



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:04 am BST

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

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

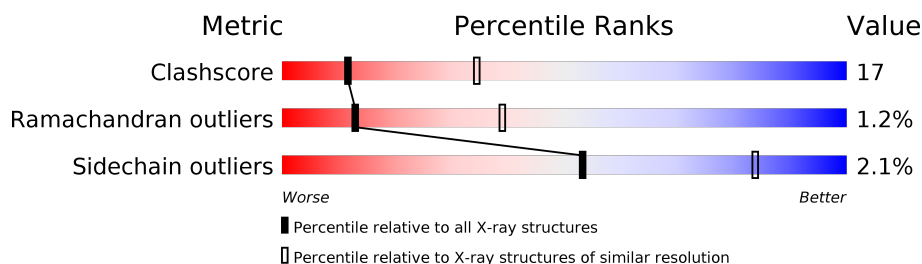
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1331	
1	B	1331	

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 [i](#)

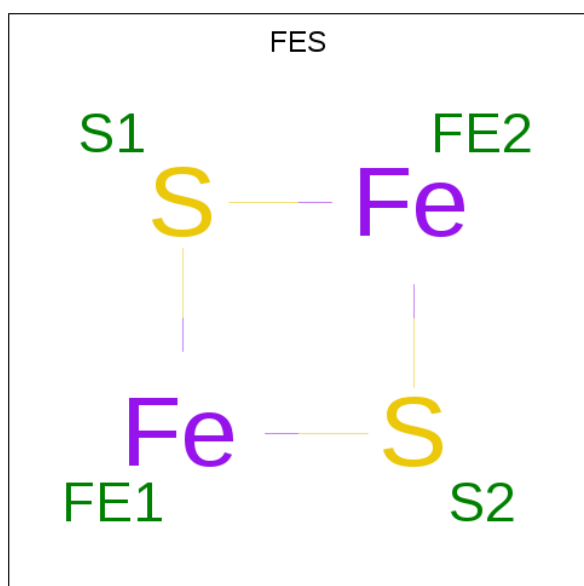
There are 6 unique types of molecules in this entry. The entry contains 20268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

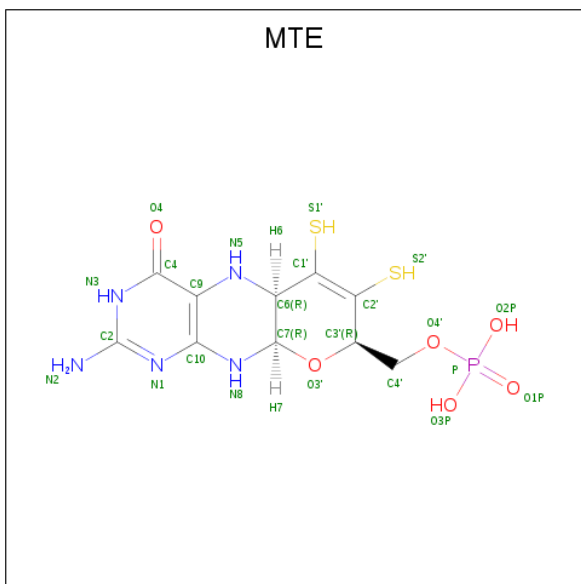
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			
1	B	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			

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



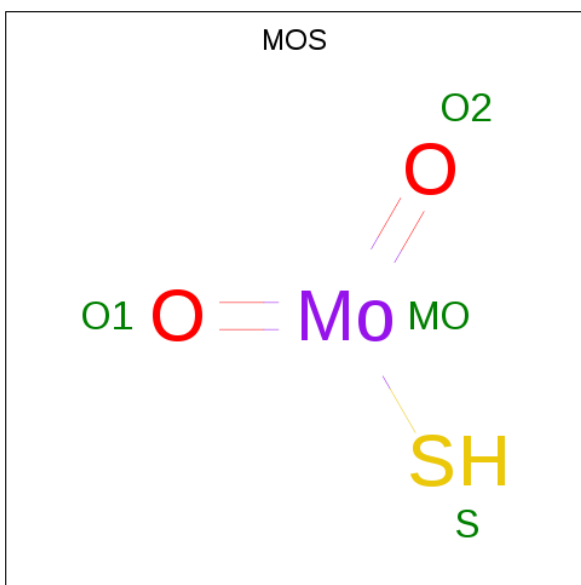
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

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



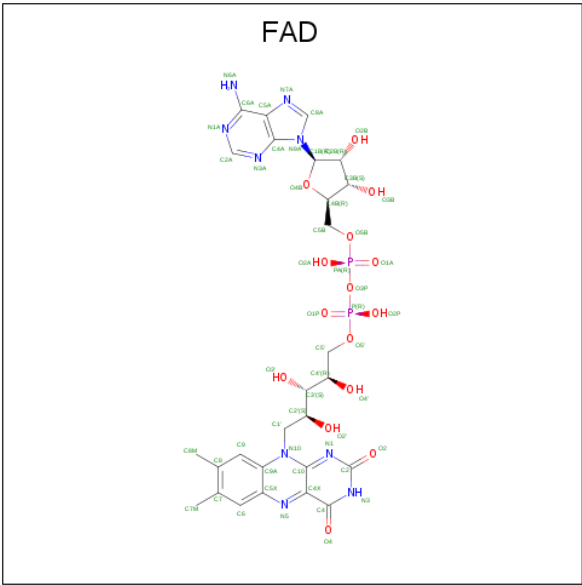
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

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



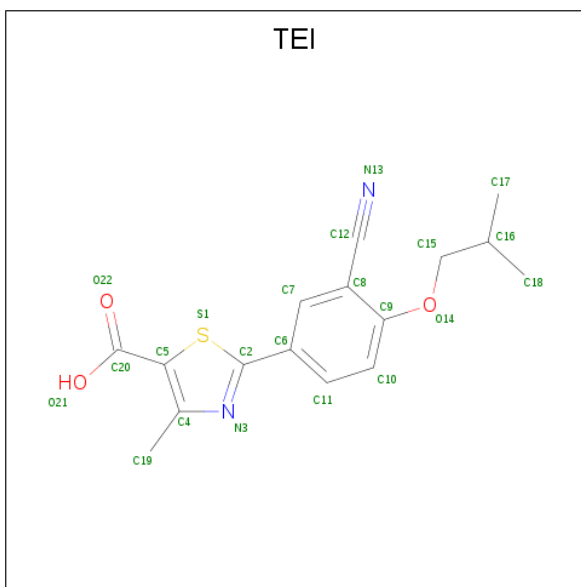
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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-CARBOXYLIC ACID (three-letter code: TEI) (formula: C₁₆H₁₆N₂O₃S).



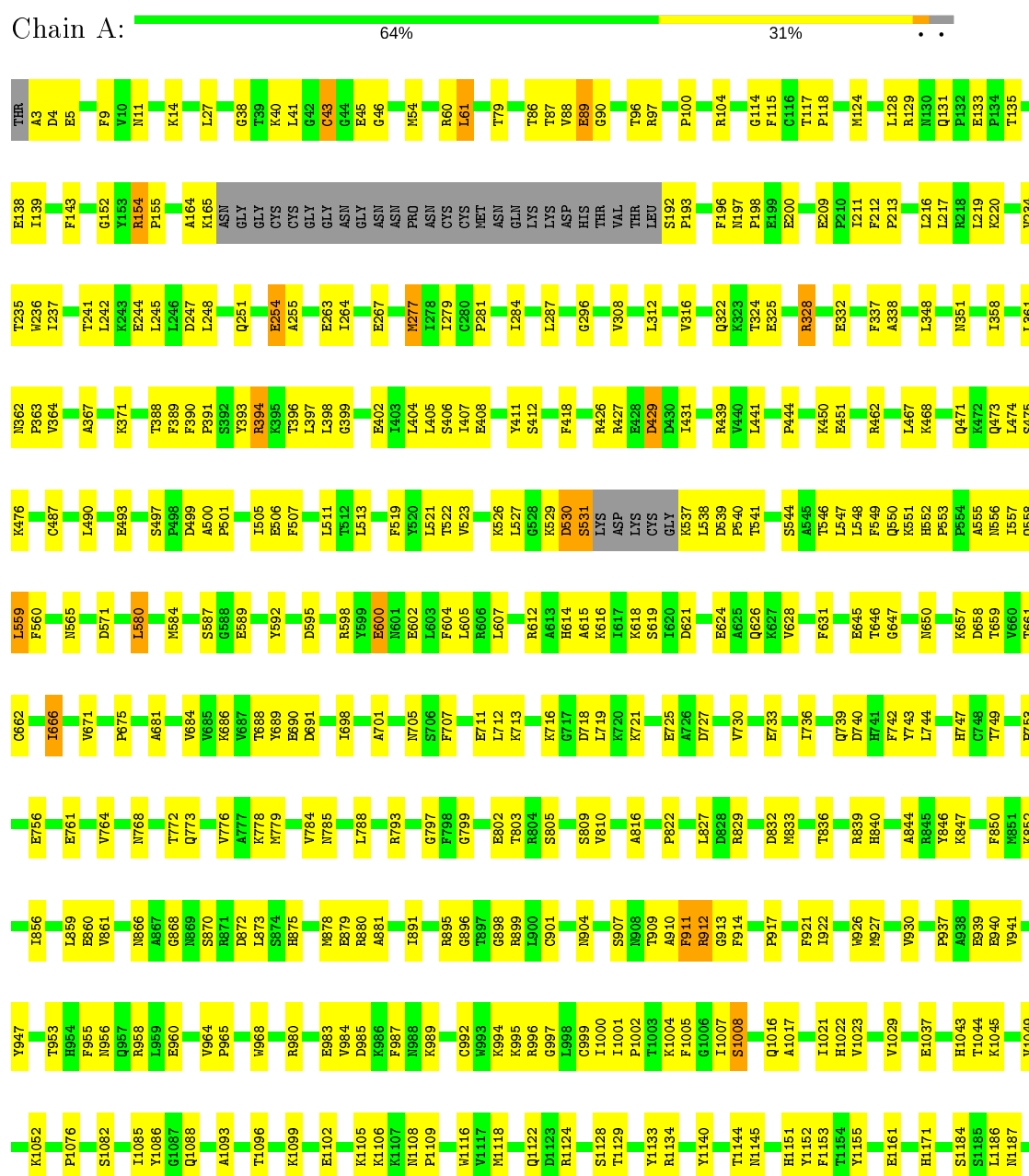
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			22	16	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			22	16	2	3	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Xanthine Dehydrogenase



T1190	D1311
D1191	K1312
T1192	F1313
E1196	T1314
T1315	L1316
V1200	CYS
L1203	VAL
Y1213	THR
S1214	GLY
P1215	ALA
E1216	PRO
P1224	GLY
K1228	ASN
T1235	K1326
E1238	L1330
F1239	R1331
L1264	V1332
H1269	
K1260	
K1251	
Y1254	
A1255	
S1256	
K1257	
A1258	
V1259	
P1262	
P1263	
L1264	
F1271	
F1272	
A1273	
A1280	
A1281	
Q1284	
H1285	
T1286	
H1287	
R1295	
S1298	
P1299	
A1300	
T1301	
P1302	
V1310	

• Molecule 1: Xanthine Dehydrogenase

Chain B:  64% 31%

THR	F143	T241	A367	E493	N584	V685	T772	G668	L959	I1085	L1203
A3	G152	T242	A371	S497	S587	K686	Q773	R669	E960	Y1086	L1203
E5	Y153	K243	K371	S497	E589	T688	A776	R671	V964	Q1088	S1214
F9	P154	E244	T388	A500	E592	V689	A777	D872	P965	A1093	P1215
Y10	P155	L245	F389	I505	T592	D691	K773	S874	W968	T1096	E1216
H11	A164	D247	F390	E506	T595	T695	H779	H575	R980	K1099	P1224
K14	K165	L248	P391	F507	T596	T696	V784	R878	E983	E1102	K1228
GLY	ASN	Q251	S392	L511	R598	L698	L788	R879	E984	K1105	I1235
ALA	GLY	E252	T393	T512	T599	D700	A701	R880	D985	K1106	E1238
PRO	CYS	A255	T396	L513	R601	A701	R793	A881	K986	P1109	F1239
GLY	CYS	E263	L397	F519	E602	N705	G797	T891	N988	K1122	K1251
ASN	GLY	T264	G399	V520	T604	S706	F798	R895	K989	Q1123	
ASN	GLY	E267	E402	L521	L605	F707	G799	G896	K994	R1124	
ASN	ASN	E277	T403	T522	R606	E711	E802	G898	K995	Y1116	
PRO	ASN	K277	L404	V523	L507	L712	T803	R899	R996	Y1117	
ASN	ASN	L278	L405	K526	R612	K713	S805	L900	G997	M1118	
CYS	CYS	L279	S406	L527	R614	K716	S809	L904	G999	Q1122	
CYS	ASN	E280	L407	L528	R615	D718	V810	N904	I1000	Q1123	
THR	ASN	P281	E408	D530	R616	L719	P822	N907	I1001	R1124	
THR	GLN	L284	Y411	S531	R617	K720	A816	S907	P1002	S1128	
VAL	LYS	L287	S412	LYS	R618	K721	T827	G913	T1003	T1129	
THR	ASP	L296	F418	ASP	S619	K725	P828	F914	K1004	Y1133	
THR	THR	G296	R426	CYS	R620	E726	R829	F917	F1005	R1134	
VAL	THR	V308	R427	GLY	R621	A728	L827	P917	G1006	Y1140	
THR	THR	L312	E428	LYS	R622	D727	D828	F921	S1007	T1144	
S192	P193	V316	D429	P540	R623	V730	R829	I922	S1008	M1145	
F196	F196	Q322	R439	T541	R624	E733	M833	P921	Q1016	H1151	
M197	M197	R323	V440	S544	R625	I736	T836	I922	A1017	Y1152	
P198	P198	T324	L441	A545	R626	Q739	H839	N926	A1017	F1153	
E199	E199	E325	P444	L547	R627	D740	H840	N927	S1028	T1154	
E200	E200	R328	P444	L548	R628	H741	A844	V930	V1029	Y1155	
E209	E209	E332	R450	F549	R629	F742	R845	V930	I1030	E1161	
I211	I211	F337	E451	K551	R631	L744	Y846	P937	V1031	H1171	
P213	P213	A338	R462	P553	R632	H747	K847	E938	E1037	A1184	
L216	L216	L348	L467	P554	R633	F748	F850	R940	H1043	S1184	
L217	L217	R351	K468	A555	R634	I749	N851	V941	T1044	S1185	
R218	R218	I358	Q471	A556	R635	P753	K852	Y947	K1045	L1186	
L219	L219	L361	Q472	N557	R636	E756	I856	K948	V1049	N1187	
K220	K220	R362	Q473	Q558	R637	E757	L859	N948	K1052	I1190	
V234	V234	V364	L474	F560	R638	E761	E854	P955	P1076	D1191	
T235	T235		S475	D571	R639	V764	R855	N956	P1076	I1192	
W236	W236		R476	L580	R640	N768	N866	Q957	F1313	E1196	
I237	I237		O487	R684	R641		A867	R958	T1314	T1315	

L1316	CYS
	VAL
	THR
	GLY
	ALA
	PRO
	GLY
	ASN
	CYS
	K1326
	P1327
	H1328
	S1329
	L1330
	R1331
	V1332

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, 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: MOS, TEI, 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	0.43	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

Continued on next page...

Continued from previous page...

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:1286:THR:HG22	1:A:1287:ASN:H	1.19	1.07
1:A:537:LYS:HG3	1:A:538:LEU:H	1.18	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:H	1:A:666:ILE:HD12	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:MO	4:B:4004:MOS:S	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:O1	4:B:4004:MOS:S	2.36	0.84
4:A:3004:MOS:O1	4:A:3004:MOS:S	2.36	0.83
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.43	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

Continued on next page...

Continued from previous page...

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:1106:LYS:O	1:A:1109:PRO:HD3	1.84	0.76
1:A:868:GLY:HA3	1:A:907:SER:HA	1.67	0.76
1:B:1330:LEU:CG	1:B:1331:ARG:H	1.97	0.76
1:B:868:GLY:HA3	1:B:907:SER:HA	1.67	0.76
4:B:4004:MOS:O2	4:B:4004:MOS:MO	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:O2	4:A:3004:MOS:MO	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:N	1:B:666:ILE:HD12	2.03	0.72
1:A:467:LEU:O	1:A:471:GLN:HG2	1.90	0.72
1:A:870:SER:HB3	1:A:907:SER:HB2	1.70	0.72
1:A:756:GLU:HB3	1:B:584:MET:SD	2.29	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:N	1:A:666:ILE:HD12	2.03	0.70
1:A:1331:ARG:O	1:A:1332:VAL:HG12	1.91	0.70
1:B:1331:ARG:O	1:B:1332:VAL:HG12	1.91	0.70
1:B:519:PHE:O	1:B:523:VAL:HG23	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

Continued on next page...

Continued from previous page...

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
4:B:4004:MOS:O1	4:B:4004:MOS:MO	1.70	0.62
1:B:60:ARG:O	1:B:61:LEU:CB	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:VAL:HG21	1:A:681:ALA:HA	1.83	0.61
4:A:3004:MOS:O1	4:A:3004:MOS:MO	1.70	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
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:1203:LEU:C	1:A:1203:LEU:HD12	2.21	0.60
1:A:196:PHE:HE1	1:A:198:PRO:HG3	1.66	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:1330:LEU:HD13	1:B:1332:VAL:H	1.67	0.60
1:B:358:ILE:HD13	1:B:431:ILE:HG23	1.84	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
4:B:4004:MOS:O2	4:B:4004:MOS:S	2.60	0.59
1:B:749:THR:HG21	1:B:809:SER:HA	1.84	0.59
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.84	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

Continued on next page...

Continued from previous page...

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:1330:LEU:HD13	1:B:1331:ARG:N	2.19	0.58
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	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:CD1	1:B:666:ILE:H	2.05	0.57
1:A:1191:ASP:OD1	1:A:1259:VAL:HG11	2.04	0.57
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.39	0.57
1:A:393:TYR:CZ	1:A:394:ARG:HD2	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:1191:ASP:O	1:A:1192:ILE:HG13	2.05	0.57
1:A:192:SER:HB3	1:A:193:PRO:HD2	1.86	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:1088:GLN:HG2	1:A:1133:TYR:CD1	2.41	0.56
1:A:450:LYS:O	1:A:474:LEU:HD22	2.05	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:999:CYS:SG	1:A:1001:ILE:HD11	2.46	0.56
1:A:744:LEU:HD23	2:A:3001:FES:S2	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:1088:GLN:HG2	1:B:1133:TYR:CD1	2.41	0.56
1:B:1330:LEU:C	1:B:1330:LEU:HD22	2.22	0.56
1:B:587:SER:OG	1:B:589:GLU:HG3	2.06	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:HG2	1:B:1326:LYS:O	2.06	0.55
1:A:506:GLU:CD	1:A:506:GLU:H	2.09	0.55

Continued on next page...

Continued from previous page...

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
5:A:3005:FAD:H51A	5:A:3005:FAD:H8A	1.89	0.55
1:A:844:ALA:HB2	1:A:922:ILE:HD13	1.89	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:911:PHE:HD2	1:B:912:ARG:N	2.03	0.55
1:B:1007:ILE:HD12	1:B:1258:ALA:HB3	1.89	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: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:B:506:GLU:H	1:B:506:GLU:CD	2.09	0.55
1:B:556:ASN:C	1:B:557:ILE:HD12	2.27	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:N	1:A:856:ILE:HD12	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
5:B:4005:FAD:H51A	5:B:4005:FAD:H8A	1.89	0.54
1:B:619:SER:HB3	1:B:688:THR:OG1	2.07	0.54
1:B:618:LYS:HD2	1:B:690:GLU:OE1	2.08	0.54
1:B:832:ASP:O	1:B:836:THR:HG23	2.08	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:1105:LYS:HG3	1:A:1116:TRP:CZ2	2.42	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

Continued on next page...

Continued from previous page...

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:1007:ILE:HD12	1:A:1258:ALA:HB3	1.89	0.53
1:A:100:PRO:O	1:A:104:ARG:HG3	2.09	0.53
1:A:3:ALA:O	1:A:5:GLU:N	2.38	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:1271:PHE:CE1	1:A:1300:ALA:HB2	2.43	0.53
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.09	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:1017:ALA:HB2	1:A:1085:ILE:HD12	1.91	0.53
1:A:736:ILE:HG12	1:A:921:PHE:CD2	2.44	0.53
1:B:856:ILE:N	1:B:856:ILE:HD12	2.23	0.53
1:A:1315:THR:HG22	1:A:1316:LEU:N	2.23	0.53
1:A:727:ASP:OD2	1:A:852:LYS:HG3	2.09	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:1315:THR:HG22	1:B:1316:LEU:N	2.23	0.53
1:B:552:HIS:ND1	1:B:553:PRO:HD2	2.24	0.53
1:B:61:LEU:HD23	1:B:61:LEU:O	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:1005:PHE:CB	1:A:1262:PRO:HG3	2.39	0.52
1:A:61:LEU:O	1:A:61:LEU:HD23	2.09	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

Continued on next page...

Continued from previous page...

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:1021:ILE:HD12	1:B:1093:ALA:HB3	1.91	0.51
1:B:560:PHE:CD2	1:B:560:PHE:N	2.79	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:1124:ARG:O	1:B:1134:ARG:HD3	2.11	0.50
1:A:507:PHE:CZ	1:A:511:LEU:HD11	2.47	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:C	1:A:605:LEU:HD23	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:1000:ILE:O	1:A:1000:ILE:HG23	2.11	0.50
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	1.94	0.50
1:A:912:ARG:O	1:A:1264:LEU:HD13	2.11	0.50
1:B:1299:PRO:HG2	1:B:1301:THR:HG23	1.94	0.50
1:B:1286:THR:CG2	1:B:1287:ASN:N	2.64	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:A:522:THR:HG22	1:A:526:LYS:HE3	1.93	0.50
1:A:560:PHE:CD2	1:A:560:PHE:N	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:1000:ILE:HG23	1:B:1000:ILE:O	2.11	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:A:592:TYR:O	1:A:595:ASP:HB2	2.12	0.49
1:B:1315:THR:HG22	1:B:1316:LEU:HD22	1.94	0.49
1:B:507:PHE:CZ	1:B:511:LEU:HD11	2.46	0.49
1:A:1140:TYR:HE1	1:A:1145:ASN:HD22	1.57	0.49
1:A:615:ALA:HB2	1:A:691:ASP:HA	1.93	0.49
1:B:237:ILE:HD12	1:B:277:MET:CE	2.42	0.49
1:B:605:LEU:HD23	1:B:605:LEU:C	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1281:ALA:O	1:A:1284:GLN:HB3	2.12	0.49
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:HH11	1:A:793:ARG:HG2	1.77	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:1330:LEU:CG	1:A:1331:ARG:N	2.68	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:B:980:ARG:NH1	1:B:1161:GLU:OE1	2.46	0.49
1:B:912:ARG:O	1:B:1264:LEU:HD13	2.11	0.49
1:A:1330:LEU:CD1	1:A:1332:VAL:N	2.70	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: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:1096:THR:HB	1:B:1129:THR:HG21	1.95	0.49
1:B:399:GLY:N	1:B:402:GLU:OE1	2.45	0.49
1:B:471:GLN:HA	1:B:471:GLN:OE1	2.13	0.49
1:B:749:THR:OG1	1:B:764:VAL:HG13	2.13	0.49
1:A:1192:ILE:O	1:A:1196:GLU:HG3	2.13	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: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: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:54:MET:HB3	1:B:86:THR:HB	1.94	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: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: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

Continued on next page...

Continued from previous page...

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: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:B:61:LEU:HD23	1:B:61:LEU:C	2.34	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:HH11	1:B:129:ARG:HG3	1.78	0.48
1:B:698:ILE:O	1:B:701:ALA:HB3	2.14	0.48
1:A:245:LEU:HB2	1:A:284:ILE:HD11	1.96	0.48
1:A:46:GLY:HA2	2:A:3002:FES:S1	2.54	0.48
1:A:308:VAL:HG21	1:A:348:LEU:HD12	1.96	0.48
1:B:1262:PRO:HB2	1:B:1263:PRO:HD3	1.95	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: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:1262:PRO:HB2	1:A:1263:PRO:HD3	1.95	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:B:418:PHE:CD1	1:B:439:ARG:HB2	2.49	0.48
1:B:46:GLY:HA2	2:B:4002:FES:S1	2.54	0.48
1:A:471:GLN:OE1	1:A:471:GLN:HA	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:NH1	1:A:328:ARG:HG2	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:1152:TYR:HE1	1:B:1257:LYS:HB3	1.79	0.47
1:B:747:HIS:ND1	1:B:805:SER:HA	2.29	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

Continued on next page...

Continued from previous page...

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:1096:THR:HB	1:A:1129:THR:HG21	1.95	0.47
1:A:154:ARG:N	1:A:155:PRO:HD2	2.29	0.47
1:A:129:ARG:NE	1:A:209:GLU:HG2	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:B:711:GLU:HA	1:B:899:ARG:HD2	1.96	0.47
1:A:1330:LEU:CD1	1:A:1332:VAL:H	2.28	0.47
1:A:747:HIS:ND1	1:A:805:SER:HA	2.29	0.47
1:B:1330:LEU:CD1	1:B:1332:VAL:H	2.28	0.47
1:B:1082:SER:HB2	3:B:4003:MTE:O1P	2.14	0.47
1:B:947:TYR:OH	1:B:953:THR:HA	2.14	0.47
1:A:1007:ILE:O	1:A:1008:SER:CB	2.62	0.47
1:A:124:MET:CE	1:A:128:LEU:HG	2.45	0.47
3:A:3003:MTE:S1'	4:A:3004:MOS:O2	2.73	0.47
1:A:418:PHE:CD1	1:A:439:ARG:HB2	2.49	0.47
1:A:872:ASP:OD1	1:A:873:LEU:N	2.47	0.47
1:B:1007:ILE:O	1:B:1008:SER:CB	2.62	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:1082:SER:HB2	3:A:3003:MTE:O1P	2.14	0.46
1:A:43:CYS:HA	1:A:829:ARG:HB2	1.97	0.46
1:B:197:ASN:O	1:B:200:GLU:HG2	2.15	0.46
1:B:43:CYS:HA	1:B:829:ARG:HB2	1.97	0.46
1:A:197:ASN:O	1:A:200:GLU:HG2	2.15	0.46
1:A:1134:ARG:HD3	1:B:1124:ARG:O	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: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:B:772:THR:O	1:B:776:VAL:HG23	2.15	0.46
1:A:537:LYS:CG	1:A:538:LEU:H	2.00	0.46
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:964:VAL:N	1:A:965:PRO:CD	2.79	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:1099:LYS:HA	1:B:1099:LYS:HD2	1.76	0.45
1:B:281:PRO:HB2	1:B:287:LEU:HD13	1.97	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:A:768:ASN:ND2	1:A:1076:PRO:HB3	2.31	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:B:473:GLN:NE2	1:B:473:GLN:HA	2.32	0.45
1:B:544:SER:HA	1:B:547:LEU:CD1	2.44	0.45
1:B:427:ARG:NE	1:B:549:PHE:CE1	2.85	0.45
1:B:846:TYR:HA	1:B:860:GLU:O	2.17	0.45
1:A:426:ARG:CZ	1:A:1228:LYS:HE3	2.47	0.45
1:A:1184:SER:HB2	1:A:1255:ALA:HB3	1.98	0.45
1:A:60:ARG:O	1:A:61:LEU:HB3	2.16	0.45
1:A:964:VAL:HB	1:A:965:PRO:HD3	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:HD23	1:A:219:LEU:N	2.32	0.45
1:A:427:ARG:NE	1:A:549:PHE:CE1	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1286:THR:CG2	1:A:1287:ASN:N	2.64	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:B:296:GLY:HA2	1:B:411:TYR:CE1	2.52	0.45
1:B:328:ARG:NH1	1:B:328:ARG:CG	2.77	0.45
1:B:79:THR:HG22	1:B:236:TRP:CZ2	2.52	0.45
1:A:1191:ASP:O	1:A:1192:ILE:CB	2.65	0.44
1:A:557:ILE:HD12	1:A:557:ILE:N	2.33	0.44
1:B:733:GLU:HG2	1:B:1295:ARG:NH1	2.32	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: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:N	1:B:557:ILE:HD12	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:1088:GLN:HG2	1:A:1133:TYR:CE1	2.52	0.44
1:A:1016:GLN:HA	1:A:1133:TYR:O	2.18	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:79:THR:HG22	1:A:236:TRP:CZ2	2.52	0.44
1:A:846:TYR:HA	1:A:860:GLU:O	2.17	0.44
1:A:705:ASN:HA	1:A:707:PHE:HE1	1.82	0.44
1:A:87:THR:HG1	1:A:89:GLU:HG2	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:HH11	1:B:612:ARG:HG3	1.82	0.44
1:A:1264:LEU:C	1:A:1264:LEU:HD23	2.38	0.44
1:A:328:ARG:NH1	1:A:328:ARG:CG	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:B:1016:GLN:HA	1:B:1133:TYR:O	2.17	0.44
1:B:719:LEU:HD13	1:B:860:GLU:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1259:VAL:O	1:B:1259:VAL:HG22	2.18	0.44
1:B:861:VAL:O	1:B:896:GLY:HA2	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:426:ARG:CZ	1:B:1228:LYS:HE3	2.47	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: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:705:ASN:HA	1:B:707:PHE:CE1	2.53	0.44
1:B:878:MET:O	1:B:881:ALA:HB3	2.18	0.44
1:B:1286:THR:O	1:B:1287:ASN:O	2.36	0.43
1:B:839:ARG:HG2	1:B:840:HIS:N	2.32	0.43
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.53	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:A:711:GLU:HA	1:A:899:ARG:CD	2.48	0.43
1:B:1152:TYR:OH	1:B:1257:LYS:HA	2.17	0.43
1:B:165:LYS:HG2	1:B:165:LYS:O	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:60:ARG:O	1:B:61:LEU:HB2	2.18	0.43
1:B:712:LEU:HD23	1:B:879:GLU:HG2	2.00	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:1264:LEU:HD23	1:B:1264:LEU:C	2.38	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: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:1023:VAL:HG13	1:B:1029:VAL:HG22	2.00	0.43
1:B:371:LYS:HB2	1:B:408:GLU:HB3	1.99	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:1249:ASN:O	1:B:1255:ALA:HA	2.18	0.43
1:B:1312:LYS:O	1:B:1316:LEU:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:CD1	1:B:164:ALA:HB2	2.48	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:521:LEU:CD2	1:A:538:LEU:HD11	2.48	0.43
1:A:115:PHE:HD2	1:A:744:LEU:HB3	1.84	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: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:A:60:ARG:O	1:A:61:LEU:HB2	2.18	0.43
1:B:1284:GLN:HG2	1:B:1285:HIS:CE1	2.54	0.43
1:B:1082:SER:HB2	3:B:4003:MTE:P	2.59	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:A:705:ASN:HA	1:A:707:PHE:CE1	2.53	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:913:GLY:HA3	1:B:917:PRO:HG2	2.00	0.42
1:B:850:PHE:CD1	1:B:930:VAL:HG13	2.53	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:HD2	1:A:1099:LYS:HA	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:NE2	1:A:473:GLN:HA	2.32	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: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:A:1082:SER:HB2	3:A:3003:MTE:P	2.59	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: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:580:LEU:HG	1:A:1044:THR:HG23	2.01	0.42
1:A:211:ILE:HG12	1:A:212:PHE:N	2.35	0.42
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.85	0.42

Continued on next page...

Continued from previous page...

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:HE3	1:B:721:LYS:HB2	1.89	0.42
1:A:1312:LYS:O	1:A:1316:LEU:HB2	2.19	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:B:799:GLY:HA2	4:B:4004:MOS:S	2.60	0.42
1:B:580:LEU:HG	1:B:1044:THR:HG23	2.00	0.42
1:B:968:TRP:CH2	1:B:1000:ILE:HG23	2.54	0.42
1:A:1214:SER:OG	1:A:1216:GLU:HG2	2.19	0.42
1:A:621:ASP:HB3	1:A:686:LYS:HB3	2.00	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:995:LYS:HD2	1:B:1280:ALA:HB1	2.02	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:A:744:LEU:HA	1:A:744:LEU:HD13	1.78	0.41
1:A:541:THR:O	1:A:992:CYS:HB3	2.20	0.41
1:B:1144:THR:O	1:B:1145:ASN:C	2.58	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: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: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:A:11:ASN:OD1	1:A:90:GLY:HA3	2.21	0.41
1:B:1286:THR:CG2	1:B:1287:ASN:H	1.94	0.41
1:B:124:MET:HB2	1:B:143:PHE:HZ	1.86	0.41
1:A:237:ILE:HD12	1:A:277:MET:HE3	2.02	0.41
1:A:38:GLY:O	1:A:40:LYS:HE2	2.20	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

Continued on next page...

Continued from previous page...

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: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:A:598:ARG:HG3	1:A:602:GLU:HB3	2.02	0.41
1:B:948:LYS:HB3	1:B:948:LYS:HE2	1.92	0.41
1:A:1105:LYS:HG3	1:A:1116:TRP:CH2	2.56	0.41
1:A:721:LYS:HB2	1:A:721:LYS:HE3	1.89	0.41
1:B:1214:SER:OG	1:B:1216:GLU:HG2	2.20	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: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:614:HIS:HB2	1:B:904:ASN:ND2	2.35	0.41
1:A:958:ARG:HH21	1:A:960:GLU:HG2	1.85	0.41
1:B:713:LYS:HD2	1:B:895:ARG:NH1	2.35	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: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: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: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:11:ASN:OD1	1:B:90:GLY:HA3	2.21	0.41
1:A:530:ASP:O	1:A:531:SER:CB	2.69	0.40
1:A:154:ARG:HD2	1:A:558:GLN:NE2	2.36	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:1151:HIS:NE2	1:B:1251:LYS:HE3	2.36	0.40
1:B:316:VAL:HA	1:B:324:THR:HG21	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:PHE:HE2	1:B:551:LYS:HG3	1.86	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: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:B:548:LEU:O	1:B:550:GLN:HG2	2.21	0.40
1:A:1144:THR:O	1:A:1145:ASN:C	2.58	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: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: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: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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Some 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

Continued on next page...

Continued from previous page...

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	MOS	B	4004	3	0,3,3	0.00	-	-		
6	TEI	A	3006	-	16,23,23	3.98	6 (37%)	16,32,32	1.48	3 (18%)
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
3	MTE	B	4003	4	21,26,26	6.04	12 (57%)	21,40,40	3.27	8 (38%)
6	TEI	B	4006	-	16,23,23	3.97	6 (37%)	16,32,32	1.48	3 (18%)
5	FAD	B	4005	-	51,58,58	5.26	37 (72%)	60,89,89	3.11	30 (50%)
5	FAD	A	3005	-	51,58,58	5.26	37 (72%)	60,89,89	3.10	30 (50%)
2	FES	B	4001	1	0,4,4	0.00	-	-		
2	FES	A	3002	1	0,4,4	0.00	-	-		
4	MOS	A	3004	3	0,3,3	0.00	-	-		
2	FES	A	3001	1	0,4,4	0.00	-	-		
2	FES	B	4002	1	0,4,4	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TEI	A	3006	-	-	0/11/15/15	0/2/2/2
3	MTE	A	3003	4	-	0/6/34/34	0/3/3/3
3	MTE	B	4003	4	-	0/6/34/34	0/3/3/3
6	TEI	B	4006	-	-	0/11/15/15	0/2/2/2
5	FAD	B	4005	-	-	7/30/50/50	0/6/6/6
5	FAD	A	3005	-	-	7/30/50/50	0/6/6/6
2	FES	B	4001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	B	4002	1	-	-	0/1/1/1

All (110) 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
5	B	4005	FAD	C9A-N10	14.88	1.58	1.38
5	A	3005	FAD	C9A-N10	14.82	1.58	1.38
5	B	4005	FAD	C4X-C10	12.59	1.51	1.38
5	A	3005	FAD	C4X-C10	12.57	1.51	1.38
3	B	4003	MTE	C9-C10	11.64	1.63	1.41
3	A	3003	MTE	C9-C10	11.63	1.63	1.41
6	B	4006	TEI	C11-C6	11.00	1.62	1.39
6	A	3006	TEI	C11-C6	10.99	1.62	1.39
5	A	3005	FAD	C5'-C4'	-10.31	1.37	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4005	FAD	C5'-C4'	-10.27	1.37	1.51
5	B	4005	FAD	C2A-N3A	9.29	1.47	1.32
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	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	C4-C4X	8.08	1.55	1.41
5	B	4005	FAD	C4-C4X	8.07	1.55	1.41
5	A	3005	FAD	C4A-N3A	7.97	1.46	1.35
5	B	4005	FAD	C4A-N3A	7.92	1.46	1.35
5	A	3005	FAD	C9A-C5X	7.77	1.58	1.42
5	B	4005	FAD	C9A-C5X	7.74	1.58	1.42
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	A	3005	FAD	C4-N3	7.62	1.46	1.33
5	B	4005	FAD	C4-N3	7.59	1.46	1.33
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	C2-N3	5.34	1.48	1.38
5	B	4005	FAD	C2-N3	5.33	1.48	1.38
5	A	3005	FAD	C4X-N5	5.32	1.40	1.33
5	A	3005	FAD	C5A-C4A	5.31	1.55	1.40
5	B	4005	FAD	C5A-C4A	5.30	1.55	1.40
5	B	4005	FAD	C4X-N5	5.26	1.40	1.33
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	C7M-C7	-4.88	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4005	FAD	C7M-C7	-4.88	1.41	1.51
5	A	3005	FAD	O2B-C2B	-4.83	1.31	1.43
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	C4-C9	4.31	1.47	1.41
3	A	3003	MTE	C4-C9	4.30	1.47	1.41
5	B	4005	FAD	C6-C5X	4.20	1.48	1.41
5	A	3005	FAD	C6-C5X	4.17	1.48	1.41
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	A	3005	FAD	C9-C9A	3.81	1.48	1.40
5	B	4005	FAD	C9-C9A	3.79	1.48	1.40
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	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	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	C10-N1	3.06	1.37	1.33
5	B	4005	FAD	C8A-N7A	-3.06	1.29	1.34
5	A	3005	FAD	C10-N1	3.05	1.37	1.33
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	C6-C7	2.70	1.44	1.37
5	B	4005	FAD	C6-C7	2.68	1.44	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	FAD	PA-O5B	-2.54	1.49	1.59
5	A	3005	FAD	C9-C8	2.53	1.44	1.37
5	B	4005	FAD	C9-C8	2.52	1.44	1.37
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
6	A	3006	TEI	C2-N3	2.21	1.34	1.31
6	B	4006	TEI	C2-N3	2.21	1.34	1.31
3	B	4003	MTE	O3'-C3'	2.17	1.46	1.43
5	A	3005	FAD	C1'-N10	2.16	1.50	1.48
3	A	3003	MTE	O3'-C3'	2.15	1.46	1.43
5	B	4005	FAD	C1'-N10	2.10	1.50	1.48
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 (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	B	4005	FAD	C5X-C9A-N10	-7.10	112.57	117.72
5	A	3005	FAD	C5X-C9A-N10	-7.08	112.58	117.72
5	B	4005	FAD	C1'-N10-C9A	7.02	123.82	118.29
5	A	3005	FAD	C1'-N10-C9A	7.02	123.82	118.29
5	B	4005	FAD	C4-N3-C2	6.59	120.71	115.14
5	A	3005	FAD	C4-N3-C2	6.58	120.70	115.14
5	A	3005	FAD	C4X-N5-C5X	6.46	123.23	116.77
5	B	4005	FAD	C4X-N5-C5X	6.46	123.22	116.77
5	B	4005	FAD	C4-C4X-C10	-6.05	115.94	119.95
5	A	3005	FAD	C4-C4X-C10	-6.02	115.96	119.95
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	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	C1'-N10-C10	-5.00	113.93	118.41
5	B	4005	FAD	C1'-N10-C10	-4.97	113.96	118.41
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4005	FAD	O5B-PA-O1A	-4.79	90.34	109.07
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	C4-N3-C2	4.51	123.09	115.93
3	A	3003	MTE	C4-N3-C2	4.49	123.07	115.93
5	A	3005	FAD	C4X-C4-N3	-4.49	117.29	123.43
5	B	4005	FAD	C4X-C4-N3	-4.47	117.32	123.43
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	C8M-C8-C9	-3.91	110.99	120.34
5	A	3005	FAD	C8M-C8-C9	-3.90	111.00	120.34
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	N3-C2-N1	-3.81	119.44	125.42
3	A	3003	MTE	N3-C2-N1	-3.79	119.47	125.42
5	A	3005	FAD	C7M-C7-C6	-3.49	112.00	120.34
5	B	4005	FAD	C7M-C7-C6	-3.48	112.01	120.34
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	B	4005	FAD	C5A-C6A-N6A	3.09	125.05	120.35
5	B	4005	FAD	C4-C4X-N5	3.07	122.10	118.60
5	A	3005	FAD	C5A-C6A-N6A	3.06	125.00	120.35
5	A	3005	FAD	C4-C4X-N5	3.05	122.08	118.60
6	B	4006	TEI	C10-C11-C6	-3.00	116.81	121.13
6	A	3006	TEI	C10-C11-C6	-2.98	116.84	121.13
6	B	4006	TEI	C11-C6-C7	2.98	122.38	118.16
6	A	3006	TEI	C11-C6-C7	2.97	122.36	118.16
5	A	3005	FAD	O2'-C2'-C1'	2.91	116.59	109.59
5	B	4005	FAD	O2'-C2'-C1'	2.90	116.58	109.59
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
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
3	A	3003	MTE	C9-C10-N8	2.67	120.57	118.13
3	B	4003	MTE	C9-C10-N8	2.61	120.52	118.13
6	A	3006	TEI	C6-C7-C8	-2.47	119.31	121.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4006	TEI	C6-C7-C8	-2.45	119.32	121.53
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
5	A	3005	FAD	N3A-C2A-N1A	-2.36	124.99	128.68
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
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	A	3005	FAD	C4X-C10-N10	-2.11	118.13	120.30
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	B	4005	FAD	C4X-C10-N10	-2.09	118.15	120.30
5	B	4005	FAD	O4'-C4'-C3'	-2.04	104.13	109.10
5	A	3005	FAD	O4'-C4'-C3'	-2.04	104.13	109.10

There are no chirality outliers.

All (14) torsion outliers are listed below:

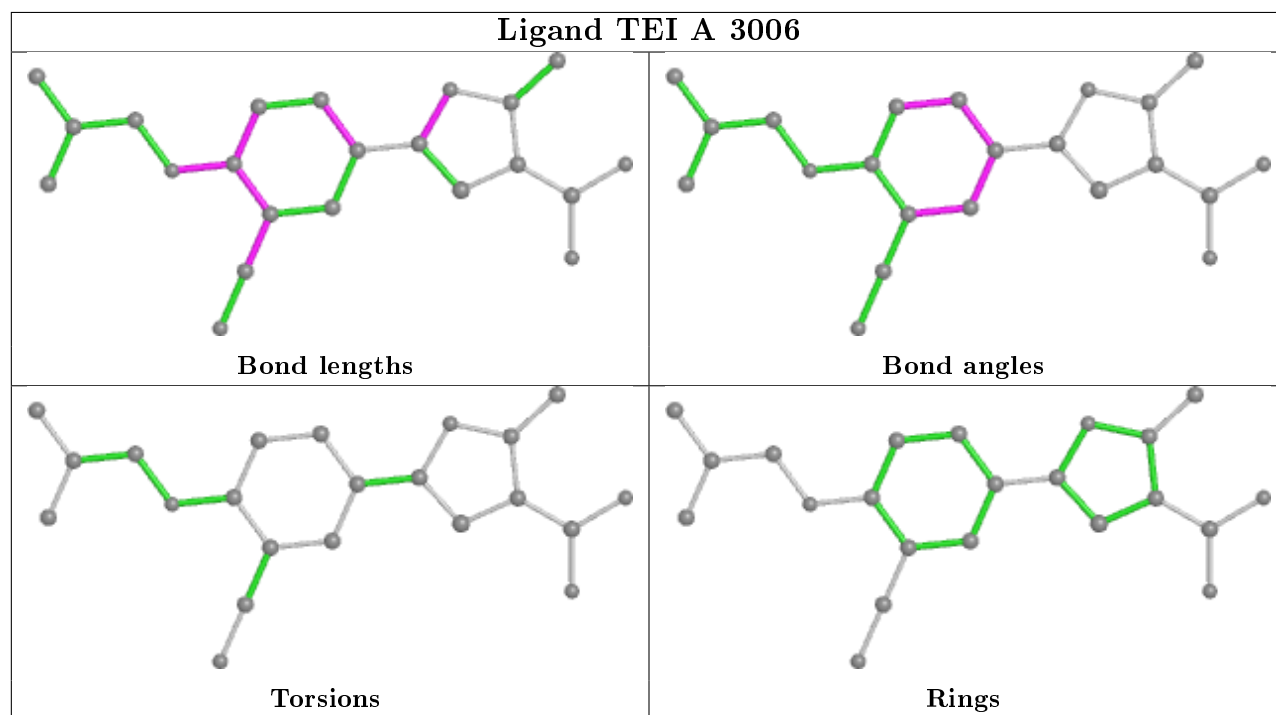
Mol	Chain	Res	Type	Atoms
5	B	4005	FAD	N10-C1'-C2'-O2'
5	B	4005	FAD	C2'-C3'-C4'-O4'
5	B	4005	FAD	O3'-C3'-C4'-O4'
5	B	4005	FAD	O3'-C3'-C4'-C5'
5	A	3005	FAD	N10-C1'-C2'-O2'
5	A	3005	FAD	C2'-C3'-C4'-O4'
5	A	3005	FAD	O3'-C3'-C4'-O4'
5	A	3005	FAD	O3'-C3'-C4'-C5'
5	B	4005	FAD	C4'-C5'-O5'-P
5	A	3005	FAD	C4'-C5'-O5'-P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

There are no ring outliers.

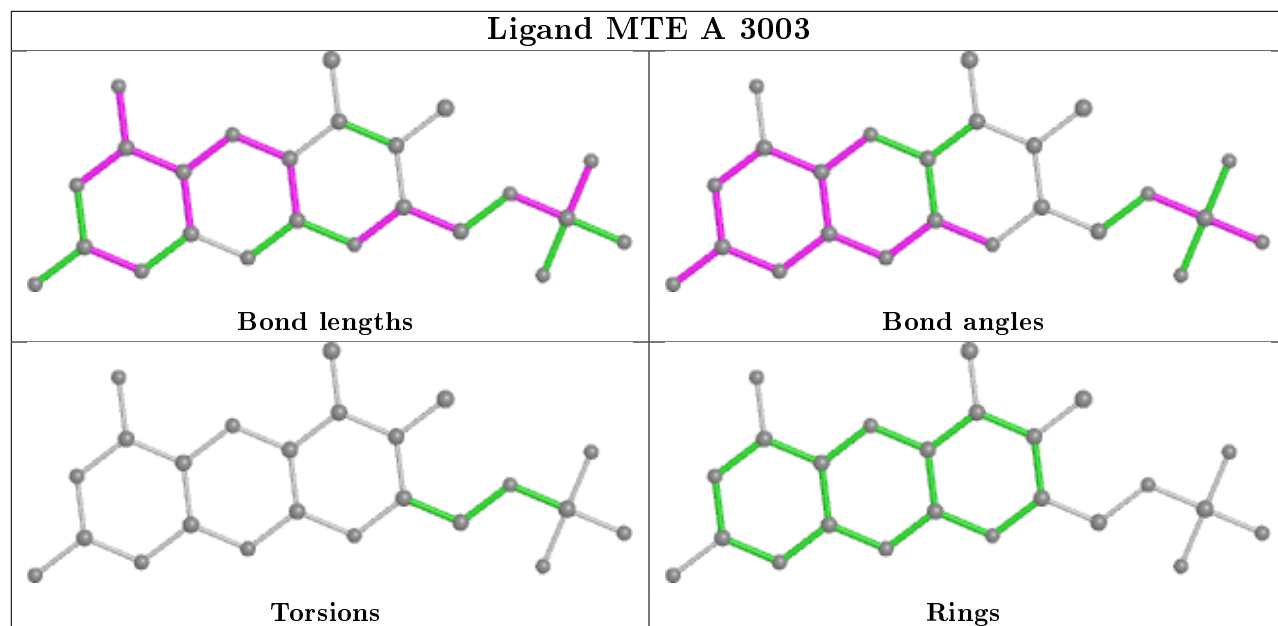
10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4004	MOS	8	0
3	A	3003	MTE	4	0
3	B	4003	MTE	4	0
5	B	4005	FAD	2	0
5	A	3005	FAD	2	0
2	B	4001	FES	1	0
2	A	3002	FES	1	0
4	A	3004	MOS	8	0
2	A	3001	FES	1	0
2	B	4002	FES	1	0

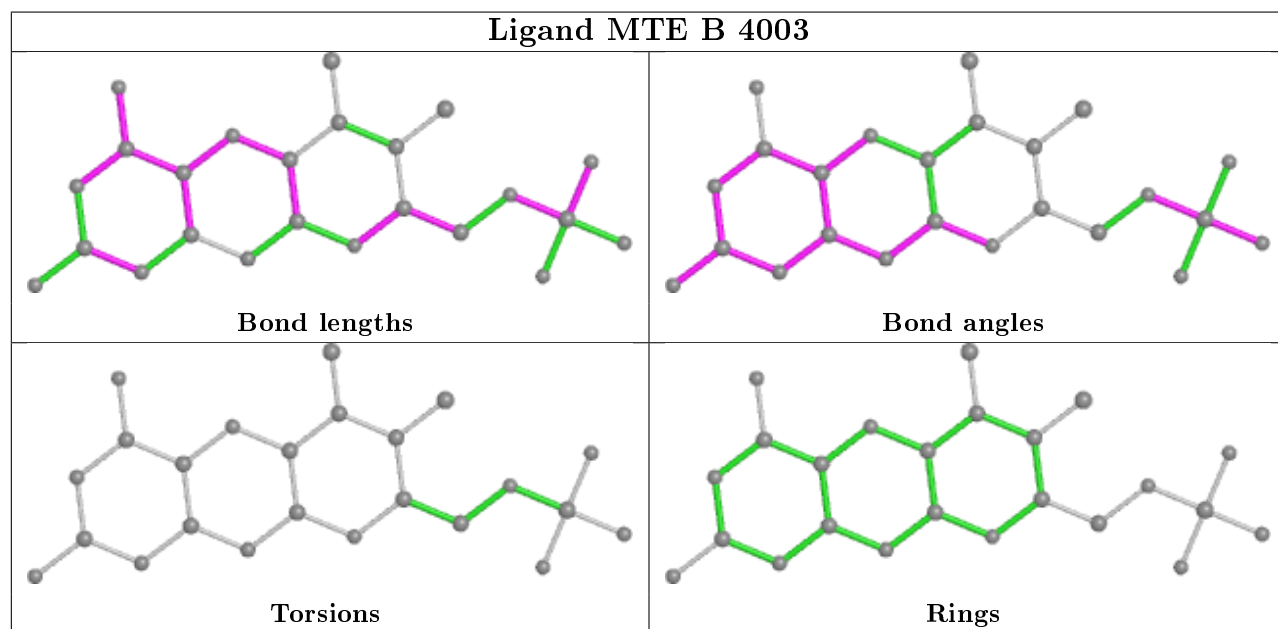
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

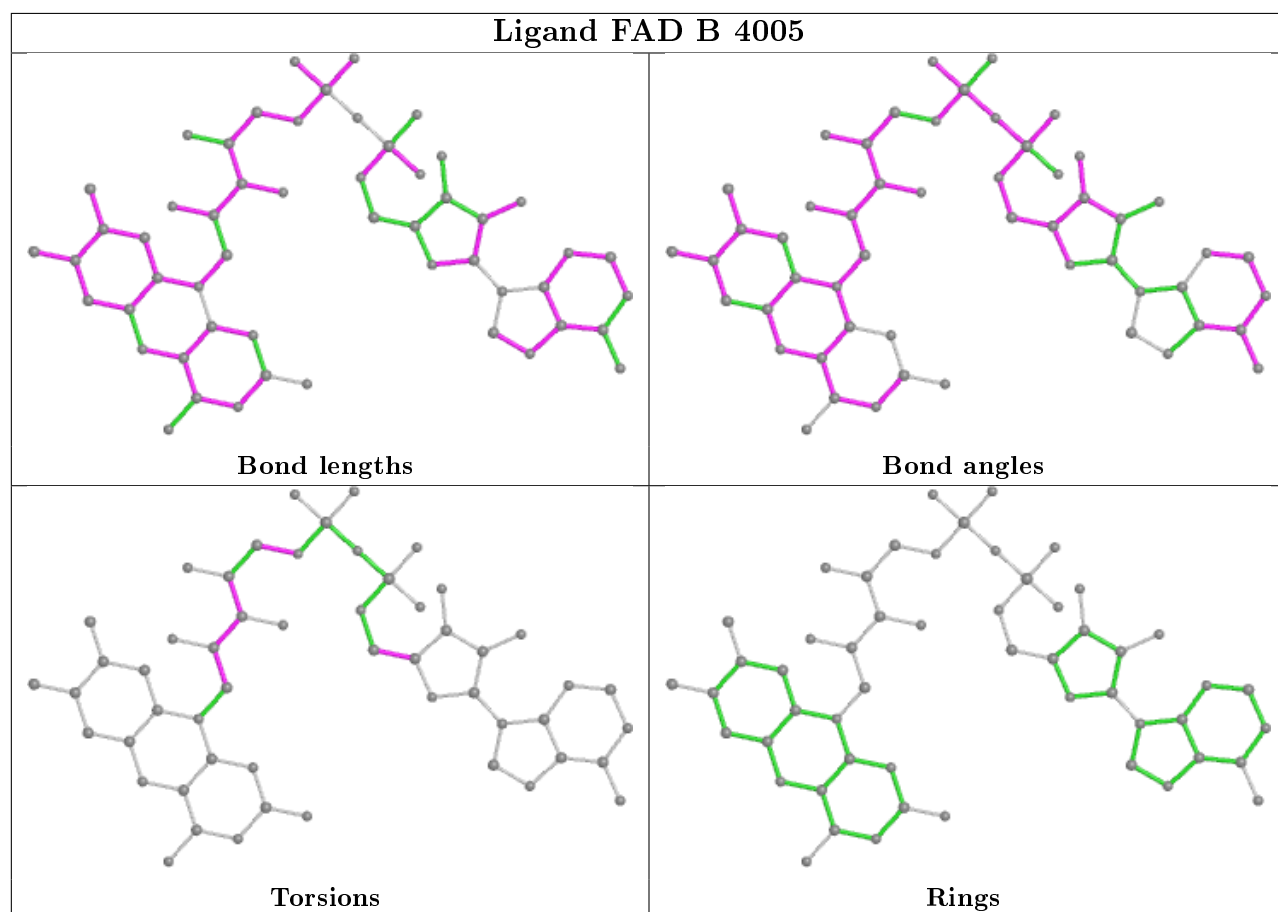
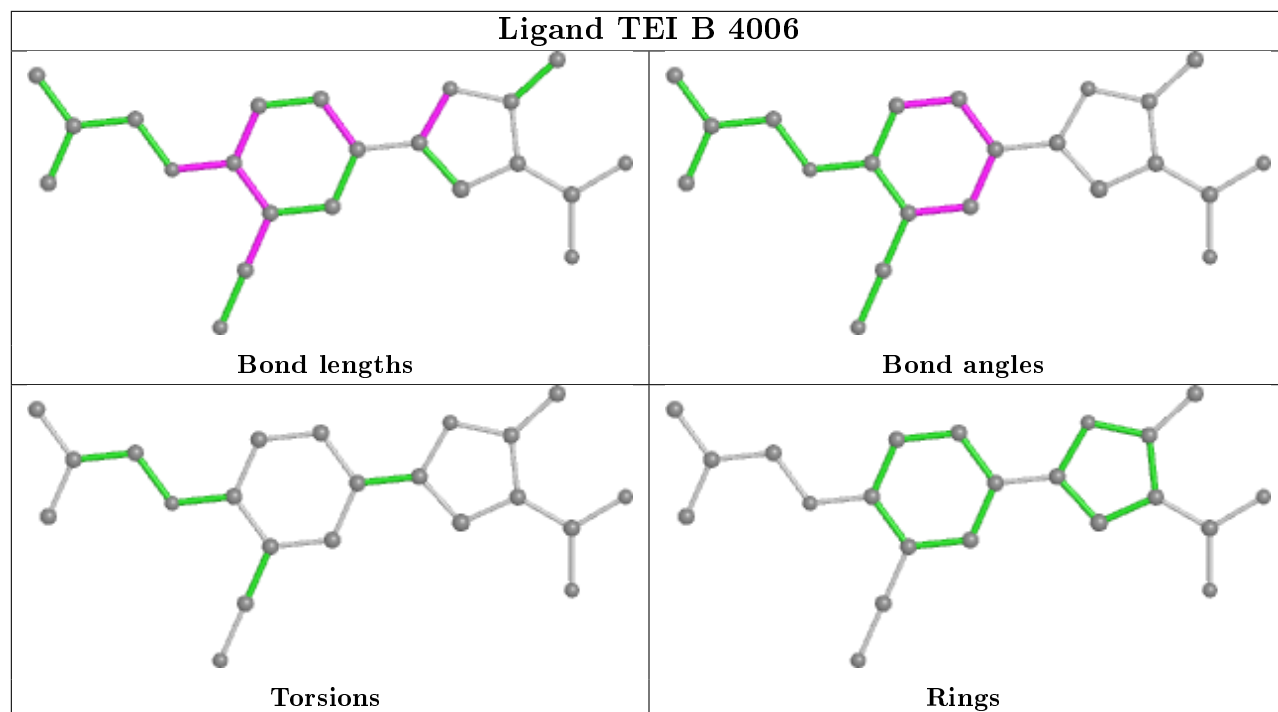


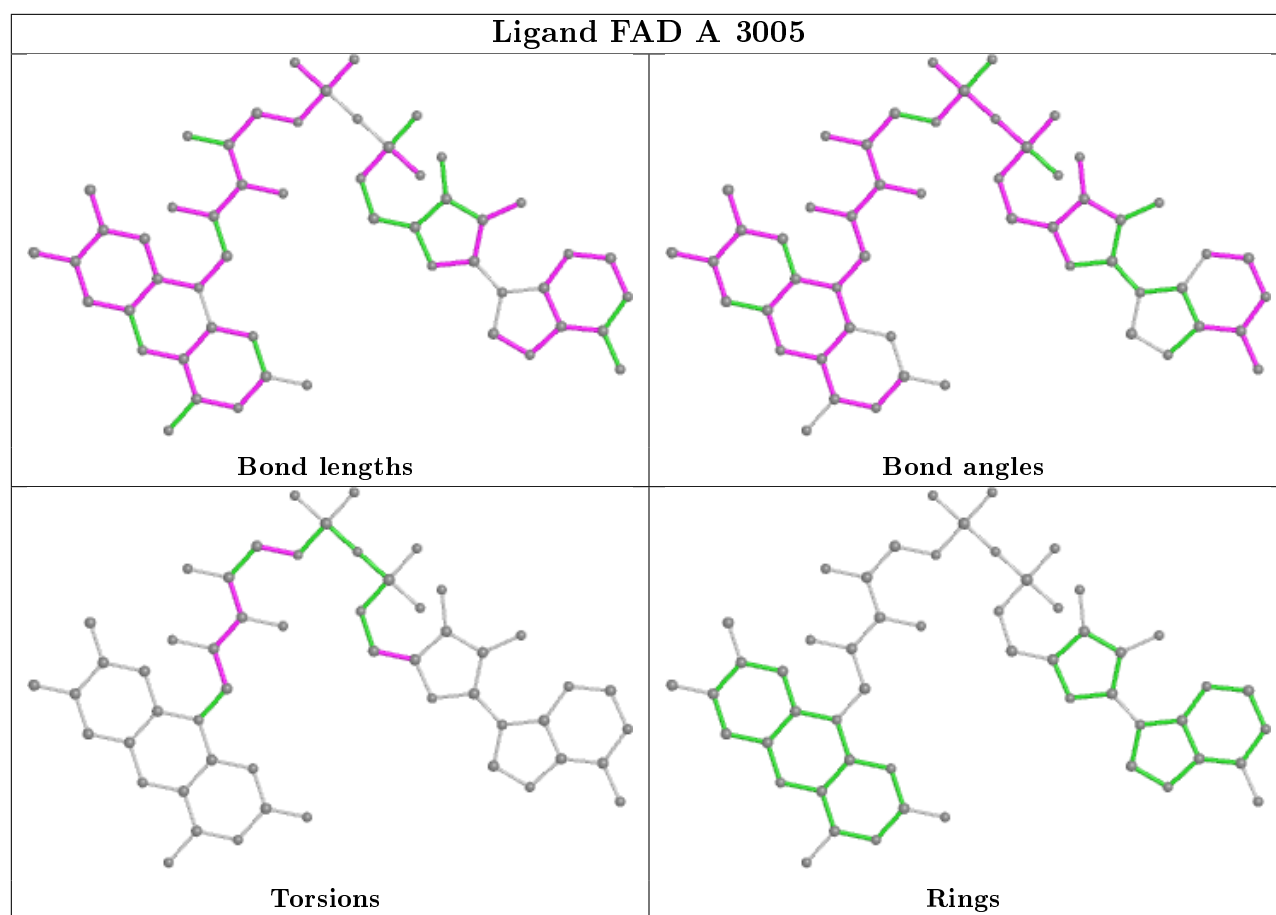
Ligand MTE A 3003



Ligand MTE B 4003







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 ⓘ

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.