



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:01 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

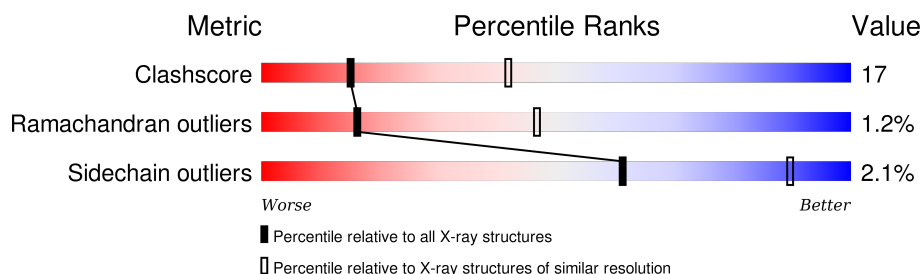
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	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](#)

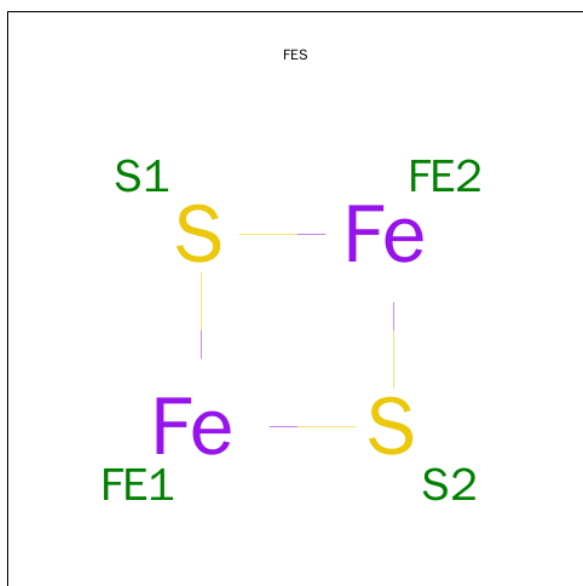
There are 6 unique types of molecules in this entry. The entry contains 20268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

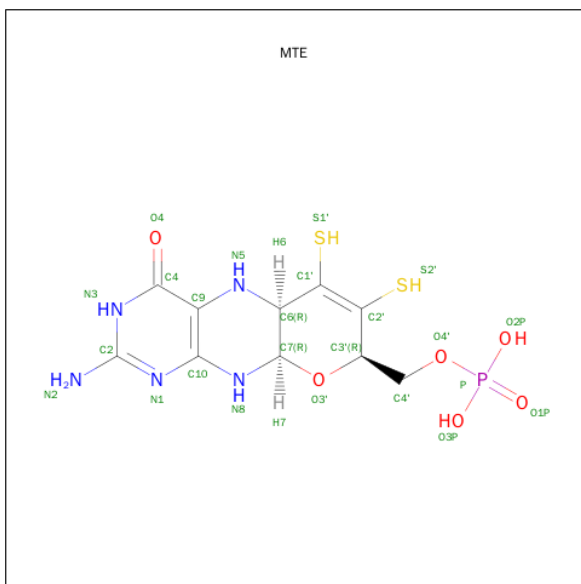
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			
1	B	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			

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



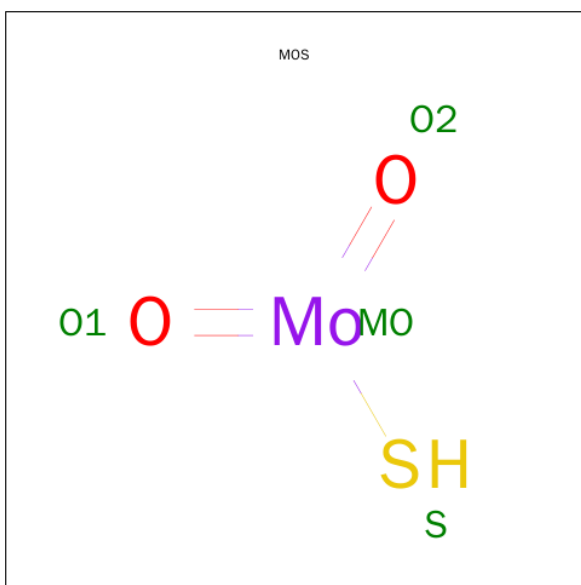
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- 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: $C_{10}H_{14}N_5O_6P S_2$).



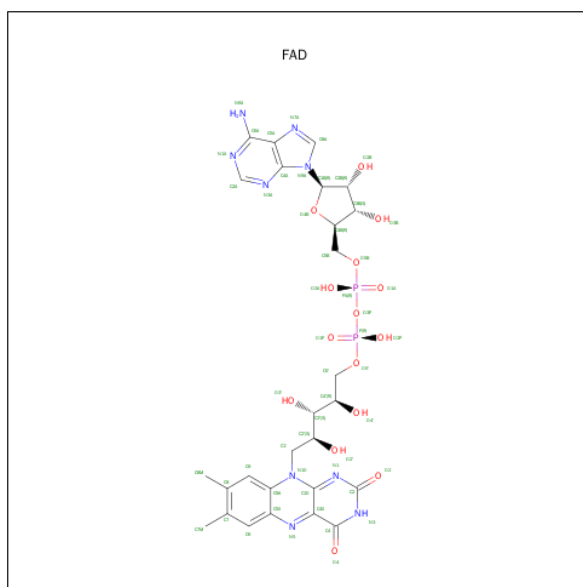
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

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



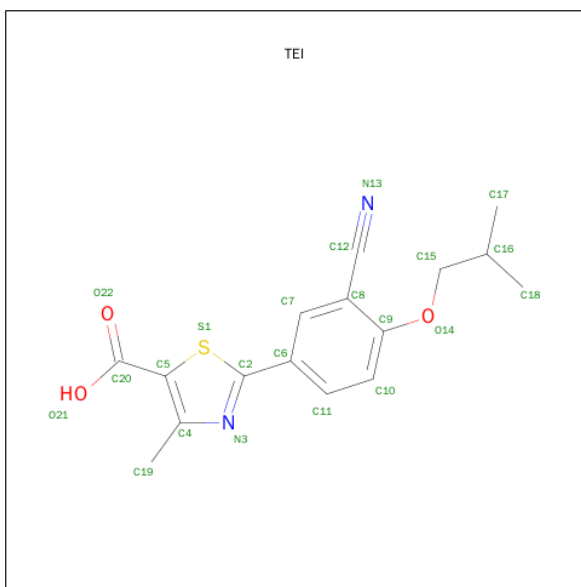
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- 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-CARBOXYLIC ACID (three-letter code: TEI) (formula: $C_{16}H_{16}N_2O_3S$).



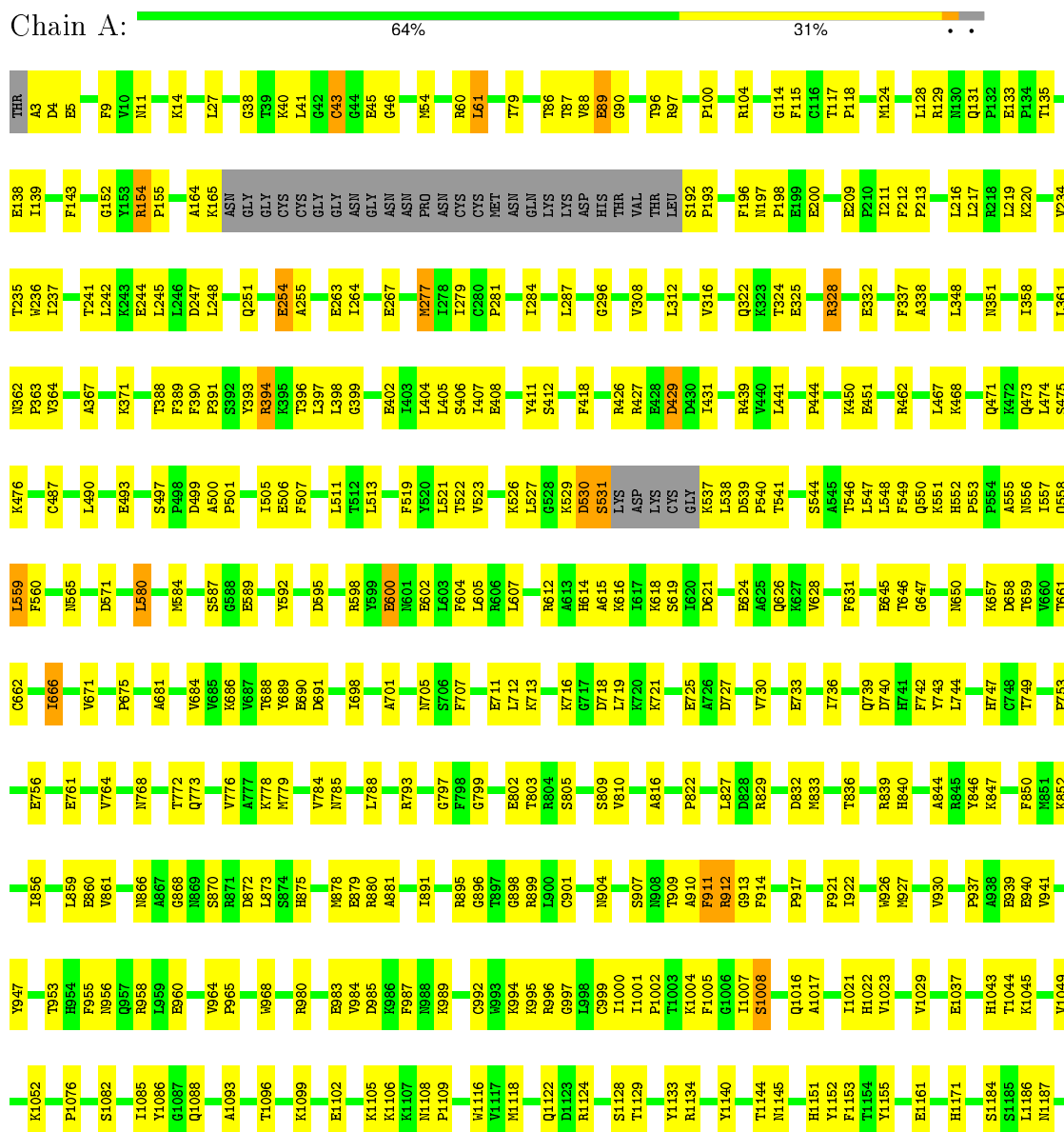
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			22	16	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			22	16	2	3	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Xanthine Dehydrogenase



I1190	D1311
D1191	K1312
I1192	F1313
E1196	T1314
V1200	T1315
L1203	L1316
Y1213	CYS
S1214	VAL
P1215	THR
E1216	GLY
P1224	ALA
K1228	PRO
I1235	GLY
E1238	ASN
F1239	GLY
N1249	ASN
K1250	CYS
K1251	K1326
Y1254	L1330
A1255	R1331
S1256	V1332
K1257	
A1258	
V1259	
P1262	
P1263	
L1264	
F1271	
F1272	
A1273	
A1280	
A1281	
Q1284	
H1285	
T1286	
N1287	
R1295	
S1298	
P1299	
A1300	
T1301	
P1302	
V1310	

• Molecule 1: Xanthine Dehydrogenase

Chain B:  64% 31%

L1316	CYS	L1203	I1085	L959	G868	T772	V685	M584	E493	A367	T241	F143
VAL	Y1086	G1087	Q1088	E960	N869	Q773	K686	S587	E493	A367	T241	G152
THR	Q1088	G1087	Q1088	V964	R871	Q773	T688	G588	S497	K371	E243	Y153
GLY	P1215	E1216	A1093	P965	D872	V776	E689	E589			E244	R154
ALA	E1216			P965	L873	A777	E690		A500	T388	L245	P155
PRO				W968	S874	K778	D691	Y592			L246	
GLY	P1224		T1096	R980	H875	K779		D595	I505	F390	D247	A164
ASN									E506	P391	L248	K165
CYS	K1228		K1099	R980	M878	V784	I695		F507	S392	Q251	ASN
				E983	R879		L698	B598	L511	Y393		GLY
K1326	I1235		E1102	V984	R880	L788	E699	B599	T512	R394	E254	CYS
W1328				D985	A881		D700	E500	L513	T396	A255	T39
S1329	E1238		K1105	K986	R871	R793	A701	H601	F519	L397		GLY
L1330	F1239		K1106	F987	L873	A777		E602	Y520	L398	E263	C43
R1331			N1107	N988	S874	G797	N705	L603	F519	L398	E263	G44
	M1249		K1107	K989	R895	G797	T706	F604	L521	C399	I264	E45
V1332	P1109		P1108	K989	G896	G799	F707	L605	L521			GLY
	K1250											G46
	K1251			K994	T897			R606	T522	E402	E267	
	Y1254		W1116	K995	E802	E802	E711	L607	V523	L403		
	A1255		V1117	K996	R898	R804	L712	L607	T522	L403		
	S1256		M1118	G997	R899	R804	K713		V523	L403	M277	PRO
	K1257		Q1122	C999	C901	S805			K526	L405	I278	ASN
	A1258		D1123	I1000	N904	S809	K716	H614	L527	S406	I279	CYS
	V1259		R1124	P1002	S907	V810	D718	H616	G528	L407	C280	CYS
							L719		D530	E408	P281	MET
	P1262		S1128	T1003	N908	A816	K720	L617	S531	Y411	I284	GLN
	P1263		T1129	K1004	T909		K721		LVS	S412		LVS
	L1264		Y1133	F1005	A910	P822	E725	S619	ASP		L287	LVS
			R1134	G1006	F911	L827	A726	D621	GLY	R426	G296	ASP
	F1271		R1134	I1007	R912	D828	D727	B624	K537	R427	V308	HIS
	F1272		Y1140	S1008	G913	B829		G626	D639	E428		THR
	A1273				F914		V730	G627	P640	D429	L312	THR
									T541	P430		LEU
	A1280		T1144	Q1016	P917	D832				I431	V316	S192
	A1281		N1145	A1017		H833	E733					P193
	R1282			I1021	F921	T836	I736	F631	S544	R439	Q322	
	A1283		H1151	H1022	I922				A545	V440	F196	R104
	Q1284		Y1152	V1023		R839	Q739	B645	T546	N197	G224	G114
	H1285		F1153		W926	H840	D740		L547	L441	P198	F115
	T1286		T1154	S1028	M927		H741	H650	L548	P444	E325	C116
	M1287		Y1155	V1029			F742		F549		E199	
				I1030	V930	A844	Y743		Q550	R328	E200	
			E1161	V1031		R845	L744		K551	E451		P118
	R1295				P937	Y846			H552			
			H1171	E1037	A938	K347			P553		E332	M124
	S1298				E939		H747	H660		R462	F337	
	P1299						C748	T661	P554		A338	L128
	A1300		S1184	H1043	E940	F850	T749	C662	A555	L467	P213	R129
	T1301		L1185	T1044	V941	K851			N556	K468	L216	H130
	P1302		L1186	K1045		R852			I557		L217	Q132
			N1187		Y947		P753		Q471		N351	P132
	A1308			V1049	K948	L856			L559	R472	L219	E133
							E756	V671			K220	P134
	C1309		I1190			L859			F560	Q473	I358	T135
	V1310		D1191	K1052	T953		E761	P675	D571	L474		
	D1311		I1192		H954	B860					L361	E138
	K1312			P1076	N956	V861				S475	N362	T235
	F1313		E1196		P956		V764	A681		K476	P263	I139
	T1314			S1082	Q957	R866			L580		P266	
			V1200		R957	A957					I237	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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: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: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:B:322:GLN:O	1:B:412:SER:HB3	1.82	0.80
1:A:322:GLN:O	1:A: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:CG	1:A:1331:ARG:H	1.97	0.74
1:A:1330:LEU:CD1	1:A:1331:ARG:H	2.00	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:B:955:PHE:HA	1:B:1145:ASN:ND2	2.01	0.71
1:A:584:MET:SD	1:B:756:GLU:HB3	2.30	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:718:ASP:HB3	1:B:721:LYS:HB3	1.74	0.70
1:B:389:PHE:O	1:B:391:PRO:HD3	1.91	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:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.95	0.67
1:A:1005:PHE:HB3	1:A:1262:PRO:HG3	1.75	0.67
1:A:325:GLU:HB2	1:A:412:SER:OG	1.93	0.67
1:B:406:SER:C	1:B:407:ILE:HD12	2.14	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: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:B:367:ALA:O	1:B:439:ARG:HD3	1.99	0.63
1:A:1187:ASN:CG	1:A:1190:ILE:HG12	2.19	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:B:487:CYS:HA	1:B:513:LEU:HD22	1.80	0.62
1:A:135:THR:OG1	1:A:138:GLU:HG3	2.00	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:B:870:SER:HB3	1:B:907:SER:CB	2.30	0.61
1:B:296:GLY:HA2	1:B:411:TYR:CD1	2.34	0.61
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.66	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:196:PHE:HE1	1:A:198:PRO:HG3	1.66	0.60
1:B:730:VAL:O	1:B:847:LYS:HA	2.02	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:A:730:VAL:O	1:A:847:LYS:HA	2.02	0.60
1:B:1330:LEU:HD13	1:B:1332:VAL:H	1.67	0.60
4:A:3004:MOS:O2	4:A:3004:MOS:S	2.60	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
4:B:4004:MOS:O2	4:B:4004:MOS:S	2.60	0.59
1:A:802:GLU:HG2	1:A:803:THR:HG23	1.82	0.59
1:B:749:THR:HG21	1:B:809:SER:HA	1.84	0.59
1:A:749:THR:HG21	1:A: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: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:358:ILE:HD13	1:A:431:ILE:HG23	1.84	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:B:1191:ASP:OD1	1:B:1259:VAL:HG11	2.04	0.58
1:A:937:PRO:O	1:A:941:VAL:HG23	2.03	0.58
1:B:255:ALA:HB2	1:B:277:MET:HG2	1.86	0.58
1:B:131:GLN:NE2	1:B:133:GLU:H	1.86	0.58
1:A:761:GLU:HG3	1:A:788:LEU:HD23	1.85	0.58

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:N	2.19	0.58
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.58
1:A:255:ALA:HB2	1:A:277:MET:HG2	1.86	0.58
1:A:196:PHE:CE1	1:A:198:PRO:HG3	2.39	0.57
1:B:544:SER:OG	1:B:994:LYS:HD2	2.04	0.57
1:B:539:ASP:OD1	1:B:541:THR:N	2.37	0.57
1:B:666:ILE:CD1	1:B:666:ILE:H	2.05	0.57
1:A:544:SER:OG	1:A:994:LYS:HD2	2.04	0.57
1:A:1191:ASP:OD1	1:A:1259:VAL:HG11	2.04	0.57
1:B:1052:LYS:HD3	1:B:1254:TYR:CZ	2.39	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:A:242:LEU:HA	1:A:284:ILE:HD13	1.87	0.57
1:B:552:HIS:CG	1:B:553:PRO:HD2	2.40	0.57
1:A:96:THR:OG1	1:A:97:ARG:N	2.38	0.57
1:B:450:LYS:O	1:B:474:LEU:HD22	2.05	0.57
1:B:602:GLU:HG3	1:B:822:PRO:HG2	1.85	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: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:196:PHE:CE1	1:B:198:PRO:HG3	2.39	0.56
1:B:192:SER:HB3	1:B:193:PRO:HD2	1.86	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:1330:LEU:HD22	1:A:1330:LEU:C	2.22	0.56
1:A:1326:LYS:O	1:A:1326:LYS:HG2	2.06	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:B:744:LEU:HD23	2:B:4001:FES:S2	2.46	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:1330:LEU:C	1:B:1330:LEU:HD22	2.22	0.56
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.41	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: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:B:999:CYS:SG	1:B:1001:ILE:HD11	2.46	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLU:CD	1:A:506:GLU:H	2.09	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:B:1105:LYS:HG3	1:B:1116:TRP:CZ2	2.42	0.55
1:A:844:ALA:HB2	1:A:922:ILE:HD13	1.89	0.55
1:B:911:PHE:HD2	1:B:912:ARG:N	2.03	0.55
5:A:3005:FAD:H51A	5:A:3005:FAD:H8A	1.89	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:1330:LEU:CG	1:B:1331:ARG:N	2.68	0.55
1:B:997:GLY:HA3	1:B:1273:ALA:O	2.05	0.55
1:B:556:ASN:C	1:B:557:ILE:HD12	2.27	0.55
1:B:506:GLU:H	1:B:506:GLU:CD	2.09	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:521:LEU:HD22	1:B:538:LEU:HD11	1.89	0.54
1:B:287:LEU:CD2	1:B:405:LEU:HD12	2.37	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
5:B:4005:FAD:H51A	5:B:4005:FAD:H8A	1.89	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:A:396:THR:OG1	1:A:398:LEU:HD23	2.08	0.54
1:B:832:ASP:O	1:B:836:THR:HG23	2.08	0.54
1:A:619:SER:HB3	1:A:688:THR:OG1	2.07	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:404:LEU:CD2	1:A:407:ILE:HD11	2.37	0.54
1:A:284:ILE:HB	1:A:287:LEU:HD12	1.88	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

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: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: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:B:773:GLN:HG2	1:B:784:VAL:HG13	1.90	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:A:1271:PHE:CE1	1:A:1300:ALA:HB2	2.43	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:HD12	1:B:856:ILE:N	2.23	0.53
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.09	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: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: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:N	1:A:559:LEU:HD23	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:B:441:LEU:HB3	1:B:451:GLU:HB2	1.91	0.52
1:A:552:HIS:ND1	1:A:553:PRO:HD2	2.24	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:441:LEU:HB3	1:A:451:GLU:HB2	1.91	0.51
1:B:880:ARG:HD2	1:B:914:PHE:O	2.11	0.51
1:A:264:ILE:HD11	5:A:3005:FAD:H3B	1.91	0.51
1:A:773:GLN:HG2	1:A:784:VAL:HG13	1.90	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:522:THR:HG22	1:B:526:LYS:HE3	1.93	0.51
1:B:263:GLU:O	1:B:267:GLU:HG3	2.11	0.51
3:B:4003:MTE:S2'	4:B:4004:MOS:O1	2.69	0.50
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
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: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:A:912:ARG:O	1:A:1264:LEU:HD13	2.11	0.50
1:A:1000:ILE:O	1:A:1000:ILE:HG23	2.11	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:B:328:ARG:HG2	1:B:328:ARG:NH1	2.21	0.50
1:A:779:MET:HG3	1:A:810:VAL:CG1	2.42	0.50
1:A:560:PHE:CD2	1:A:560:PHE:N	2.79	0.50
1:B:364:VAL:HG13	1:B:418:PHE:CE2	2.46	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:793:ARG:HH11	1:B:793:ARG:HG2	1.77	0.50
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:592:TYR:O	1:A:595:ASP:HB2	2.12	0.49
1:A:1140:TYR:HE1	1:A:1145:ASN:HD22	1.57	0.49
1:B:719:LEU:HD13	1:B:860:GLU:OE2	2.12	0.49
1:B:237:ILE:HD12	1:B:277:MET:CE	2.42	0.49
1:B:739:GLN:HG2	1:B:911:PHE:CE1	2.47	0.49
1:B:605:LEU:HD23	1:B:605:LEU:C	2.32	0.49
1:A:615:ALA:HB2	1:A:691:ASP:HA	1.93	0.49

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD23	1:B:61:LEU:C	2.34	0.48
1:A:615:ALA:CB	1:A:691:ASP:HA	2.43	0.48
1:B:615:ALA:CB	1:B:691:ASP:HA	2.43	0.48
1:A:362:ASN:HB2	1:A:363:PRO:HD3	1.95	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:A:607:LEU:HD22	1:A:666:ILE:HG21	1.96	0.48
1:B:607:LEU:HD22	1:B:666:ILE:HG21	1.96	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:A:698:ILE:O	1:A:701:ALA:HB3	2.14	0.48
1:A:213:PRO:HB2	1:A:216:LEU:HB3	1.96	0.48
1:B:698:ILE:O	1:B:701:ALA:HB3	2.14	0.48
1:A:114:GLY:HA2	1:A:117:THR:OG1	2.13	0.48
1:B:129:ARG:HH11	1:B:129:ARG:HG3	1.78	0.48
1:B:1262:PRO:HB2	1:B:1263:PRO:HD3	1.95	0.48
1:A:245:LEU:HB2	1:A:284:ILE:HD11	1.96	0.48
1:B:245:LEU:HB2	1:B:284:ILE:HD11	1.96	0.48
1:A:308:VAL:HG21	1:A:348:LEU:HD12	1.96	0.48
1:A:46:GLY:HA2	2:A:3002:FES:S1	2.54	0.48
1:B:213:PRO:HB2	1:B:216:LEU:HB3	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:1262:PRO:HB2	1:A:1263:PRO:HD3	1.95	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: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:HA	1:A:471:GLN:OE1	2.13	0.47
1:B:154:ARG:N	1:B:155:PRO:HD2	2.29	0.47
1:B:129:ARG:NE	1:B:209:GLU:HG2	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: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:88:VAL:HG13	1:A:89:GLU:N	2.28	0.47
1:B:616:LYS:HA	1:B:659:THR:HG22	1.95	0.47
1:A:1022:HIS:CE1	1:A:1128:SER:HG	2.32	0.47
1:B:124:MET:CE	1:B:128:LEU:HG	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ILE:CD1	1:A:921:PHE:HD2	2.27	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:129:ARG:NE	1:A:209:GLU:HG2	2.29	0.47
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.96	0.47
1:A:1096:THR:HB	1:A:1129:THR:HG21	1.95	0.47
1:A:772:THR:O	1:A:776:VAL:HG23	2.15	0.47
1:A:1330:LEU:CD1	1:A:1332:VAL:H	2.28	0.47
1:B:1330:LEU:CD1	1:B:1332:VAL:H	2.28	0.47
1:A:124:MET:CE	1:A:128:LEU:HG	2.45	0.47
1:B:1082:SER:HB2	3:B:4003:MTE:O1P	2.14	0.47
3:B:4003:MTE:S1'	4:B:4004:MOS:O2	2.73	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:B:1007:ILE:O	1:B:1008:SER:CB	2.62	0.47
1:A:747:HIS:ND1	1:A:805:SER:HA	2.29	0.47
1:A:1007:ILE:O	1:A:1008:SER:CB	2.62	0.47
1:B:947:TYR:OH	1:B:953:THR:HA	2.14	0.47
1:A:872:ASP:OD1	1:A:873:LEU:N	2.47	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.53	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:439:ARG:NH2	1:B:451:GLU:OE1	2.46	0.47
1:A:712:LEU:HD11	1:A:875:HIS:CE1	2.50	0.47
1:B:712:LEU:HD11	1:B:875:HIS:CE1	2.50	0.47
1:B:308:VAL:HG21	1:B:348:LEU:HD12	1.96	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: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:B:1102:GLU:OE1	1:B:1106:LYS:HE3	2.16	0.46
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.50	0.46
1:A:947:TYR:OH	1:A:953:THR:HA	2.14	0.46
1:A:45:GLU:OE1	1:A:1224:PRO:HD2	2.15	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: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:A:87:THR:OG1	1:A:89:GLU:HG2	2.15	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:B:87:THR:OG1	1:B:89:GLU:HG2	2.15	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:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.50	0.46
1:B:736:ILE:CD1	1:B:921:PHE:HD2	2.27	0.46
1:A:911:PHE:O	1:A:912:ARG:C	2.53	0.46
1:A:711:GLU:HA	1:A:899:ARG:HD2	1.96	0.46
1:A:657:LYS:O	1:A:658:ASP:HB2	2.16	0.46
1:B:657:LYS:O	1:B:658:ASP:HB2	2.16	0.46
1:B:60:ARG:O	1:B:61:LEU:HB3	2.16	0.46
1:A:234:VAL:HG12	1:A:235:THR:N	2.31	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:B:872:ASP:OD1	1:B:873:LEU:N	2.47	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:964:VAL:N	1:B:965:PRO:CD	2.79	0.45
1:B:281:PRO:HB2	1:B:287:LEU:HD13	1.97	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:A:1102:GLU:OE1	1:A:1106:LYS:HE3	2.16	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: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:1153:PHE:HB2	1:B:1155:TYR:CZ	2.51	0.45
1:B:427:ARG:NE	1:B:549:PHE:CE1	2.85	0.45
1:B:473:GLN:NE2	1:B:473:GLN:HA	2.32	0.45
1:A:60:ARG:O	1:A:61:LEU:HB3	2.16	0.45
1:B:468:LYS:HB2	1:B:493:GLU:CD	2.37	0.45
1:A:1184:SER:HB2	1:A:1255:ALA:HB3	1.98	0.45
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.98	0.45
1:B:624:GLU:HB3	1:B:684:VAL:CG2	2.46	0.45
1:B:254:GLU:CD	1:B:254:GLU:H	2.19	0.45
1:A:426:ARG:CZ	1:A:1228:LYS:HE3	2.47	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:B:1330:LEU:CD1	1:B:1332:VAL:N	2.70	0.45
1:B:1191:ASP:O	1:B:1192:ILE:CB	2.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.98	0.45
1:B:217:LEU:CD1	1:B:220:LYS:HD3	2.46	0.45
1:A:427:ARG:NE	1:A:549:PHE:CE1	2.85	0.45
1:B:926:TRP:CE3	1:B:927:MET:N	2.85	0.45
1:A:219:LEU:HD23	1:A:219:LEU:N	2.32	0.45
1:A:1286:THR:CG2	1:A:1287:ASN:N	2.64	0.45
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.77	0.45
1:B:296:GLY:HA2	1:B:411:TYR:CE1	2.52	0.45
1:A:736:ILE:HG23	1:A:1298:SER:HB3	1.99	0.45
1:B:79:THR:HG22	1:B:236:TRP:CZ2	2.52	0.45
1:A:254:GLU:H	1:A:254:GLU:CD	2.19	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:705:ASN:HA	1:B:707:PHE:HE1	1.82	0.44
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.53	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:733:GLU:O	1:B:1295:ARG:HD2	2.18	0.44
1:B:557:ILE:N	1:B:557:ILE:HD12	2.32	0.44
1:B:747:HIS:HB2	1:B:827:LEU:HD12	1.99	0.44
1:B:604:PHE:O	1:B:671:VAL:HA	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:A:281:PRO:HB2	1:A:287:LEU:HD13	1.97	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: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:B:1184:SER:HB2	1:B:1255:ALA:HB3	1.98	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:A:612:ARG:HH11	1:A:612:ARG:HG3	1.83	0.44
1:B:612:ARG:HH11	1:B:612:ARG:HG3	1.82	0.44
1:B:571:ASP:OD2	1:B:1052:LYS:NZ	2.47	0.44
1:A:328:ARG:NH1	1:A:328:ARG:CG	2.77	0.44
1:B:719:LEU:HD13	1:B:860:GLU:HG3	1.99	0.44
1:A:1264:LEU:HD23	1:A:1264:LEU:C	2.38	0.44
1:B:1016:GLN:HA	1:B:1133:TYR:O	2.17	0.44
1:A:859:LEU:HD22	1:A:891:ILE:HD13	2.00	0.44
1:A:733:GLU:HG2	1:A:1295:ARG:NH1	2.32	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:B:736:ILE:HG23	1:B:1298:SER:HB3	1.99	0.44
1:A:212:PHE:CD1	1:A:213:PRO:HD2	2.53	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:733:GLU:HG2	1:B:1295:ARG:HH12	1.83	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:878:MET:O	1:B:881:ALA:HB3	2.18	0.44
1:B:152:GLY:O	1:B:1235:ILE:HG21	2.18	0.44
1:A:371:LYS:HB2	1:A:408:GLU:HB3	1.99	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:B:389:PHE:C	1:B:391:PRO:HD3	2.38	0.43
1:B:165:LYS:HG2	1:B:165:LYS:O	2.18	0.43
1:B:60:ARG:O	1:B:61:LEU:HB2	2.18	0.43
1:A:747:HIS:HB2	1:A:827:LEU:HD12	1.99	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:711:GLU:HA	1:A:899:ARG:CD	2.48	0.43
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.53	0.43
1:B:497:SER:O	1:B:500:ALA:N	2.51	0.43
1:A:839:ARG:HG2	1:A:840:HIS:N	2.32	0.43
1:B:115:PHE:HD2	1:B:744:LEU:HB3	1.84	0.43
1:B:1264:LEU:HD23	1:B:1264:LEU:C	2.38	0.43
1:B:898:GLY:O	1:B:899:ARG:HD2	2.18	0.43
1:A:861:VAL:O	1:A:896:GLY:HA2	2.17	0.43
1:A:497:SER:O	1:A:500:ALA:N	2.51	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:B:521:LEU:CD2	1:B:538:LEU:HD11	2.48	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:139:ILE:CD1	1:B:164:ALA:HB2	2.48	0.43
1:B:1312:LYS:O	1:B:1316:LEU:HB2	2.19	0.43
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:PHE:O	1:A:462:ARG:HD2	2.19	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: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: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:B:1082:SER:HB2	3:B:4003:MTE:P	2.59	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:A:1023:VAL:HG13	1:A:1029:VAL:HG22	2.00	0.43
1:A:1286:THR:O	1:A:1287:ASN:O	2.36	0.43
1:B:117:THR:HB	1:B:118:PRO:HD3	2.01	0.43
1:A:705:ASN:HA	1:A:707:PHE:CE1	2.53	0.43
1:A:1311:ASP:OD1	1:A:1313:PHE:HB2	2.19	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: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:1099:LYS:HA	1:A:1099:LYS:HD2	1.76	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:473:GLN:NE2	1:A:473:GLN:HA	2.32	0.42
1:A:128:LEU:HA	1:A:131:GLN:O	2.20	0.42
1:A:1082:SER:HB2	3:A:3003:MTE:P	2.59	0.42
1:A:612:ARG:HH12	1:A:689:TYR:HB2	1.84	0.42
1:B:539:ASP:OD2	1:B:540:PRO:HD2	2.20	0.42
1:A:995:LYS:HD2	1:A:1280:ALA:HB1	2.02	0.42
1:B:859:LEU:HD22	1:B:891:ILE:HD13	2.00	0.42
1:B:721:LYS:HB2	1:B:721:LYS:HE3	1.89	0.42
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.85	0.42
1:B:237:ILE:HD12	1:B:277:MET:HE1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:799:GLY:HA2	4:B:4004:MOS:S	2.60	0.42
1:A:1312:LYS:O	1:A:1316:LEU:HB2	2.19	0.42
1:B:968:TRP:CH2	1:B:1000:ILE:HG23	2.54	0.42
1:A:427:ARG:NH2	1:A:1171:HIS:O	2.53	0.42
1:B:580:LEU:HG	1:B:1044:THR:HG23	2.00	0.42
1:A:753:PRO:HD3	1:A:816:ALA:HB1	2.02	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:A:621:ASP:HB3	1:A:686:LYS:HB3	2.00	0.42
1:B:753:PRO:HD3	1:B:816:ALA:HB1	2.02	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: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: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: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:621:ASP:HB3	1:B:686:LYS:HB3	2.00	0.42
1:B:1144:THR:O	1:B:1145:ASN:C	2.58	0.41
1:A:541:THR:O	1:A:992:CYS:HB3	2.20	0.41
1:A:744:LEU:HA	1:A:744:LEU:HD13	1.78	0.41
1:B:427:ARG:NH2	1:B:1171:HIS:O	2.53	0.41
1:B:390:PHE:O	1:B:462:ARG:HD2	2.19	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: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:124:MET:HB2	1:A:143:PHE:HZ	1.86	0.41
1:A:117:THR:HB	1:A:118:PRO:HD3	2.01	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:248:LEU:HB3	1:A:279:ILE:HD13	2.02	0.41
1:A:11:ASN:OD1	1:A:90:GLY:HA3	2.21	0.41
1:B:718:ASP:CB	1:B:721:LYS:HB3	2.48	0.41
1:A:523:VAL:O	1:A:527:LEU:N	2.54	0.41
1:B:530:ASP:O	1:B:531:SER:CB	2.69	0.41
1:A:237:ILE:HD12	1:A:277:MET:HE3	2.02	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:A:38:GLY:O	1:A:40:LYS:HE2	2.20	0.41
1:A:646:THR:OG1	1:A:647:GLY:N	2.53	0.41
1:B:612:ARG:HH12	1:B:689:TYR:HB2	1.84	0.41
1:A:707:PHE:CD2	1:A:899:ARG:HB3	2.56	0.41
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	2.02	0.41
1:B:958:ARG:HH21	1:B:960:GLU:HG2	1.85	0.41
1:B:248:LEU:HB3	1:B:279:ILE:HD13	2.03	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:1049:VAL:HG13	1:A:1254:TYR:HE1	1.85	0.41
1:A:1004:LYS:HB2	1:A:1155:TYR:CE2	2.54	0.41
1:B:948:LYS:HB3	1:B:948:LYS:HE2	1.92	0.41
1:A:721:LYS:HB2	1:A:721:LYS:HE3	1.89	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:B:557:ILE:HG22	1:B:559:LEU:HD22	2.01	0.41
1:A:1105:LYS:HG3	1:A:1116:TRP:CH2	2.56	0.41
1:B:211:ILE:HG12	1:B:212:PHE:N	2.35	0.41
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	2.03	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: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: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:A:612:ARG:NH1	1:A:612:ARG:HG3	2.36	0.41
1:A:135:THR:O	1:A:139:ILE:HG13	2.21	0.41
1:B:1105:LYS:HG3	1:B:1116:TRP:CH2	2.56	0.41
1:B:506:GLU:N	1:B:506:GLU:CD	2.74	0.41
1:B:707:PHE:CD2	1:B:899:ARG:HB3	2.56	0.41
1:B:312:LEU:O	1:B:316:VAL:HG23	2.20	0.41
1:B:11:ASN:OD1	1:B:90:GLY:HA3	2.21	0.41
1:B:695:ILE:HG23	1:B:700:ASP:HB2	2.02	0.41
1:A:785:ASN:ND2	1:B:1028:SER:HB2	2.36	0.41
1:B:1282:ARG:NH1	1:B:1308:ALA:O	2.51	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:B:549:PHE:HE2	1:B:551:LYS:HG3	1.86	0.40
1:B:316:VAL:HA	1:B:324:THR:HG21	2.04	0.40
1:B:1151:HIS:NE2	1:B:1251:LYS:HE3	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:LYS:HE3	1:A:956:ASN:OD1	2.22	0.40
1:A:490:LEU:HB2	1:A:513:LEU:CD2	2.51	0.40
1:A:1045:LYS:O	1:A:1049:VAL:HG23	2.21	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:1249:ASN:HD22	1:A:1257:LYS:HG2	1.85	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:1045:LYS:O	1:B:1049:VAL:HG23	2.21	0.40
1:B:1021:ILE:HG12	1:B:1031:VAL:HG13	2.03	0.40
1:B:1249:ASN:HD22	1:B:1257:LYS:HG2	1.85	0.40
1:A:549:PHE:HE2	1:A:551:LYS:HG3	1.86	0.40
1:B:716:LYS:HE3	1:B:956:ASN:OD1	2.22	0.40
1:A:312:LEU:O	1:A:316:VAL:HG23	2.20	0.40
1:B:523:VAL:O	1:B:527:LEU:N	2.54	0.40
1:A:316:VAL:HA	1:A:324:THR:HG21	2.04	0.40
1:A:27:LEU:HD21	1:A:41:LEU:HB2	2.03	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%)	16	47
1	B	1282/1331 (96%)	1172 (91%)	95 (7%)	15 (1%)	16	47
All	All	2564/2662 (96%)	2345 (92%)	189 (7%)	30 (1%)	16	47

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%)	61	90
1	B	1095/1127 (97%)	1072 (98%)	23 (2%)	61	90
All	All	2190/2254 (97%)	2144 (98%)	46 (2%)	61	90

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	$\# Z > 2$
2	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	MTE	A	3003	4	19,26,26	6.07	11 (57%)	19,40,40	2.79	9 (47%)
4	MOS	A	3004	3	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	A	3005	-	48,58,58	4.83	34 (70%)	54,89,89	3.06	27 (50%)
6	TEI	A	3006	-	17,23,23	3.81	5 (29%)	16,32,32	1.77	4 (25%)
2	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	MTE	B	4003	4	19,26,26	6.07	11 (57%)	19,40,40	2.79	8 (42%)
4	MOS	B	4004	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	B	4005	-	48,58,58	4.83	34 (70%)	54,89,89	3.07	27 (50%)
6	TEI	B	4006	-	17,23,23	3.81	5 (29%)	16,32,32	1.76	4 (25%)

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	3001	1	-	0/0/4/4	0/1/1/1
2	FES	A	3002	1	-	0/0/4/4	0/1/1/1
3	MTE	A	3003	4	-	0/6/34/34	0/3/3/3
4	MOS	A	3004	3	-	0/0/0/0	0/0/0/0
5	FAD	A	3005	-	-	0/30/50/50	0/6/6/6
6	TEI	A	3006	-	-	0/11/15/15	0/2/2/2
2	FES	B	4001	1	-	0/0/4/4	0/1/1/1
2	FES	B	4002	1	-	0/0/4/4	0/1/1/1
3	MTE	B	4003	4	-	0/6/34/34	0/3/3/3
4	MOS	B	4004	3	-	0/0/0/0	0/0/0/0
5	FAD	B	4005	-	-	0/30/50/50	0/6/6/6
6	TEI	B	4006	-	-	0/11/15/15	0/2/2/2

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	FAD	C5'-C4'	-9.42	1.37	1.51
5	B	4005	FAD	C5'-C4'	-9.38	1.37	1.51
3	A	3003	MTE	P-O4'	-7.39	1.35	1.60
3	B	4003	MTE	P-O4'	-7.38	1.35	1.60
3	B	4003	MTE	P-O3P	-5.60	1.34	1.54
3	A	3003	MTE	P-O3P	-5.59	1.34	1.54
5	A	3005	FAD	C7M-C7	-4.83	1.41	1.51
5	B	4005	FAD	C7M-C7	-4.83	1.41	1.51
5	A	3005	FAD	O2B-C2B	-4.75	1.31	1.43
5	B	4005	FAD	O2B-C2B	-4.72	1.31	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4005	FAD	PA-O2A	-4.71	1.34	1.54
5	A	3005	FAD	PA-O2A	-4.69	1.34	1.54
5	B	4005	FAD	C2'-C3'	-4.36	1.44	1.53
5	A	3005	FAD	C2'-C3'	-4.35	1.44	1.53
5	B	4005	FAD	O2'-C2'	-3.66	1.35	1.43
5	A	3005	FAD	O2'-C2'	-3.65	1.35	1.43
5	A	3005	FAD	P-O2P	-3.47	1.40	1.54
5	B	4005	FAD	P-O2P	-3.45	1.40	1.54
5	A	3005	FAD	C5A-N7A	-3.22	1.28	1.39
5	B	4005	FAD	C5A-N7A	-3.20	1.28	1.39
5	B	4005	FAD	C8M-C8	-2.94	1.45	1.51
5	A	3005	FAD	C8M-C8	-2.92	1.45	1.51
5	A	3005	FAD	C8A-N7A	-2.81	1.29	1.34
5	B	4005	FAD	C8A-N7A	-2.80	1.29	1.34
5	B	4005	FAD	P-O5'	-2.70	1.46	1.59
5	A	3005	FAD	P-O5'	-2.70	1.46	1.59
5	B	4005	FAD	P-O1P	-2.57	1.41	1.51
5	A	3005	FAD	P-O1P	-2.57	1.41	1.51
5	B	4005	FAD	PA-O5B	-2.18	1.49	1.59
5	A	3005	FAD	PA-O5B	-2.18	1.49	1.59
5	A	3005	FAD	C6A-N6A	-2.07	1.28	1.34
5	B	4005	FAD	C6A-N6A	-2.07	1.28	1.34
3	A	3003	MTE	O3'-C3'	2.00	1.46	1.43
3	B	4003	MTE	O3'-C3'	2.02	1.46	1.43
6	B	4006	TEI	C2-N3	2.21	1.34	1.31
6	A	3006	TEI	C2-N3	2.21	1.34	1.31
5	B	4005	FAD	C9-C8	2.31	1.44	1.37
5	A	3005	FAD	C9-C8	2.31	1.44	1.37
3	A	3003	MTE	C2-N1	2.39	1.39	1.35
3	B	4003	MTE	C2-N1	2.42	1.39	1.35
5	B	4005	FAD	C6-C7	2.45	1.44	1.37
5	A	3005	FAD	C6-C7	2.47	1.44	1.37
3	A	3003	MTE	O4-C4	2.48	1.30	1.24
3	B	4003	MTE	O4-C4	2.48	1.30	1.24
3	A	3003	MTE	C10-N8	2.64	1.40	1.35
3	B	4003	MTE	C10-N8	2.66	1.40	1.35
6	B	4006	TEI	O14-C9	2.94	1.43	1.37
6	A	3006	TEI	O14-C9	2.97	1.43	1.37
5	A	3005	FAD	C10-N10	3.38	1.43	1.39
5	B	4005	FAD	C10-N10	3.39	1.43	1.39
5	B	4005	FAD	C9-C9A	3.46	1.48	1.40
5	A	3005	FAD	C9-C9A	3.48	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	FAD	O5'-C5'	3.51	1.59	1.44
5	B	4005	FAD	O5'-C5'	3.52	1.59	1.44
3	A	3003	MTE	C4-N3	3.62	1.39	1.33
3	B	4003	MTE	C4-N3	3.63	1.39	1.33
5	A	3005	FAD	O4B-C1B	3.87	1.46	1.41
5	B	4005	FAD	O4B-C1B	3.89	1.46	1.41
5	A	3005	FAD	C6-C5X	4.34	1.48	1.41
5	B	4005	FAD	C6-C5X	4.38	1.48	1.41
5	B	4005	FAD	C4X-N5	4.78	1.40	1.33
5	A	3005	FAD	C4X-N5	4.83	1.40	1.33
5	A	3005	FAD	C4X-C10	5.53	1.51	1.41
5	B	4005	FAD	C4X-C10	5.55	1.51	1.41
5	A	3005	FAD	C4'-C3'	5.74	1.65	1.53
5	B	4005	FAD	C4'-C3'	5.75	1.65	1.53
5	A	3005	FAD	O3'-C3'	5.75	1.56	1.43
5	B	4005	FAD	O3'-C3'	5.76	1.56	1.43
6	B	4006	TEI	C8-C12	5.90	1.53	1.44
6	A	3006	TEI	C8-C12	5.93	1.53	1.44
3	B	4003	MTE	C9-N5	5.95	1.51	1.38
3	A	3003	MTE	C9-N5	5.97	1.51	1.38
5	A	3005	FAD	C8-C7	6.35	1.58	1.41
5	B	4005	FAD	C8-C7	6.37	1.58	1.41
5	B	4005	FAD	C5A-C4A	6.41	1.55	1.40
5	A	3005	FAD	C5A-C4A	6.42	1.55	1.40
5	B	4005	FAD	C4-C4X	7.00	1.55	1.41
5	A	3005	FAD	C4-C4X	7.01	1.55	1.41
5	B	4005	FAD	C4-N3	7.08	1.46	1.33
5	A	3005	FAD	C4-N3	7.11	1.46	1.33
5	B	4005	FAD	C4A-N3A	7.39	1.46	1.35
5	A	3005	FAD	C4A-N3A	7.44	1.46	1.35
5	B	4005	FAD	C9A-C5X	7.59	1.58	1.42
5	A	3005	FAD	C9A-C5X	7.62	1.58	1.42
6	A	3006	TEI	C10-C9	8.18	1.57	1.39
6	B	4006	TEI	C10-C9	8.19	1.57	1.39
5	A	3005	FAD	C2A-N3A	8.43	1.47	1.32
5	B	4005	FAD	C2A-N3A	8.44	1.47	1.32
5	B	4005	FAD	C2A-N1A	8.62	1.50	1.33
5	A	3005	FAD	C2A-N1A	8.63	1.50	1.33
3	B	4003	MTE	C6-N5	8.74	1.57	1.45
3	A	3003	MTE	C6-N5	8.75	1.57	1.45
3	A	3003	MTE	C9-C10	10.78	1.63	1.41
3	B	4003	MTE	C9-C10	10.80	1.63	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3006	TEI	C11-C6	10.89	1.62	1.39
6	B	4006	TEI	C11-C6	10.89	1.62	1.39
5	A	3005	FAD	C9A-N10	14.33	1.58	1.38
5	B	4005	FAD	C9A-N10	14.39	1.58	1.38
3	B	4003	MTE	C7-C6	18.57	1.67	1.53
3	A	3003	MTE	C7-C6	18.57	1.67	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4005	FAD	C5X-C9A-N10	-6.65	112.57	117.62
5	A	3005	FAD	C5X-C9A-N10	-6.62	112.58	117.62
5	B	4005	FAD	C4-C4X-C10	-6.25	115.94	119.94
5	A	3005	FAD	C4-C4X-C10	-6.21	115.96	119.94
5	B	4005	FAD	O4'-C4'-C5'	-6.00	97.12	110.19
5	A	3005	FAD	O4'-C4'-C5'	-6.00	97.13	110.19
5	B	4005	FAD	N3A-C2A-N1A	-5.16	124.94	128.89
5	A	3005	FAD	N3A-C2A-N1A	-5.10	124.99	128.89
5	A	3005	FAD	O5B-PA-O1A	-4.97	90.33	109.62
5	B	4005	FAD	O5B-PA-O1A	-4.97	90.34	109.62
5	A	3005	FAD	C4X-C4-N3	-4.61	117.29	123.59
5	B	4005	FAD	C4X-C4-N3	-4.59	117.32	123.59
6	A	3006	TEI	C6-C7-C8	-4.13	119.31	121.58
6	B	4006	TEI	C6-C7-C8	-4.10	119.32	121.58
5	A	3005	FAD	C4X-C10-N10	-4.05	118.13	120.52
5	B	4005	FAD	C4X-C10-N10	-4.02	118.15	120.52
3	B	4003	MTE	N3-C2-N1	-3.72	119.44	125.53
3	A	3003	MTE	N3-C2-N1	-3.70	119.47	125.53
5	B	4005	FAD	O4B-C4B-C5B	-3.53	96.71	109.32
5	A	3005	FAD	O4B-C4B-C5B	-3.51	96.75	109.32
5	B	4005	FAD	C8M-C8-C9	-3.42	110.99	120.28
5	A	3005	FAD	C8M-C8-C9	-3.41	111.00	120.28
5	B	4005	FAD	O5'-P-O1P	-3.04	97.80	109.62
5	A	3005	FAD	C7M-C7-C6	-3.04	112.00	120.28
5	A	3005	FAD	O5'-P-O1P	-3.04	97.80	109.62
5	B	4005	FAD	C7M-C7-C6	-3.04	112.01	120.28
6	B	4006	TEI	C10-C11-C6	-2.96	116.81	121.14
6	A	3006	TEI	C10-C11-C6	-2.94	116.84	121.14
6	A	3006	TEI	C9-C8-C12	-2.66	117.66	119.43
6	B	4006	TEI	C9-C8-C12	-2.66	117.66	119.43
3	A	3003	MTE	C9-C10-N1	-2.35	113.89	118.76
3	B	4003	MTE	C9-C10-N1	-2.33	113.92	118.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3003	MTE	C9-N5-C6	-2.00	113.26	118.65
3	B	4003	MTE	C9-C10-N8	2.08	120.52	118.34
5	A	3005	FAD	O2'-C2'-C3'	2.12	114.34	109.02
5	B	4005	FAD	O2'-C2'-C3'	2.12	114.34	109.02
3	A	3003	MTE	C9-C10-N8	2.13	120.57	118.34
5	A	3005	FAD	C2A-N1A-C6A	2.14	122.60	118.77
5	B	4005	FAD	C2A-N1A-C6A	2.16	122.63	118.77
5	A	3005	FAD	O3B-C3B-C2B	2.23	119.09	111.83
5	B	4005	FAD	O3B-C3B-C2B	2.24	119.12	111.83
3	B	4003	MTE	O2P-P-O4'	2.30	113.20	106.56
3	A	3003	MTE	O2P-P-O4'	2.31	113.23	106.56
5	B	4005	FAD	C4B-O4B-C1B	2.49	112.45	109.72
5	A	3005	FAD	C4B-O4B-C1B	2.49	112.46	109.72
5	B	4005	FAD	O2'-C2'-C1'	2.70	116.58	109.94
5	A	3005	FAD	O2'-C2'-C1'	2.70	116.59	109.94
5	A	3005	FAD	C4-C4X-N5	2.77	122.08	118.72
5	B	4005	FAD	C4-C4X-N5	2.79	122.10	118.72
5	B	4005	FAD	O5B-C5B-C4B	2.95	119.98	109.12
5	A	3005	FAD	O5B-C5B-C4B	2.95	119.99	109.12
5	A	3005	FAD	C2B-C1B-N9A	2.97	118.83	114.29
5	B	4005	FAD	C2B-C1B-N9A	3.00	118.87	114.29
5	B	4005	FAD	C7M-C7-C8	3.08	127.49	120.73
5	A	3005	FAD	C7M-C7-C8	3.09	127.52	120.73
6	A	3006	TEI	C11-C6-C7	3.16	122.36	118.17
6	B	4006	TEI	C11-C6-C7	3.17	122.38	118.17
5	A	3005	FAD	P-O3P-PA	3.90	143.69	132.73
5	B	4005	FAD	P-O3P-PA	3.90	143.69	132.73
5	A	3005	FAD	C8M-C8-C7	3.98	129.47	120.73
5	B	4005	FAD	C8M-C8-C7	3.99	129.50	120.73
3	A	3003	MTE	N2-C2-N3	4.31	124.33	117.20
3	B	4003	MTE	N2-C2-N3	4.32	124.36	117.20
5	A	3005	FAD	C1'-N10-C9A	4.41	123.82	118.86
5	B	4005	FAD	C1'-N10-C9A	4.42	123.82	118.86
5	B	4005	FAD	O3'-C3'-C4'	4.74	120.69	108.75
5	A	3005	FAD	O3'-C3'-C4'	4.74	120.70	108.75
5	B	4005	FAD	O3'-C3'-C2'	4.96	121.25	108.75
5	A	3005	FAD	O3'-C3'-C2'	4.96	121.25	108.75
3	A	3003	MTE	C4-N3-C2	5.14	123.07	115.94
3	B	4003	MTE	C4-N3-C2	5.16	123.09	115.94
3	A	3003	MTE	N8-C10-N1	5.60	125.53	116.62
3	B	4003	MTE	N8-C10-N1	5.62	125.56	116.62
5	B	4005	FAD	C4X-N5-C5X	5.62	123.22	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3005	FAD	C4X-N5-C5X	5.62	123.23	116.76
3	B	4003	MTE	C2-N1-C10	5.88	127.76	114.54
3	A	3003	MTE	C2-N1-C10	5.88	127.76	114.54
5	A	3005	FAD	C4-N3-C2	6.31	120.70	115.25
5	B	4005	FAD	C4-N3-C2	6.32	120.71	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 28 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.