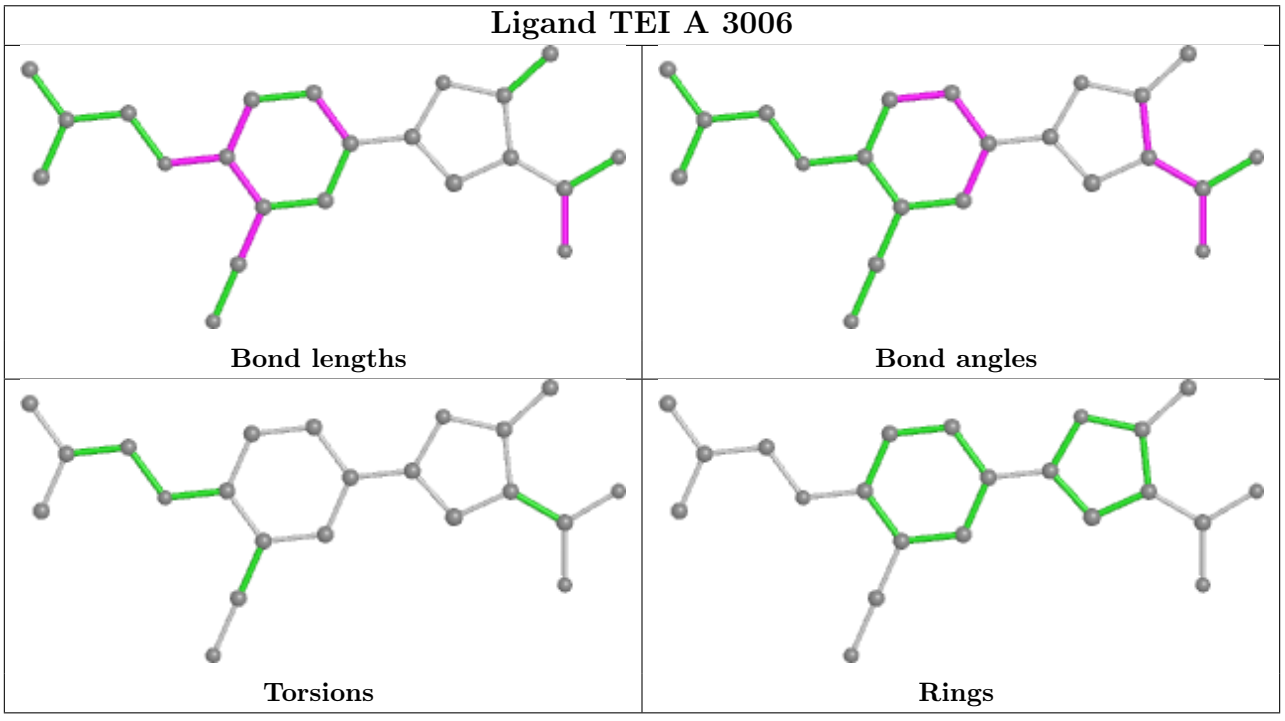
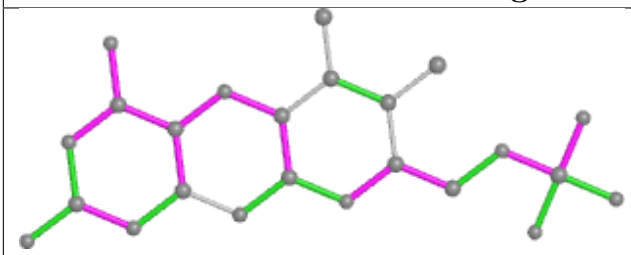
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4001	FES	1	0
4	A	3004	MOS	8	0
4	B	4004	MOS	8	0
5	A	3005	FAD	2	0
5	B	4005	FAD	2	0
3	B	4003	MTE	4	0
2	B	4002	FES	1	0
2	A	3001	FES	1	0

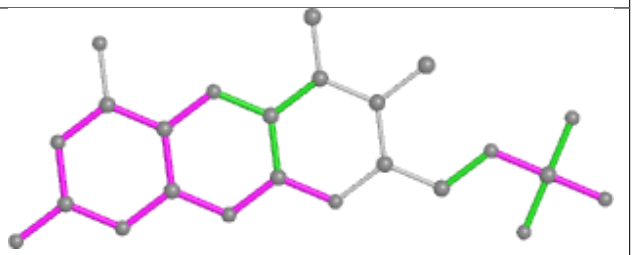
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



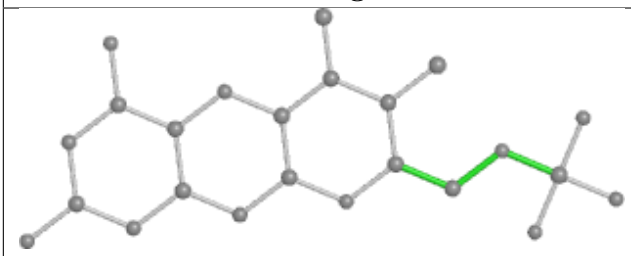
Ligand MTE A 3003



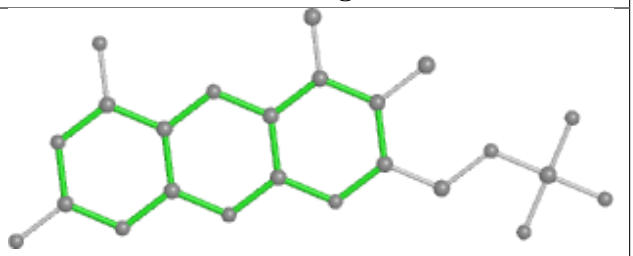
Bond lengths



Bond angles

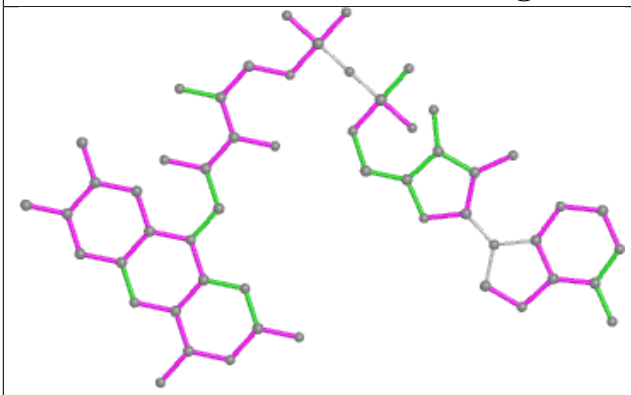


Torsions

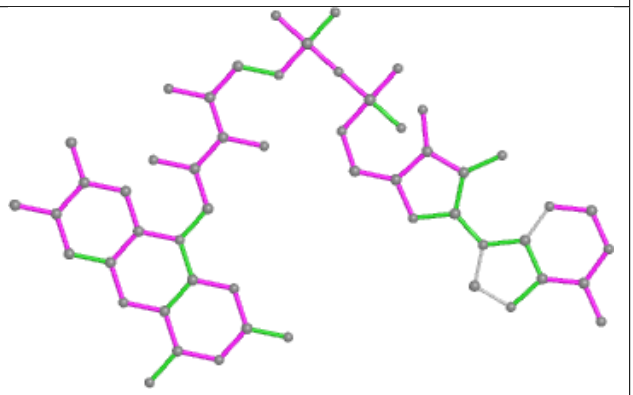


Rings

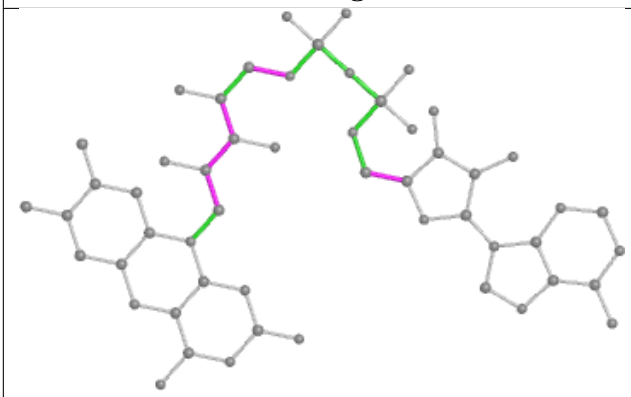
Ligand FAD A 3005



Bond lengths



Bond angles



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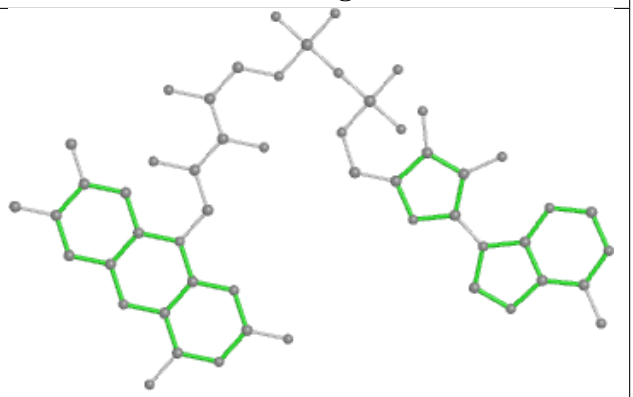
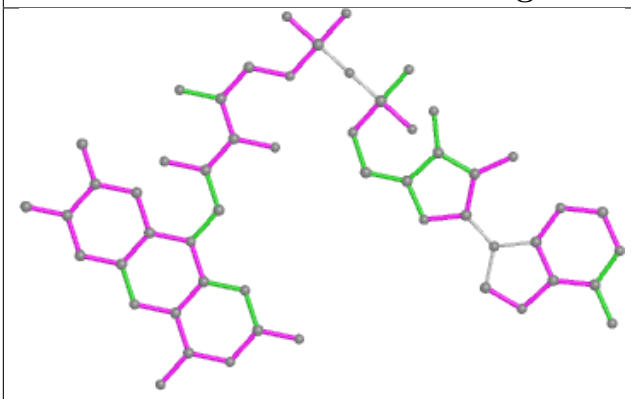
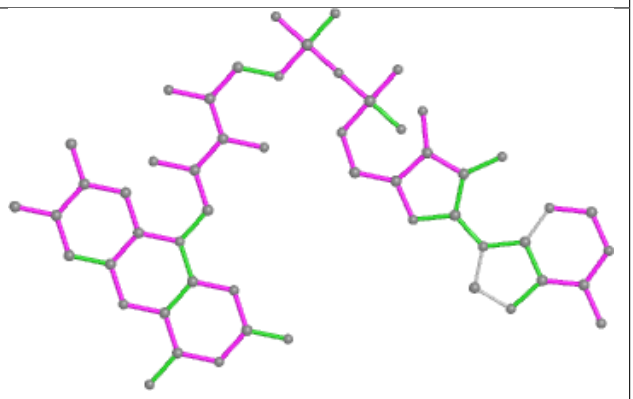


Rings

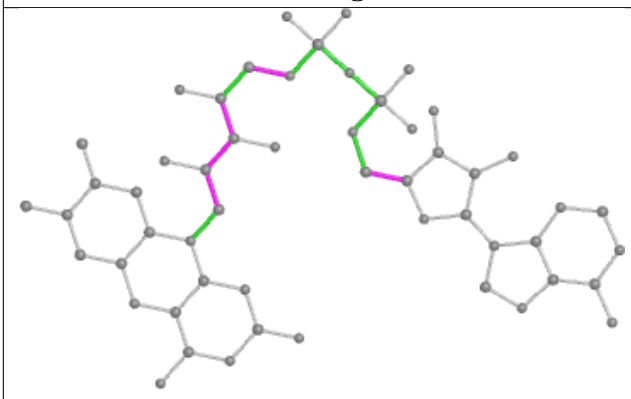
Ligand FAD B 4005



Bond lengths



Bond angles



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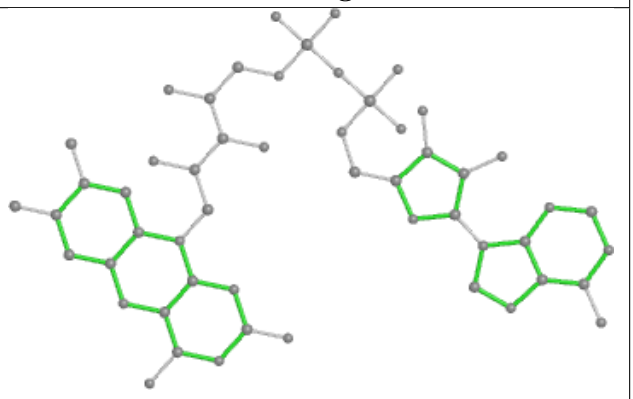
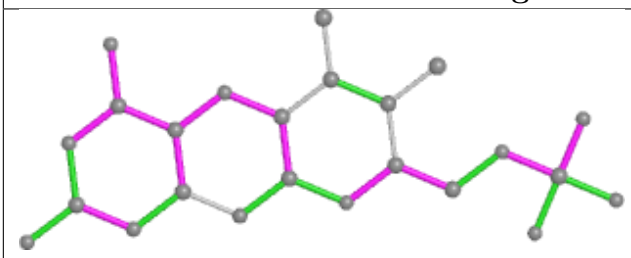
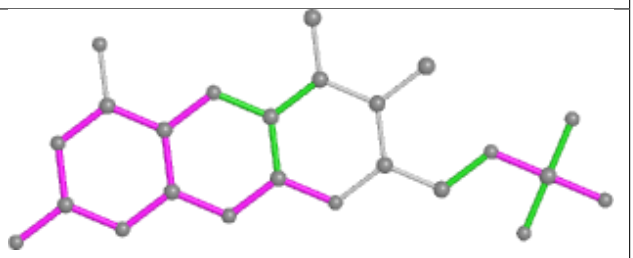


Rings

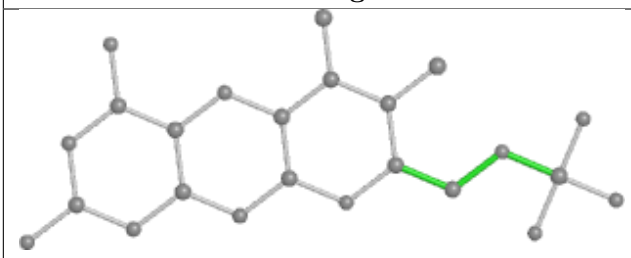
Ligand MTE B 4003



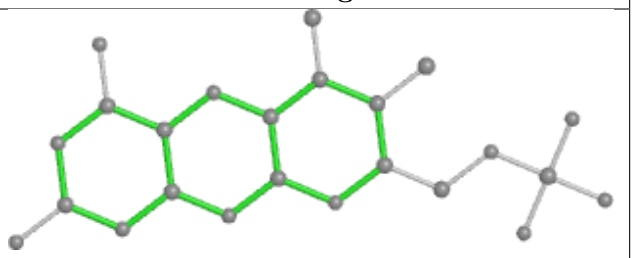
Bond lengths



Bond angles

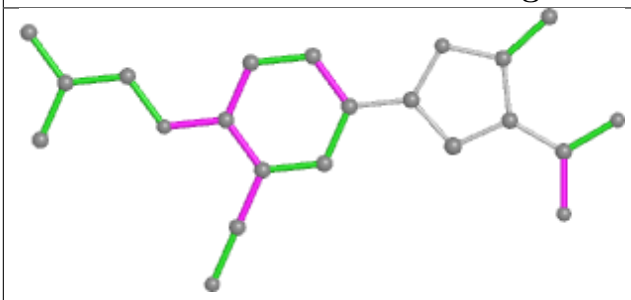


Torsions

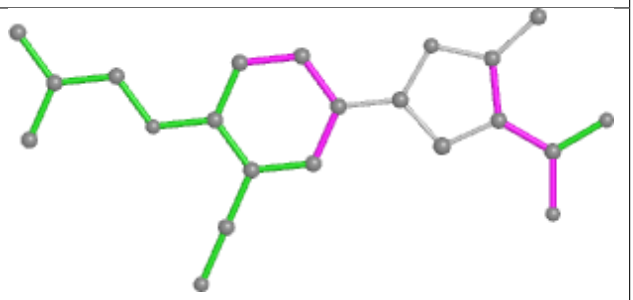


Rings

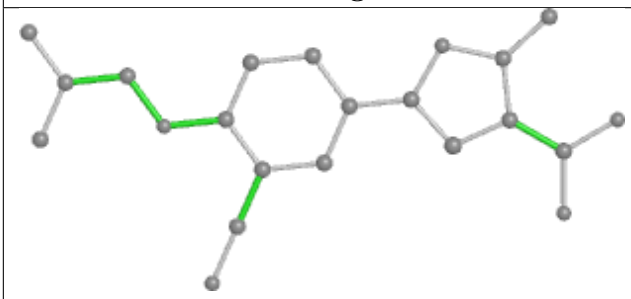
Ligand TEI B 4006



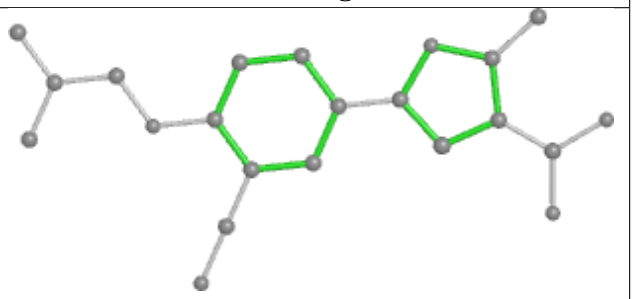
Bond lengths



Bond angles



Torsions



Rings

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.