



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 03:41 AM EDT

PDB ID : 2E1Q
Title : Crystal Structure of Human Xanthine Oxidoreductase mutant, Glu803Val
Authors : Yamaguchi, Y.; Matsumura, T.; Ichida, K.; Okamoto, K.; Nishino, T.
Deposited on : 2006-10-27
Resolution : 2.60 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) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

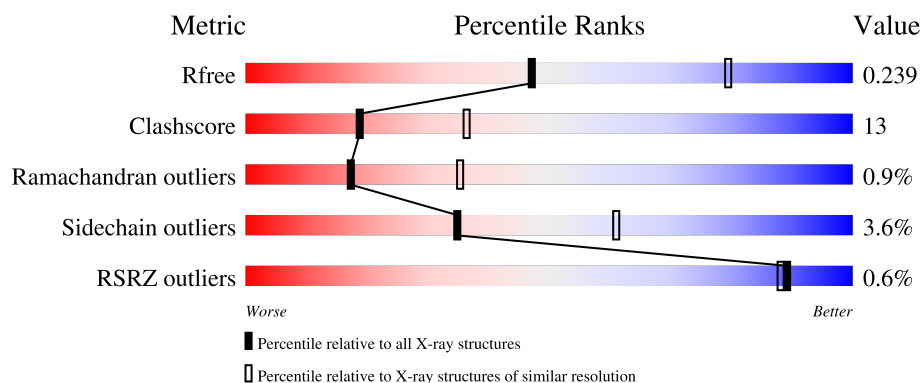
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	1333	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	1333	<div> <div></div> <div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
1	C	1333	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>..</div> </div> </div>
1	D	1333	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>..</div> </div> </div>

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
7	MOM	A	2005	-	-	X	-
7	MOM	B	3005	-	-	X	-
7	MOM	C	4005	-	-	X	-
7	MOM	D	5005	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 41721 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.

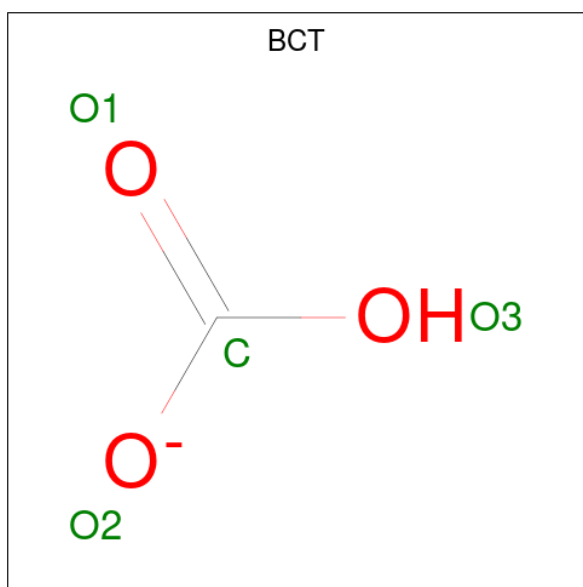
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	B	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	C	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	D	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P47989
A	803	VAL	GLU	engineered mutation	UNP P47989
B	1	MET	-	initiating methionine	UNP P47989
B	803	VAL	GLU	engineered mutation	UNP P47989
C	1	MET	-	initiating methionine	UNP P47989
C	803	VAL	GLU	engineered mutation	UNP P47989
D	1	MET	-	initiating methionine	UNP P47989
D	803	VAL	GLU	engineered mutation	UNP P47989

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

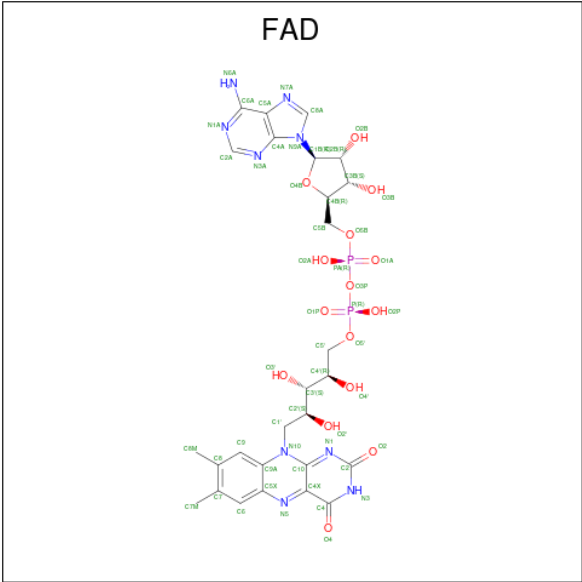
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



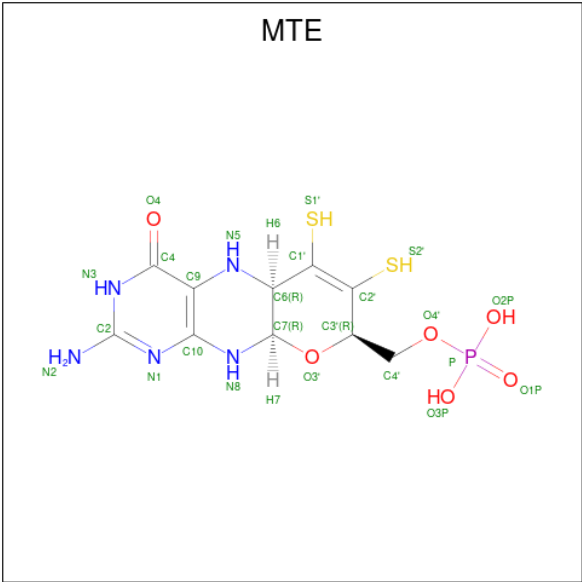
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		

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



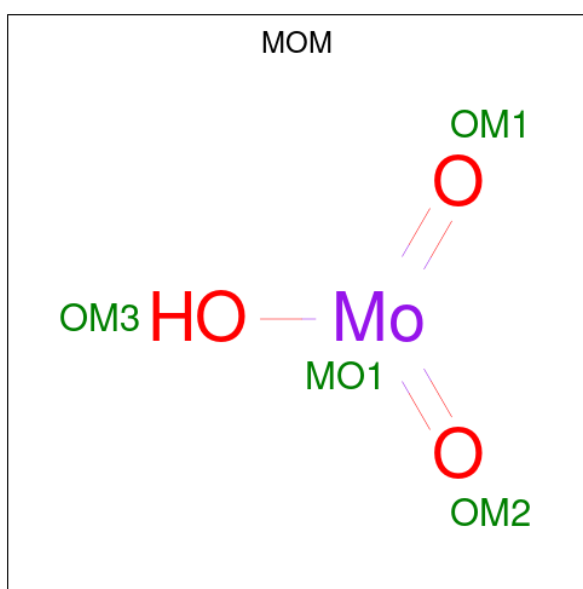
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 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: C₁₀H₁₄N₅O₆PS₂).



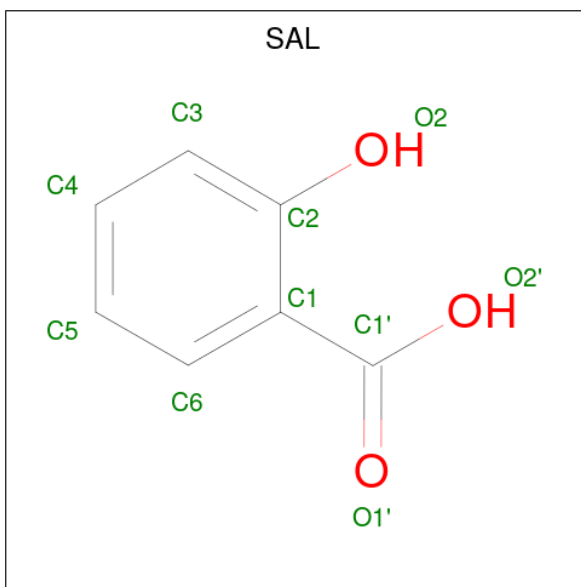
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
6	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
6	C	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
6	D	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0

- Molecule 7 is HYDROXY(DIOXO)MOLYBDENUM (three-letter code: MOM) (formula: HMoO_3).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mo O	0	0
			4 1 3			
7	B	1	Total	Mo O	0	0
			4 1 3			
7	C	1	Total	Mo O	0	0
			4 1 3			
7	D	1	Total	Mo O	0	0
			4 1 3			

- Molecule 8 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $\text{C}_7\text{H}_6\text{O}_3$).



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

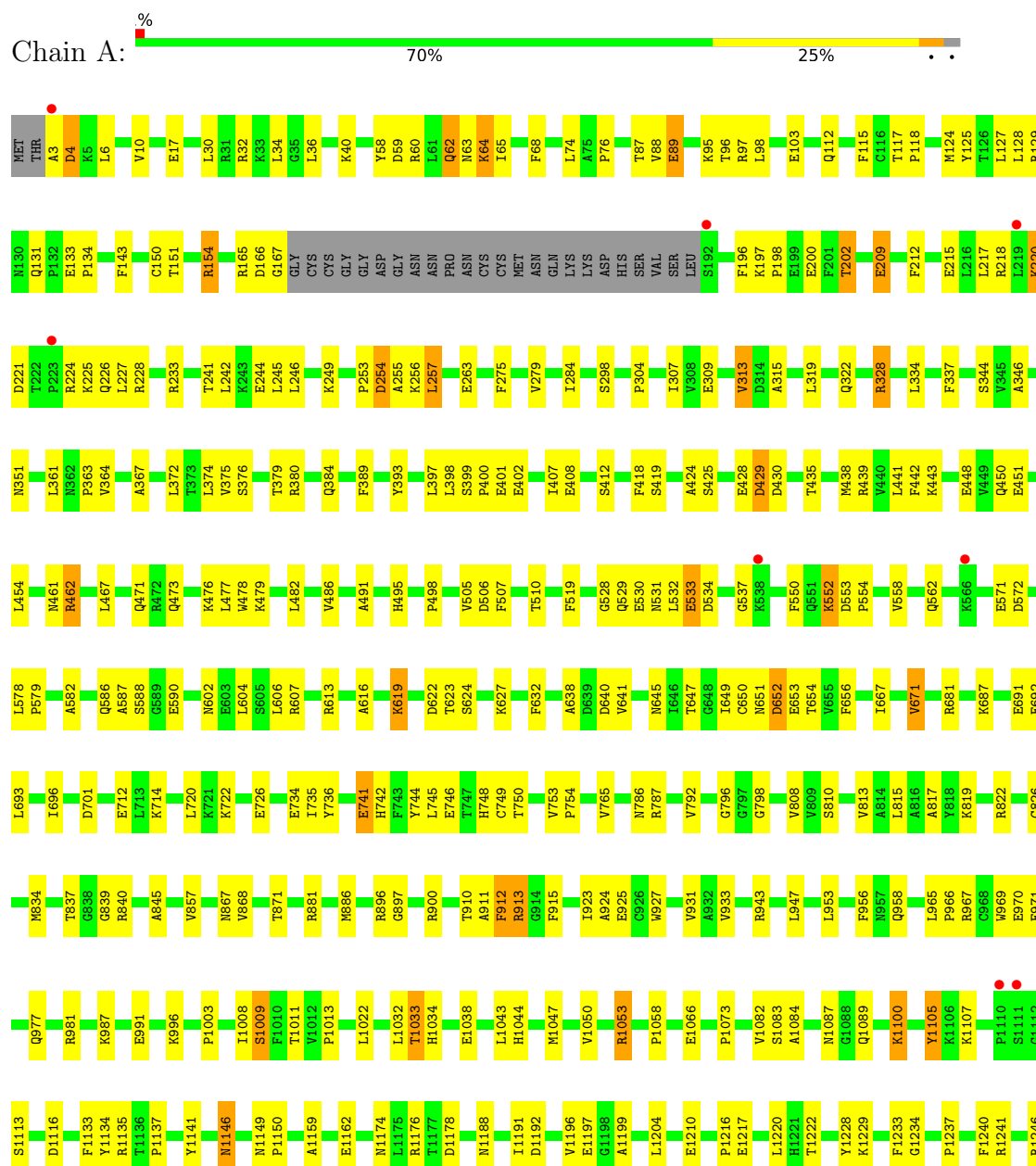
- Molecule 9 is water.

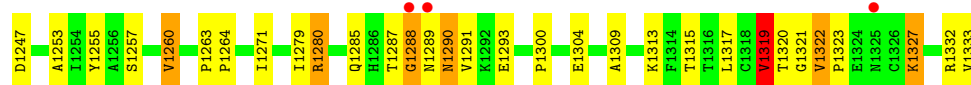
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	234	Total	O	0	0
			234	234		
9	B	245	Total	O	0	0
			245	245		
9	C	237	Total	O	0	0
			237	237		
9	D	233	Total	O	0	0
			233	233		

3 Residue-property plots

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

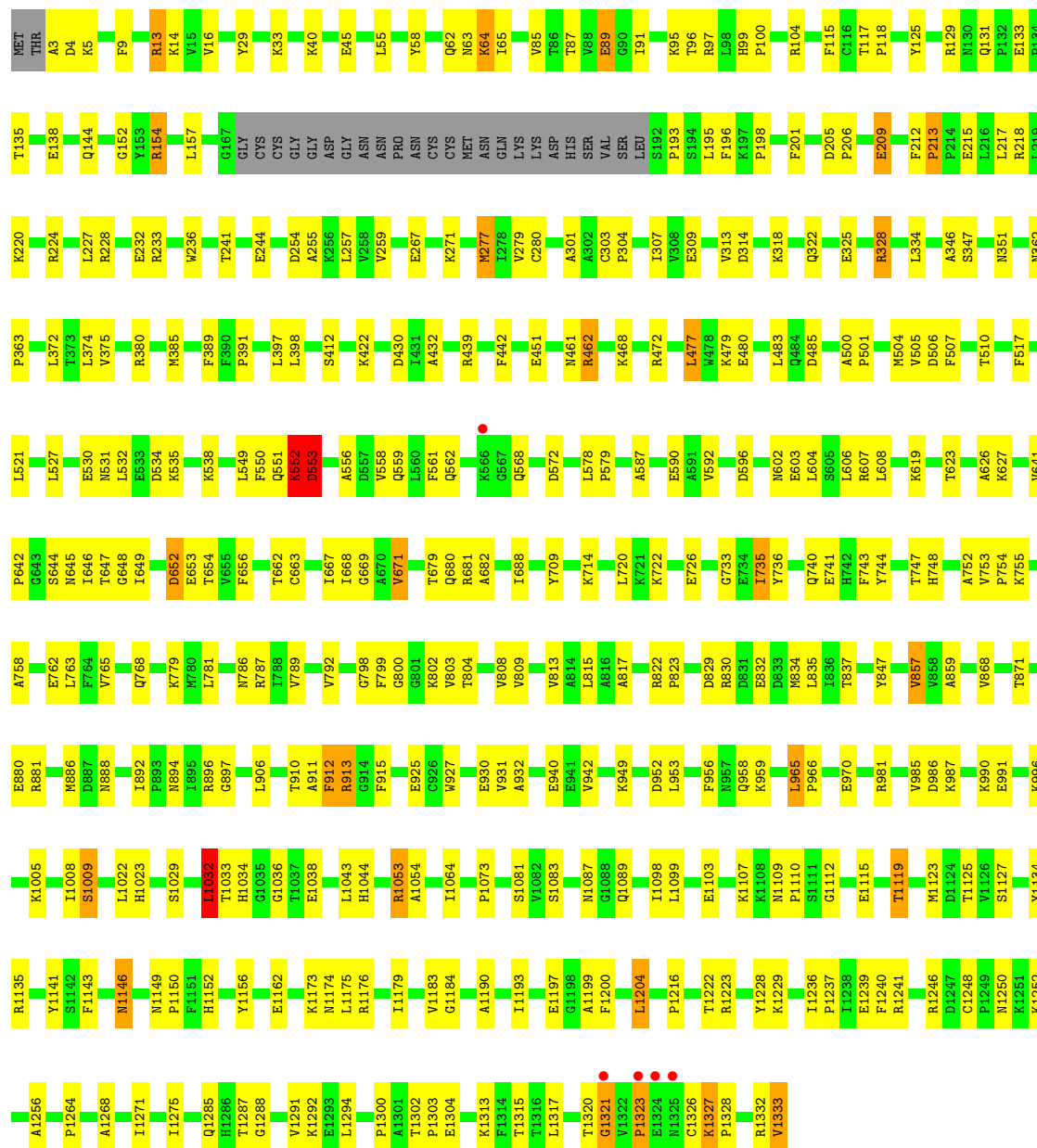
• Molecule 1: Xanthine dehydrogenase/oxidase





• Molecule 1: Xanthine dehydrogenase/oxidase

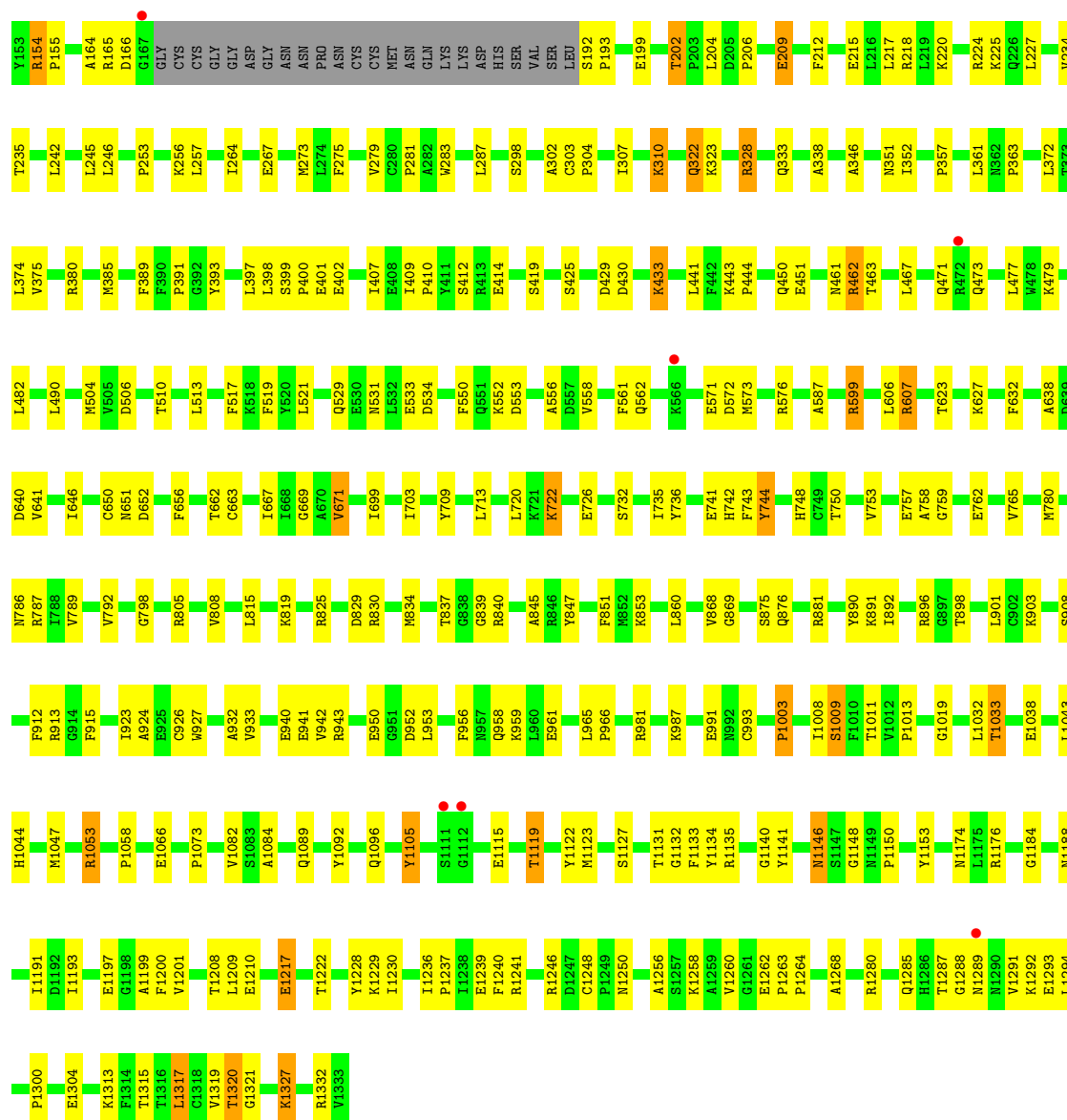
Chain B: 71% 25% ..



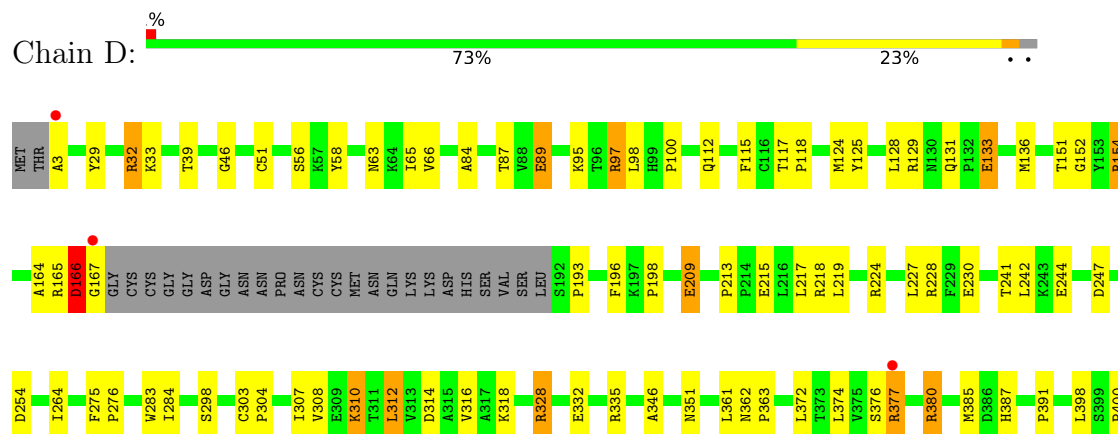
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain C: 72% 24% ..





• Molecule 1: Xanthine dehydrogenase/oxidase



F1240	R1241	V1242	S1243	R1246	N1250	K1251	K1252	A1253	I1254	Y1255	A1256	S1257	E1262	P1263	P1264	L1265	I1271	D1277	R1283	H1286	T1287	G1288	N1289	N1290	V1291	K1292	E1293	P1300	A1301	T1302	P1303	T1315	V1319	T1320	G1321	V1322	P1323	E1324	N1325	G1326	K1327	P1328	V1331	R1332	V1333
K1106	K1107	F956	N1108	N1109	G1112	E1115	D1116	W1117	V1118	T1119	M1123	S1127	T1131	G1132	F1133	Y1134	R1135	Y1141	S1142	F1143	N1146	P1150	V1163	N1174	I1193	E1197	G1198	A1199	F1200	V1201	L1204	T1208	L1209	S1215	P1216	E1217	T1222	A1232	P1237	T1238	E1239				
D952	F956	L965	P966	E970	E971	Y978	K982	N989	K996	R997	G998	L999	C1000	I1001	I1002	P1003	I1008	S1009	L1021	L1022	S1029	H1034	G1035	G1036	T1037	E1038	M1039	L1043	H1044	M1047	V1050	A1051	S1052	P1058	T1059	P1073	A1079	A1080	S1081	G1088	Q1089				
A816	A817	Y818	K819	R822	P823	R830	M834	T837	H841	Y847	V857	L860	E861	N867	V868	D873	T878	H879	E880	R881	R896	C902	N905	T910	F912	R913	G914	F915	A924	W927	E940	E941	V942	R943	R944	L947	Y948	K949							
C650	N651	D652	F656	V661	H666	V671	V672	T679	G680	R681	A682	E692	E716	F743	Y744	L745	H748	C749	T750	V753	P754	A758	R765	Q768	R787	I788	V789	G798	F799	K802	V803	T804	V808	L815											
E533	D534	K535	D553	P554	P555	A556	D557	S425	Q559	L560	F561	Q562	K566	G567	E571	L578	P579	D584	A587	E590	A591	V592	D596	E603	L604	S605	L606	R607	T612	R613	A614	S620	T623	A626	P630	V633	D640	V641	N645	T646	T649				
E401	E408	F418	K422	Q423	A424	S425	R426	D429	D430	I431	A432	R439	V440	L441	F442	K443	P444	G445	T446	Q450	E451	N461	R462	L467	K468	Q471	L474	P498	D499	A500	P501	V505	D506	T510	L513	F517	K518	F519	Y520	L521	T522	V523	L532		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.57Å 140.94Å 176.48Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.47 – 2.58	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.60) 94.0 (49.47-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.246 0.186 , 0.239	Depositor DCC
R_{free} test set	3840 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l 0.014 for k,h,-l 0.146 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41721	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MOM, FAD, MTE, BCT, FES, SAL, CA

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	0.35	0/10303	0.62	0/13950
1	B	0.36	0/10303	0.63	1/13950 (0.0%)
1	C	0.36	0/10303	0.62	0/13950
1	D	0.36	0/10303	0.62	0/13950
All	All	0.36	0/41212	0.63	1/55800 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1032	LEU	CA-CB-CG	5.62	128.22	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1105	TYR	Sidechain
1	C	1105	TYR	Sidechain

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	10088	0	10112	281	0
1	B	10088	0	10111	275	0
1	C	10088	0	10110	266	0
1	D	10088	0	10112	237	0
2	A	4	0	0	1	0
2	B	4	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	1	0
5	A	53	0	31	2	0
5	B	53	0	31	3	0
5	C	53	0	31	2	0
5	D	53	0	31	3	0
6	A	24	0	10	4	0
6	B	24	0	8	2	0
6	C	24	0	10	2	0
6	D	24	0	10	2	0
7	A	4	0	0	2	0
7	B	4	0	0	2	0
7	C	4	0	0	2	0
7	D	4	0	0	3	0
8	A	10	0	4	0	0
8	B	10	0	4	0	0
8	C	10	0	4	0	0
8	D	10	0	4	0	0
9	A	234	0	0	7	0
9	B	245	0	0	3	0
9	C	237	0	0	2	0
9	D	233	0	0	6	0
All	All	41721	0	40623	1063	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1063) 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)
6:A:2004:MTE:C9	6:A:2004:MTE:N5	1.68	1.52
6:C:4004:MTE:C9	6:C:4004:MTE:N5	1.68	1.51
1:A:133:GLU:HG2	1:A:165:ARG:HB3	1.40	1.03
1:D:1320:THR:HG23	1:D:1321:GLY:H	1.26	1.00
1:A:3:ALA:HB1	1:A:228:ARG:H	1.28	0.99
1:C:1287:THR:HG22	1:C:1288:GLY:H	1.31	0.95
1:C:154:ARG:HD3	1:C:1197:GLU:OE2	1.67	0.93
1:C:956:PHE:HA	1:C:1146:ASN:HD21	1.31	0.93
1:C:131:GLN:HE21	1:C:133:GLU:H	1.15	0.92
1:B:558:VAL:HG22	1:B:1241:ARG:HG2	1.53	0.90
1:B:1141:TYR:HB2	1:B:1150:PRO:HG3	1.51	0.90
1:B:538:LYS:H	1:B:538:LYS:HD2	1.36	0.89
1:D:314:ASP:O	1:D:318:LYS:HD3	1.72	0.88
1:B:64:LYS:HD2	1:B:65:ILE:H	1.38	0.88
1:D:264:ILE:HD11	5:D:5003:FAD:H3B	1.56	0.87
1:B:3:ALA:HB1	1:B:228:ARG:H	1.39	0.86
1:B:64:LYS:HD2	1:B:65:ILE:N	1.91	0.86
1:C:558:VAL:HG22	1:C:1241:ARG:HG2	1.59	0.85
1:B:1313:LYS:O	1:B:1317:LEU:HD23	1.77	0.84
1:B:1323:PRO:HG2	1:B:1326:CYS:HB3	1.62	0.82
1:D:741:GLU:HG3	1:D:834:MET:HG2	1.62	0.82
1:D:380:ARG:HH11	1:D:380:ARG:HB2	1.45	0.81
1:B:461:ASN:OD1	1:B:462:ARG:HD3	1.81	0.81
1:D:649:ILE:HD12	1:D:649:ILE:H	1.45	0.80
1:A:558:VAL:HG22	1:A:1241:ARG:HG2	1.64	0.79
1:D:671:VAL:HG11	1:D:682:ALA:HB3	1.63	0.79
1:A:309:GLU:O	1:A:313:VAL:HG12	1.82	0.79
1:C:133:GLU:HG2	1:C:165:ARG:HB2	1.64	0.79
1:C:736:TYR:CE2	1:C:1332:ARG:HD2	2.19	0.78
1:C:556:ALA:HB3	1:C:1239:GLU:HG2	1.65	0.78
1:D:154:ARG:HD3	1:D:1197:GLU:OE2	1.83	0.78
1:D:646:ILE:HD11	1:D:651:ASN:ND2	1.98	0.78
1:B:538:LYS:HD2	1:B:538:LYS:N	1.99	0.78
1:B:480:GLU:CD	1:B:480:GLU:H	1.85	0.78
1:C:667:ILE:HD12	1:C:808:VAL:HG22	1.65	0.78
1:B:193:PRO:HG2	1:B:561:PHE:CE2	2.20	0.77
1:D:125:TYR:OH	1:D:209:GLU:HG3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLU:HG3	1:C:218:ARG:HH22	1.51	0.75
1:D:424:ALA:HB1	1:D:430:ASP:OD2	1.87	0.75
1:A:741:GLU:HG3	1:A:834:MET:HG2	1.68	0.74
1:A:956:PHE:HA	1:A:1146:ASN:HD21	1.51	0.74
1:D:646:ILE:HD11	1:D:651:ASN:CG	2.06	0.74
1:A:376:SER:HB3	1:A:379:THR:OG1	1.87	0.74
1:D:649:ILE:HD12	1:D:649:ILE:N	2.03	0.74
1:D:506:ASP:OD1	1:D:1320:THR:HG22	1.87	0.74
1:C:748:HIS:CD2	1:C:837:THR:HG21	2.23	0.74
1:C:987:LYS:O	1:C:991:GLU:HG3	1.88	0.73
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.71	0.73
1:C:374:LEU:HD13	1:C:398:LEU:HD13	1.71	0.73
1:D:372:LEU:HD11	1:D:385:MET:HE2	1.71	0.73
1:C:1115:GLU:O	1:C:1119:THR:HG23	1.88	0.72
1:C:125:TYR:OH	1:C:209:GLU:HG3	1.90	0.72
1:C:374:LEU:HD22	1:C:398:LEU:HD11	1.72	0.72
1:B:374:LEU:HD22	1:B:398:LEU:HD21	1.71	0.72
1:D:736:TYR:CE2	1:D:1332:ARG:HD2	2.24	0.72
1:C:477:LEU:HD23	1:C:479:LYS:HE3	1.71	0.71
1:A:1204:LEU:HD13	1:A:1271:ILE:HD12	1.70	0.71
1:B:241:THR:OG1	1:B:244:GLU:HG3	1.91	0.71
1:C:433:LYS:HE2	1:C:504:MET:SD	2.30	0.71
1:D:1036:GLY:HA3	1:D:1043:LEU:HD21	1.72	0.71
1:D:867:ASN:ND2	1:D:1333:VAL:HG13	2.06	0.71
1:D:310:LYS:HE2	1:D:310:LYS:HA	1.71	0.71
1:D:374:LEU:HD13	1:D:398:LEU:HD22	1.72	0.71
1:B:1115:GLU:O	1:B:1119:THR:HG23	1.90	0.70
1:C:981:ARG:NH1	1:C:1176:ARG:HD3	2.06	0.70
1:B:215:GLU:HA	1:B:218:ARG:NH1	2.06	0.70
1:A:97:ARG:NH1	1:A:97:ARG:HB2	2.07	0.70
1:B:953:LEU:HD23	1:B:959:LYS:HA	1.73	0.70
1:C:97:ARG:HB2	1:C:97:ARG:NH1	2.07	0.70
1:D:164:ALA:C	1:D:166:ASP:H	1.95	0.70
1:D:623:THR:O	1:D:623:THR:HG22	1.92	0.69
1:B:649:ILE:HD11	1:B:804:THR:HG21	1.75	0.69
1:B:765:VAL:O	1:B:792:VAL:HG22	1.93	0.69
1:D:312:LEU:O	1:D:316:VAL:HG23	1.92	0.69
1:B:125:TYR:OH	1:B:209:GLU:HG3	1.93	0.69
6:C:4004:MTE:C9	6:C:4004:MTE:C6	2.69	0.68
1:D:559:GLN:HB3	1:D:1193:ILE:HD13	1.76	0.68
1:B:753:VAL:HG13	1:B:762:GLU:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:PRO:HG2	1:D:561:PHE:CE2	2.28	0.68
1:C:765:VAL:O	1:C:792:VAL:HG22	1.93	0.68
1:B:956:PHE:HA	1:B:1146:ASN:HD21	1.58	0.68
1:B:736:TYR:CD2	1:B:1332:ARG:HD2	2.28	0.68
1:C:1250:ASN:O	1:C:1256:ALA:HA	1.94	0.68
1:A:154:ARG:HD3	1:A:1197:GLU:OE2	1.93	0.68
1:D:1320:THR:HG23	1:D:1321:GLY:N	2.05	0.67
1:A:1135:ARG:HD3	1:B:1125:THR:OG1	1.94	0.67
1:B:3:ALA:HA	1:B:227:LEU:HD22	1.77	0.67
6:A:2004:MTE:C9	6:A:2004:MTE:C6	2.73	0.67
1:C:215:GLU:HG3	1:C:218:ARG:NH2	2.08	0.67
1:C:322:GLN:HA	1:C:322:GLN:HE21	1.60	0.67
1:D:1141:TYR:HB2	1:D:1150:PRO:HG3	1.76	0.67
1:D:956:PHE:HA	1:D:1146:ASN:HD21	1.59	0.67
1:A:103:GLU:OE2	1:A:202:THR:HG23	1.95	0.67
1:A:351:ASN:ND2	1:A:361:LEU:HB2	2.11	0.67
1:B:552:LYS:O	1:B:553:ASP:HB2	1.95	0.67
1:B:623:THR:HG22	1:B:623:THR:O	1.94	0.66
1:C:741:GLU:HG3	1:C:834:MET:HG2	1.77	0.66
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.77	0.66
1:B:656:PHE:HE2	1:B:815:LEU:HD23	1.60	0.66
1:D:1204:LEU:HD13	1:D:1271:ILE:HD12	1.78	0.66
1:C:164:ALA:C	1:C:166:ASP:H	1.99	0.66
1:C:993:CYS:HA	1:C:1285:GLN:HE22	1.60	0.66
1:B:472:ARG:HD2	1:B:485:ASP:OD1	1.95	0.66
1:A:604:LEU:HD21	1:A:822:ARG:NH2	2.10	0.66
1:B:1089:GLN:HG2	1:B:1134:TYR:CD1	2.31	0.65
1:A:748:HIS:CD2	1:A:837:THR:HG21	2.31	0.65
1:C:1320:THR:HG23	1:C:1321:GLY:H	1.61	0.65
1:B:309:GLU:O	1:B:313:VAL:HG13	1.96	0.65
1:B:748:HIS:CD2	1:B:837:THR:HG21	2.31	0.65
1:C:881:ARG:HD2	1:C:915:PHE:HB3	1.77	0.65
1:D:578:LEU:HD12	1:D:579:PRO:HD2	1.79	0.65
1:A:400:PRO:HG2	1:A:401:GLU:OE2	1.97	0.65
1:A:473:GLN:HA	1:A:476:LYS:HD3	1.79	0.65
1:D:328:ARG:HG2	1:D:328:ARG:HH11	1.60	0.65
1:D:604:LEU:HD21	1:D:822:ARG:NH2	2.12	0.65
1:B:95:LYS:HG3	1:B:590:GLU:OE2	1.97	0.64
1:D:32:ARG:HG3	1:D:32:ARG:HH11	1.62	0.64
1:D:446:THR:HB	1:D:535:LYS:NZ	2.12	0.64
1:D:944:ARG:O	1:D:947:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:CD	1:B:65:ILE:H	2.08	0.64
1:B:255:ALA:HB2	1:B:277:MET:HG2	1.79	0.64
1:A:3:ALA:CB	1:A:228:ARG:H	2.06	0.64
1:A:1135:ARG:HH12	1:A:1137:PRO:HB3	1.63	0.64
1:B:531:ASN:O	1:B:532:LEU:HD12	1.97	0.64
1:D:1174:ASN:O	1:D:1237:PRO:HA	1.97	0.64
1:A:64:LYS:HE2	1:A:65:ILE:H	1.62	0.64
1:D:649:ILE:H	1:D:649:ILE:CD1	2.11	0.64
1:B:218:ARG:CB	1:B:218:ARG:HH11	2.11	0.64
1:B:1141:TYR:CB	1:B:1150:PRO:HG3	2.26	0.64
1:C:933:VAL:HG11	1:C:1280:ARG:HH21	1.63	0.64
1:D:193:PRO:HG2	1:D:561:PHE:CZ	2.33	0.64
1:D:241:THR:OG1	1:D:244:GLU:HG3	1.97	0.63
1:C:1287:THR:HG22	1:C:1288:GLY:N	2.09	0.63
1:D:1115:GLU:O	1:D:1119:THR:HG22	1.98	0.63
1:C:667:ILE:HD12	1:C:808:VAL:CG2	2.28	0.63
1:B:389:PHE:HA	1:B:397:LEU:HG	1.80	0.63
1:C:389:PHE:HA	1:C:397:LEU:HG	1.81	0.63
1:A:987:LYS:O	1:A:991:GLU:HG3	1.99	0.63
1:C:1293:GLU:HG2	1:C:1294:LEU:N	2.14	0.62
1:D:748:HIS:CD2	1:D:837:THR:HG21	2.34	0.62
1:A:1008:ILE:O	1:A:1009:SER:HB2	1.98	0.62
1:A:131:GLN:HE21	1:A:133:GLU:H	1.48	0.62
1:D:607:ARG:NH1	1:D:679:THR:OG1	2.32	0.62
1:A:125:TYR:OH	1:A:209:GLU:HG3	2.00	0.62
1:A:1089:GLN:HG2	1:A:1134:TYR:CD1	2.35	0.62
1:C:1011:THR:O	1:C:1013:PRO:HD3	1.99	0.62
1:A:722:LYS:O	1:A:726:GLU:HG3	1.99	0.62
7:D:5005:MOM:OM2	7:D:5005:MOM:MO1	1.71	0.62
1:C:103:GLU:OE2	1:C:202:THR:HG23	2.00	0.62
1:C:933:VAL:HG11	1:C:1280:ARG:NH2	2.15	0.62
1:A:981:ARG:HH11	1:A:981:ARG:HB3	1.64	0.62
1:B:1216:PRO:HG2	1:B:1327:LYS:CD	2.29	0.61
1:B:949:LYS:HG2	1:B:952:ASP:OD2	2.00	0.61
1:C:958:GLN:OE1	1:C:1150:PRO:HD2	2.01	0.61
1:D:303:CYS:SG	1:D:307:ILE:HD11	2.40	0.61
1:C:1313:LYS:O	1:C:1317:LEU:HD23	2.01	0.61
7:C:4005:MOM:OM2	7:C:4005:MOM:MO1	1.72	0.61
1:A:1313:LYS:O	1:A:1317:LEU:HD23	2.01	0.61
7:A:2005:MOM:OM2	7:A:2005:MOM:MO1	1.72	0.61
1:A:1280:ARG:HG2	1:A:1280:ARG:HH11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:754:PRO:HD3	1:D:817:ALA:HB1	1.83	0.61
1:A:443:LYS:HG3	1:A:448:GLU:HG3	1.82	0.61
1:D:131:GLN:HE21	1:D:133:GLU:H	1.49	0.61
1:A:528:GLY:HA2	1:A:533:GLU:HB3	1.82	0.61
1:B:722:LYS:O	1:B:726:GLU:HG3	2.01	0.61
1:D:971:GLU:HG2	9:D:7225:HOH:O	2.00	0.61
1:C:868:VAL:HB	1:C:875:SER:OG	2.01	0.60
1:A:735:ILE:HD12	1:A:735:ILE:O	2.01	0.60
7:A:2005:MOM:MO1	7:A:2005:MOM:OM3	1.72	0.60
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.82	0.60
1:C:753:VAL:CG2	1:C:762:GLU:HB3	2.31	0.60
7:C:4005:MOM:MO1	7:C:4005:MOM:OM3	1.72	0.60
1:D:982:LYS:HG2	1:D:999:LEU:HD23	1.83	0.60
7:B:3005:MOM:OM2	7:B:3005:MOM:MO1	1.72	0.60
1:C:623:THR:O	1:C:627:LYS:HG3	2.01	0.60
1:D:1324:GLU:O	1:D:1325:ASN:HB2	2.02	0.60
7:D:5005:MOM:MO1	7:D:5005:MOM:OM3	1.72	0.60
1:A:304:PRO:HD2	1:A:307:ILE:HD12	1.83	0.60
1:C:638:ALA:O	1:C:641:VAL:HG22	2.02	0.60
1:A:1332:ARG:HG2	1:A:1332:ARG:HH11	1.67	0.60
1:D:372:LEU:HD11	1:D:385:MET:CE	2.32	0.60
1:D:671:VAL:HG11	1:D:682:ALA:CB	2.30	0.60
1:C:310:LYS:HE2	1:C:310:LYS:HA	1.84	0.59
7:B:3005:MOM:MO1	7:B:3005:MOM:OM3	1.73	0.59
1:A:562:GLN:HG3	1:A:1246:ARG:CZ	2.32	0.59
1:A:1100:LYS:HE3	1:A:1100:LYS:O	2.01	0.59
1:A:3:ALA:HB1	1:A:228:ARG:N	2.10	0.59
1:A:30:LEU:HD23	1:A:34:LEU:HD12	1.84	0.59
1:A:322:GLN:O	1:A:412:SER:HB3	2.02	0.59
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.67	0.59
1:D:566:LYS:HD3	1:D:567:GLY:N	2.17	0.59
1:C:131:GLN:HE21	1:C:133:GLU:N	1.95	0.59
1:C:1008:ILE:O	1:C:1009:SER:HB2	2.01	0.59
1:A:720:LEU:HD11	1:A:896:ARG:CB	2.33	0.59
1:B:259:VAL:HG11	1:B:347:SER:HB3	1.84	0.59
1:B:649:ILE:HD11	1:B:804:THR:CG2	2.31	0.59
1:C:1141:TYR:HB2	1:C:1150:PRO:HG3	1.83	0.59
1:A:389:PHE:HA	1:A:397:LEU:HG	1.85	0.59
1:A:613:ARG:HH11	1:A:692:GLU:HG3	1.66	0.59
1:A:638:ALA:O	1:A:641:VAL:HG22	2.02	0.59
1:D:242:LEU:HA	1:D:284:ILE:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ARG:NH1	1:A:692:GLU:HG3	2.18	0.59
1:C:1043:LEU:O	1:C:1047:MET:HG2	2.03	0.59
1:A:197:LYS:HD2	1:A:200:GLU:OE2	2.03	0.58
1:B:267:GLU:HA	1:B:271:LYS:HG2	1.83	0.58
1:C:400:PRO:HG2	1:C:401:GLU:OE2	2.03	0.58
1:C:1089:GLN:HG2	1:C:1134:TYR:CD1	2.38	0.58
1:C:1280:ARG:NH2	1:C:1293:GLU:O	2.36	0.58
1:D:471:GLN:NE2	1:D:474:LEU:HD11	2.18	0.58
1:A:881:ARG:HD2	1:A:915:PHE:HB3	1.86	0.58
1:B:131:GLN:HE21	1:B:133:GLU:H	1.51	0.58
1:D:656:PHE:HE2	1:D:815:LEU:HD23	1.66	0.58
1:D:860:LEU:HD12	1:D:861:GLU:H	1.68	0.58
1:B:558:VAL:CG2	1:B:1241:ARG:HG2	2.30	0.58
1:D:1324:GLU:CD	1:D:1325:ASN:H	2.06	0.58
1:C:407:ILE:N	1:C:407:ILE:HD12	2.19	0.58
1:A:443:LYS:HG3	1:A:448:GLU:CG	2.33	0.58
1:D:215:GLU:O	1:D:219:LEU:HG	2.03	0.58
1:D:418:PHE:CD1	1:D:439:ARG:HB2	2.38	0.58
1:A:1011:THR:O	1:A:1013:PRO:HD3	2.04	0.58
1:B:562:GLN:HG3	1:B:1246:ARG:HG2	1.86	0.58
1:C:965:LEU:HB3	1:C:966:PRO:HD3	1.85	0.58
1:D:1250:ASN:O	1:D:1256:ALA:HA	2.04	0.58
1:C:1332:ARG:HG2	1:C:1332:ARG:HH11	1.69	0.58
1:D:351:ASN:ND2	1:D:361:LEU:HB2	2.19	0.58
1:A:245:LEU:HD11	1:A:257:LEU:HD11	1.86	0.58
1:B:304:PRO:HA	1:B:346:ALA:O	2.02	0.58
1:B:1034:HIS:HB2	1:B:1087:ASN:HD22	1.69	0.58
1:C:1153:TYR:CE1	1:C:1258:LYS:HG2	2.39	0.58
1:D:1286:HIS:O	1:D:1287:THR:HG23	2.03	0.58
1:B:880:GLU:HG2	1:B:1143:PHE:CZ	2.39	0.58
1:C:1222:THR:HG22	1:C:1228:TYR:HB2	1.86	0.58
1:D:641:VAL:HG21	1:D:645:ASN:HB2	1.85	0.57
1:A:786:ASN:ND2	1:B:1029:SER:HB2	2.19	0.57
1:B:559:GLN:HB3	1:B:1193:ILE:HD13	1.86	0.57
1:B:649:ILE:CD1	1:B:804:THR:HG21	2.34	0.57
1:D:868:VAL:HG13	1:D:902:CYS:O	2.04	0.57
1:B:1287:THR:HG22	1:B:1288:GLY:N	2.19	0.57
1:D:510:THR:HG21	1:D:1315:THR:HG22	1.86	0.57
1:B:374:LEU:HD22	1:B:398:LEU:CD2	2.35	0.57
1:B:372:LEU:HD11	1:B:385:MET:CE	2.35	0.57
1:C:713:LEU:HD21	1:C:876:GLN:HE21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLY:O	1:B:1236:ILE:HG21	2.05	0.57
1:A:645:ASN:O	1:A:654:THR:HA	2.05	0.57
1:B:996:LYS:NZ	1:B:1285:GLN:HE22	2.03	0.57
1:A:215:GLU:HG3	1:A:218:ARG:HH22	1.70	0.56
1:A:1280:ARG:NH2	1:A:1293:GLU:O	2.32	0.56
1:B:375:VAL:HG12	1:B:380:ARG:HG3	1.86	0.56
1:A:606:LEU:C	1:A:606:LEU:HD23	2.26	0.56
1:A:720:LEU:HD11	1:A:896:ARG:HB3	1.87	0.56
1:D:553:ASP:HB3	1:D:554:PRO:HD2	1.85	0.56
1:A:367:ALA:O	1:A:439:ARG:HD3	2.05	0.56
1:B:743:PHE:HA	1:B:830:ARG:HH21	1.70	0.56
1:C:504:MET:HG2	1:C:1304:GLU:OE2	2.04	0.56
1:A:479:LYS:HG2	1:A:537:GLY:N	2.21	0.56
1:C:32:ARG:HD2	9:C:7058:HOH:O	2.04	0.56
1:C:328:ARG:HH11	1:C:328:ARG:HG2	1.70	0.56
1:C:735:ILE:HD12	1:C:735:ILE:O	2.06	0.56
1:C:131:GLN:NE2	1:C:133:GLU:H	1.95	0.56
1:D:881:ARG:HD2	1:D:915:PHE:HB3	1.86	0.56
1:B:1174:ASN:O	1:B:1237:PRO:HA	2.06	0.56
1:C:662:THR:O	1:C:663:CYS:HB3	2.05	0.56
1:A:650:CYS:HB2	1:A:652:ASP:OD2	2.05	0.56
1:B:809:VAL:O	1:B:813:VAL:HG23	2.05	0.56
1:B:1216:PRO:HG2	1:B:1327:LYS:HD2	1.88	0.56
1:A:505:VAL:HG21	1:A:1320:THR:HG21	1.86	0.56
1:B:215:GLU:HA	1:B:218:ARG:HH11	1.69	0.56
1:B:1216:PRO:HG2	1:B:1327:LYS:HD3	1.88	0.56
1:C:193:PRO:HG2	1:C:561:PHE:CE2	2.41	0.56
1:A:510:THR:HG21	1:A:1315:THR:HG22	1.86	0.56
1:A:622:ASP:HB3	1:A:687:LYS:HB3	1.87	0.56
1:C:1291:VAL:HG13	1:C:1292:LYS:HG3	1.88	0.56
1:B:218:ARG:HH11	1:B:218:ARG:HB3	1.70	0.55
1:B:218:ARG:NH1	1:B:218:ARG:HB2	2.22	0.55
1:B:720:LEU:HD11	1:B:896:ARG:HB3	1.89	0.55
1:C:217:LEU:O	1:C:220:LYS:HG2	2.07	0.55
1:A:374:LEU:HD13	1:A:398:LEU:CD2	2.37	0.55
1:B:1332:ARG:HG2	1:B:1332:ARG:HH11	1.71	0.55
1:A:477:LEU:HD23	1:A:479:LYS:HE2	1.87	0.55
1:A:667:ILE:HD12	1:A:808:VAL:HG13	1.89	0.55
1:A:712:GLU:N	1:A:900:ARG:HH11	2.04	0.55
1:C:372:LEU:CD2	1:C:407:ILE:HG23	2.36	0.55
1:C:1127:SER:HB2	1:D:1133:PHE:CG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:THR:HG23	1:D:626:ALA:HB3	1.88	0.55
1:A:124:MET:HE3	1:A:127:LEU:HD23	1.89	0.55
1:B:1204:LEU:HD12	1:B:1204:LEU:O	2.06	0.55
1:C:1008:ILE:O	1:C:1009:SER:CB	2.55	0.55
1:D:498:PRO:HG2	1:D:1323:PRO:CD	2.37	0.55
1:D:880:GLU:HG2	1:D:1143:PHE:CZ	2.41	0.55
1:A:507:PHE:HB2	1:A:1304:GLU:HG3	1.89	0.55
1:C:744:TYR:O	1:C:830:ARG:NH2	2.31	0.55
1:C:558:VAL:CG2	1:C:1241:ARG:HG2	2.34	0.55
1:B:799:PHE:HA	6:B:3004:MTE:S1'	2.48	0.54
1:C:281:PRO:HB2	1:C:287:LEU:CD1	2.37	0.54
1:A:1199:ALA:HB3	1:A:1264:PRO:HB2	1.89	0.54
1:B:603:GLU:HG3	1:B:823:PRO:HB2	1.88	0.54
1:D:196:PHE:CE2	1:D:198:PRO:HG3	2.42	0.54
1:D:1290:ASN:ND2	1:D:1292:LYS:H	2.05	0.54
1:A:473:GLN:HA	1:A:476:LYS:CD	2.36	0.54
1:A:656:PHE:HE2	1:A:815:LEU:HD23	1.71	0.54
1:D:535:LYS:O	1:D:535:LYS:HG2	2.07	0.54
1:A:133:GLU:CG	1:A:165:ARG:HB3	2.25	0.54
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.72	0.54
1:C:709:TYR:CZ	1:C:903:LYS:HG3	2.43	0.54
1:B:322:GLN:HA	1:B:322:GLN:OE1	2.07	0.54
1:B:538:LYS:H	1:B:538:LYS:CD	2.16	0.54
1:C:3:ALA:HB2	1:C:225:LYS:NZ	2.23	0.54
1:C:667:ILE:CD1	1:C:808:VAL:HG22	2.36	0.54
1:C:1217:GLU:CD	1:C:1217:GLU:H	2.10	0.54
1:D:95:LYS:HG3	1:D:590:GLU:OE2	2.07	0.54
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.08	0.54
1:A:249:LYS:HD3	1:A:257:LEU:HD21	1.88	0.54
1:C:940:GLU:HG2	1:C:941:GLU:N	2.22	0.54
1:A:550:PHE:CE2	1:A:552:LYS:HD2	2.42	0.53
1:B:714:LYS:HD2	1:B:896:ARG:NH1	2.23	0.53
1:C:473:GLN:NE2	1:C:482:LEU:HG	2.23	0.53
1:C:891:LYS:HD2	1:C:952:ASP:OD2	2.09	0.53
1:D:940:GLU:HG2	1:D:941:GLU:N	2.22	0.53
1:B:996:LYS:NZ	1:B:1285:GLN:NE2	2.56	0.53
1:B:1109:ASN:ND2	1:B:1112:GLY:HA3	2.23	0.53
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.08	0.53
1:A:150:CYS:HB3	6:A:2004:MTE:N2	2.24	0.53
1:D:758:ALA:HB1	1:D:787:ARG:HE	1.72	0.53
1:D:1324:GLU:CD	1:D:1325:ASN:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:ALA:HA	1:A:693:LEU:HG	1.90	0.53
1:A:958:GLN:OE1	1:A:1150:PRO:HD2	2.08	0.53
1:B:196:PHE:CE2	1:B:198:PRO:HG3	2.43	0.53
1:D:444:PRO:O	1:D:446:THR:HG23	2.08	0.53
1:A:742:HIS:HA	1:A:912:PHE:CE2	2.44	0.53
1:B:578:LEU:HD12	1:B:579:PRO:HD2	1.89	0.53
1:B:888:ASN:O	1:B:1005:LYS:HE2	2.07	0.53
1:C:322:GLN:HA	1:C:322:GLN:NE2	2.21	0.53
1:D:1263:PRO:HB2	1:D:1264:PRO:HD3	1.90	0.53
1:A:212:PHE:CE2	1:A:217:LEU:HD13	2.44	0.53
1:A:910:THR:OG1	1:A:911:ALA:N	2.42	0.53
1:B:910:THR:OG1	1:B:911:ALA:N	2.41	0.53
1:C:245:LEU:HD22	1:C:281:PRO:HB3	1.90	0.53
1:B:753:VAL:CG1	1:B:762:GLU:HB3	2.37	0.53
1:C:441:LEU:HB3	1:C:451:GLU:HB2	1.90	0.53
1:D:517:PHE:CZ	1:D:521:LEU:HD11	2.43	0.53
1:B:881:ARG:HD2	1:B:915:PHE:O	2.09	0.53
1:D:1008:ILE:O	1:D:1009:SER:CB	2.56	0.53
1:A:124:MET:CE	1:A:127:LEU:HD23	2.38	0.53
1:A:242:LEU:HA	1:A:284:ILE:HD13	1.90	0.53
1:A:253:PRO:HB3	1:A:400:PRO:HB2	1.91	0.53
1:C:164:ALA:C	1:C:166:ASP:N	2.59	0.53
1:C:805:ARG:O	1:C:808:VAL:HG12	2.07	0.53
1:A:787:ARG:HG2	1:A:787:ARG:HH11	1.75	0.52
1:C:1332:ARG:HG2	1:C:1332:ARG:NH1	2.23	0.52
1:A:438:MET:HG2	1:A:454:LEU:HD22	1.90	0.52
1:A:1008:ILE:O	1:A:1009:SER:CB	2.57	0.52
1:A:1135:ARG:O	1:A:1135:ARG:HG3	2.09	0.52
1:B:754:PRO:HD3	1:B:817:ALA:HB1	1.92	0.52
1:B:996:LYS:HZ1	1:B:1285:GLN:NE2	2.07	0.52
1:C:192:SER:N	1:C:193:PRO:CD	2.71	0.52
1:D:65:ILE:HD11	1:D:217:LEU:HD11	1.92	0.52
1:D:881:ARG:HD2	1:D:915:PHE:O	2.09	0.52
1:A:364:VAL:HG13	1:A:418:PHE:CZ	2.45	0.52
1:C:120:ILE:HD13	1:C:146:ASN:HB3	1.91	0.52
1:A:220:LYS:HE2	1:A:221:ASP:OD1	2.09	0.52
1:B:800:GLY:HA2	1:B:803:VAL:HG23	1.91	0.52
1:A:462:ARG:HB3	9:A:7121:HOH:O	2.09	0.52
1:C:389:PHE:O	1:C:391:PRO:HD3	2.09	0.52
1:D:1332:ARG:HG2	1:D:1332:ARG:HH11	1.74	0.52
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:VAL:HG23	1:B:506:ASP:N	2.23	0.52
1:D:949:LYS:HG2	1:D:952:ASP:OD2	2.09	0.52
1:D:1300:PRO:HG2	1:D:1302:THR:HG23	1.90	0.52
1:B:422:LYS:HE3	1:B:432:ALA:HB2	1.92	0.52
1:C:375:VAL:HG12	1:C:380:ARG:HG3	1.92	0.52
1:A:881:ARG:HD2	1:A:915:PHE:O	2.10	0.52
1:A:1089:GLN:HG2	1:A:1134:TYR:CE1	2.45	0.52
1:B:154:ARG:HD3	1:B:1197:GLU:OE2	2.10	0.52
1:B:218:ARG:NH1	1:B:218:ARG:CB	2.72	0.52
1:B:743:PHE:HA	1:B:830:ARG:NH2	2.24	0.52
1:B:857:VAL:CG2	1:B:892:ILE:HG12	2.40	0.52
1:C:607:ARG:NH2	1:C:829:ASP:OD2	2.43	0.52
1:C:713:LEU:HD21	1:C:876:GLN:NE2	2.24	0.52
1:D:467:LEU:O	1:D:471:GLN:HB2	2.10	0.52
1:D:1038:GLU:HB2	1:D:1044:HIS:CD2	2.44	0.52
1:D:1208:THR:O	1:D:1209:LEU:HD12	2.09	0.52
1:C:322:GLN:HG2	1:C:414:GLU:CD	2.31	0.51
1:C:606:LEU:HD23	1:C:606:LEU:C	2.31	0.51
1:B:389:PHE:O	1:B:391:PRO:HD3	2.10	0.51
1:C:303:CYS:HB3	1:C:307:ILE:HD11	1.92	0.51
1:C:736:TYR:CZ	1:C:1332:ARG:HD2	2.45	0.51
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.11	0.51
1:C:517:PHE:CZ	1:C:521:LEU:HD11	2.45	0.51
1:A:1260:VAL:O	1:A:1260:VAL:HG22	2.10	0.51
1:D:443:LYS:HD2	1:D:450:GLN:NE2	2.24	0.51
1:D:633:VAL:HB	1:D:672:VAL:O	2.11	0.51
1:B:720:LEU:HD11	1:B:896:ARG:CB	2.41	0.51
1:A:117:THR:CG2	1:A:587:ALA:HA	2.40	0.51
1:D:32:ARG:HG3	1:D:32:ARG:NH1	2.24	0.51
1:A:531:ASN:HA	1:A:533:GLU:OE1	2.11	0.51
1:B:1179:ILE:HD11	1:B:1200:PHE:CD1	2.46	0.51
1:C:224:ARG:HG2	1:C:224:ARG:HH11	1.75	0.51
1:C:646:ILE:HG13	1:C:646:ILE:O	2.10	0.51
1:A:88:VAL:HG13	1:A:89:GLU:N	2.26	0.51
1:A:981:ARG:HB3	1:A:981:ARG:NH1	2.26	0.51
1:A:233:ARG:CZ	1:A:681:ARG:HD3	2.41	0.51
1:A:389:PHE:HA	1:A:397:LEU:CD1	2.41	0.51
1:B:608:LEU:HD13	1:B:667:ILE:CD1	2.40	0.51
1:C:490:LEU:HB2	1:C:513:LEU:HD22	1.93	0.51
1:C:510:THR:HG21	1:C:1315:THR:HG22	1.92	0.51
1:A:965:LEU:N	1:A:966:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:GLU:HB2	1:B:1044:HIS:CD2	2.46	0.51
1:C:787:ARG:HG2	1:C:787:ARG:HH11	1.76	0.51
1:C:956:PHE:CA	1:C:1146:ASN:HD21	2.15	0.51
1:C:1320:THR:HG23	1:C:1321:GLY:N	2.26	0.51
1:D:136:MET:HE3	1:D:167:GLY:HA2	1.92	0.51
1:A:653:GLU:HB3	1:A:871:THR:CG2	2.41	0.50
1:A:750:THR:HG21	1:A:810:SER:HA	1.93	0.50
1:A:953:LEU:HA	1:A:958:GLN:O	2.11	0.50
1:A:1038:GLU:HB2	1:A:1044:HIS:CD2	2.46	0.50
1:B:1022:LEU:HD22	1:B:1098:ILE:HG13	1.93	0.50
1:A:553:ASP:HB3	1:A:554:PRO:HD2	1.93	0.50
1:D:556:ALA:HB3	1:D:1239:GLU:HG2	1.93	0.50
1:D:1081:SER:OG	1:D:1262:GLU:HG3	2.11	0.50
1:D:1332:ARG:HG2	1:D:1332:ARG:NH1	2.26	0.50
1:A:1280:ARG:HH11	1:A:1280:ARG:CG	2.24	0.50
1:B:374:LEU:CD2	1:B:398:LEU:HD21	2.41	0.50
1:D:1021:LEU:HD13	1:D:1131:THR:HG22	1.93	0.50
1:B:915:PHE:HA	2:B:6002:BCT:O3	2.12	0.50
1:C:753:VAL:HG23	1:C:753:VAL:O	2.12	0.50
1:D:400:PRO:HG2	1:D:401:GLU:OE2	2.11	0.50
1:A:491:ALA:O	1:A:495:HIS:HB2	2.11	0.50
1:B:607:ARG:HH11	1:B:680:GLN:N	2.09	0.50
1:C:531:ASN:HA	1:C:533:GLU:OE1	2.11	0.50
1:C:699:ILE:O	1:C:703:ILE:HG13	2.11	0.50
1:D:716:GLU:HB2	1:D:896:ARG:HG3	1.93	0.50
1:D:1320:THR:CG2	1:D:1321:GLY:H	2.09	0.50
1:A:696:ILE:HG23	1:A:701:ASP:CB	2.41	0.50
1:A:867:ASN:ND2	1:A:1333:VAL:HG13	2.26	0.50
1:A:1084:ALA:HB3	9:A:7178:HOH:O	2.11	0.50
1:C:562:GLN:HG3	1:C:1246:ARG:CZ	2.42	0.50
1:A:736:TYR:CD2	1:A:1332:ARG:HD2	2.46	0.50
1:B:104:ARG:HD3	1:B:201:PHE:CD2	2.47	0.50
1:B:881:ARG:HD2	1:B:915:PHE:HB3	1.93	0.50
1:B:932:ALA:HA	1:B:942:VAL:HG21	1.93	0.50
1:C:323:LYS:HA	1:C:412:SER:O	2.12	0.50
1:A:65:ILE:HD12	1:A:212:PHE:CD2	2.46	0.50
1:A:1141:TYR:OH	1:A:1146:ASN:ND2	2.45	0.50
1:B:3:ALA:O	1:B:5:LYS:N	2.41	0.50
1:D:58:TYR:OH	1:D:63:ASN:ND2	2.45	0.50
1:B:1271:ILE:O	1:B:1275:ILE:HG13	2.12	0.50
1:A:399:SER:HB2	1:A:400:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:SER:OG	1:A:402:GLU:HG3	2.11	0.49
1:A:212:PHE:HE2	1:A:217:LEU:HD13	1.75	0.49
1:B:958:GLN:OE1	1:B:1150:PRO:HD2	2.12	0.49
1:B:986:ASP:O	1:B:990:LYS:HG3	2.12	0.49
1:C:264:ILE:HD11	5:C:4003:FAD:H3B	1.92	0.49
1:D:380:ARG:HH11	1:D:380:ARG:CB	2.22	0.49
1:D:640:ASP:HB3	1:D:819:LYS:HE3	1.93	0.49
1:A:131:GLN:O	1:A:134:PRO:HD3	2.12	0.49
1:A:572:ASP:OD1	1:A:1053:ARG:HD3	2.12	0.49
1:B:325:GLU:HB2	1:B:412:SER:OG	2.11	0.49
1:B:374:LEU:HD13	1:B:398:LEU:CD2	2.41	0.49
1:B:623:THR:HG22	1:B:627:LYS:HG3	1.95	0.49
1:A:1073:PRO:HD3	1:B:1023:HIS:CE1	2.47	0.49
1:B:530:GLU:O	1:B:531:ASN:HB2	2.12	0.49
1:B:958:GLN:HG3	1:B:1149:ASN:OD1	2.12	0.49
1:B:1184:GLY:HA2	1:B:1248:CYS:O	2.13	0.49
1:C:322:GLN:HG2	1:C:414:GLU:OE1	2.12	0.49
1:D:224:ARG:HD3	1:D:283:TRP:CE3	2.47	0.49
1:D:1008:ILE:O	1:D:1009:SER:HB2	2.11	0.49
1:D:1324:GLU:OE2	1:D:1325:ASN:N	2.45	0.49
1:A:1033:THR:CG2	1:A:1066:GLU:O	2.60	0.49
1:A:1050:VAL:HG13	1:A:1255:TYR:HE2	1.78	0.49
1:B:117:THR:HB	1:B:118:PRO:HD3	1.94	0.49
1:B:1083:SER:HB2	6:B:3004:MTE:O3P	2.13	0.49
1:B:1152:HIS:CE1	1:B:1252:LYS:HD2	2.47	0.49
1:C:430:ASP:CG	1:C:1229:LYS:HE2	2.32	0.49
1:C:742:HIS:HA	1:C:912:PHE:CZ	2.48	0.49
1:D:736:TYR:CZ	1:D:1332:ARG:HD2	2.47	0.49
1:A:696:ILE:HG23	1:A:701:ASP:HB3	1.94	0.49
1:B:372:LEU:HD11	1:B:385:MET:HE2	1.93	0.49
1:D:1001:ILE:HG23	1:D:1001:ILE:O	2.12	0.49
1:A:712:GLU:N	1:A:900:ARG:NH1	2.60	0.49
1:B:374:LEU:HD13	1:B:398:LEU:HD23	1.93	0.49
1:B:602:ASN:ND2	1:B:823:PRO:HD2	2.27	0.49
1:D:376:SER:O	1:D:377:ARG:C	2.50	0.49
1:D:910:THR:OG1	1:D:911:ALA:N	2.43	0.49
1:B:5:LYS:HE3	1:B:16:VAL:HG13	1.93	0.49
1:B:1326:CYS:O	1:B:1328:PRO:HD3	2.13	0.49
1:C:419:SER:HB2	1:C:519:PHE:CD1	2.47	0.49
1:D:1265:LEU:HD23	1:D:1265:LEU:C	2.33	0.49
1:A:473:GLN:O	1:A:476:LYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:GLN:HG3	9:A:7061:HOH:O	2.12	0.49
1:A:58:TYR:OH	1:A:63:ASN:ND2	2.45	0.49
1:C:742:HIS:CE1	1:C:839:GLY:HA2	2.48	0.49
1:D:519:PHE:O	1:D:523:VAL:HG23	2.13	0.49
1:D:1283:ARG:HH21	1:D:1293:GLU:CD	2.16	0.49
1:B:87:THR:OG1	1:B:89:GLU:HG2	2.13	0.48
1:B:193:PRO:HG2	1:B:561:PHE:CZ	2.48	0.48
1:C:1188:ASN:CG	1:C:1191:ILE:HG12	2.33	0.48
1:A:393:TYR:N	1:A:461:ASN:HD21	2.11	0.48
1:B:556:ALA:HB3	1:B:1239:GLU:HG2	1.94	0.48
1:D:742:HIS:HA	1:D:912:PHE:CZ	2.48	0.48
1:A:1174:ASN:O	1:A:1237:PRO:HA	2.14	0.48
1:A:1321:GLY:O	1:A:1322:VAL:HB	2.14	0.48
1:B:58:TYR:HE1	1:B:63:ASN:HD22	1.59	0.48
1:B:505:VAL:HG23	1:B:506:ASP:H	1.77	0.48
1:B:646:ILE:HG13	1:B:646:ILE:O	2.12	0.48
1:C:124:MET:HE3	1:C:127:LEU:HD23	1.96	0.48
1:C:351:ASN:ND2	1:C:361:LEU:HB2	2.28	0.48
1:D:748:HIS:CE1	1:D:802:LYS:HG2	2.48	0.48
1:D:965:LEU:HB3	1:D:966:PRO:HD3	1.95	0.48
1:D:1089:GLN:HG2	1:D:1134:TYR:CD1	2.47	0.48
1:A:1263:PRO:HB2	1:A:1264:PRO:HD3	1.96	0.48
1:B:40:LYS:HB3	1:B:115:PHE:CZ	2.48	0.48
1:B:1250:ASN:O	1:B:1256:ALA:HA	2.12	0.48
1:C:419:SER:HB2	1:C:519:PHE:HD1	1.79	0.48
1:C:868:VAL:O	1:C:868:VAL:HG23	2.11	0.48
1:A:131:GLN:NE2	1:A:133:GLU:H	2.11	0.48
1:A:346:ALA:HB1	5:A:2003:FAD:H4'	1.94	0.48
1:C:62:GLN:HB3	1:C:64:LYS:HG2	1.95	0.48
1:D:471:GLN:HE22	1:D:474:LEU:HD11	1.78	0.48
1:A:653:GLU:HB3	1:A:871:THR:HG21	1.95	0.48
1:B:735:ILE:H	1:B:735:ILE:HD12	1.79	0.48
1:D:743:PHE:HA	1:D:830:ARG:NH2	2.27	0.48
1:D:1331:VAL:HG22	1:D:1332:ARG:N	2.28	0.48
1:A:1033:THR:HG21	9:A:7095:HOH:O	2.13	0.48
1:C:1131:THR:HG23	1:D:1131:THR:HG23	1.94	0.48
1:C:1320:THR:OG1	1:C:1321:GLY:N	2.45	0.48
1:D:912:PHE:O	1:D:913:ARG:C	2.51	0.48
1:A:623:THR:HG22	1:A:627:LYS:HG3	1.94	0.48
1:C:338:ALA:HA	1:C:429:ASP:OD1	2.14	0.48
1:C:709:TYR:HB2	1:C:901:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1199:ALA:HB3	1:C:1264:PRO:HB2	1.96	0.48
1:C:372:LEU:HD11	1:C:385:MET:CE	2.44	0.48
1:C:389:PHE:HD1	1:C:397:LEU:HD12	1.77	0.48
1:C:1122:TYR:CD2	1:C:1123:MET:HE3	2.49	0.48
1:D:603:GLU:HA	1:D:823:PRO:HG2	1.95	0.48
1:B:736:TYR:CE2	1:B:1332:ARG:HD2	2.48	0.48
1:B:748:HIS:CE1	1:B:802:LYS:HG2	2.49	0.48
1:C:786:ASN:OD1	1:C:787:ARG:NH1	2.47	0.48
1:C:1009:SER:HA	1:C:1082:VAL:HG11	1.94	0.48
1:D:351:ASN:HB2	5:D:5003:FAD:O4'	2.14	0.48
1:C:97:ARG:HB2	1:C:97:ARG:CZ	2.43	0.47
1:C:1089:GLN:HB3	1:C:1134:TYR:CG	2.49	0.47
1:D:228:ARG:HE	1:D:230:GLU:CD	2.17	0.47
1:D:623:THR:O	1:D:623:THR:CG2	2.61	0.47
1:C:27:LEU:HD21	1:C:41:LEU:HB2	1.96	0.47
1:C:287:LEU:O	1:C:302:ALA:HB3	2.15	0.47
1:C:346:ALA:HB1	5:C:4003:FAD:H4'	1.96	0.47
1:C:606:LEU:HD23	1:C:607:ARG:N	2.29	0.47
1:D:117:THR:HB	1:D:118:PRO:HD3	1.95	0.47
1:D:646:ILE:HD12	1:D:646:ILE:C	2.34	0.47
1:D:799:PHE:HA	6:D:5004:MTE:S1'	2.54	0.47
1:D:943:ARG:HD2	9:D:7129:HOH:O	2.13	0.47
1:A:1192:ASP:O	1:A:1196:VAL:HG23	2.15	0.47
1:B:592:VAL:HG13	1:B:596:ASP:HB2	1.96	0.47
1:B:1162:GLU:HG2	1:B:1175:LEU:HD12	1.96	0.47
1:C:88:VAL:HG13	1:C:89:GLU:N	2.29	0.47
1:C:96:THR:OG1	1:C:97:ARG:N	2.44	0.47
1:C:736:TYR:CD2	1:C:1332:ARG:HD2	2.49	0.47
1:A:1288:GLY:O	1:A:1289:ASN:HB3	2.13	0.47
1:B:517:PHE:CZ	1:B:521:LEU:HD11	2.49	0.47
1:B:741:GLU:HB3	1:B:1228:TYR:CE2	2.50	0.47
1:B:786:ASN:OD1	1:B:787:ARG:NH1	2.46	0.47
1:C:571:GLU:OE2	1:C:1058:PRO:HG3	2.14	0.47
1:D:129:ARG:NE	1:D:209:GLU:HG2	2.30	0.47
1:A:363:PRO:HG2	1:A:435:THR:HG23	1.96	0.47
1:B:1119:THR:O	1:B:1123:MET:HG2	2.14	0.47
1:D:115:PHE:HD2	1:D:745:LEU:HB3	1.80	0.47
1:D:247:ASP:OD1	1:D:377:ARG:HD3	2.15	0.47
1:D:346:ALA:HB1	5:D:5003:FAD:H4'	1.96	0.47
1:A:845:ALA:CB	1:A:923:ILE:HD13	2.44	0.47
1:B:510:THR:HG21	1:B:1315:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:THR:HG23	1:B:648:GLY:N	2.29	0.47
1:B:709:TYR:CE2	1:B:868:VAL:HG22	2.49	0.47
1:B:912:PHE:O	1:B:913:ARG:C	2.52	0.47
1:C:741:GLU:OE1	1:C:743:PHE:N	2.46	0.47
1:D:3:ALA:HA	1:D:227:LEU:CD2	2.44	0.47
1:A:124:MET:HE2	1:A:128:LEU:HG	1.97	0.47
1:A:217:LEU:O	1:A:220:LYS:HG2	2.15	0.47
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.80	0.47
1:A:1033:THR:HG23	1:A:1066:GLU:O	2.14	0.47
1:B:91:ILE:O	1:B:99:HIS:HB2	2.15	0.47
1:B:535:LYS:HG2	1:B:535:LYS:O	2.15	0.47
1:B:607:ARG:NH1	1:B:680:GLN:HB2	2.30	0.47
1:B:733:GLY:HA3	1:B:847:TYR:CZ	2.50	0.47
1:B:741:GLU:HG2	1:B:834:MET:CE	2.44	0.47
1:B:930:GLU:OE2	1:B:1294:LEU:HB3	2.15	0.47
1:B:1287:THR:HG22	1:B:1288:GLY:H	1.80	0.47
1:C:253:PRO:HB3	1:C:400:PRO:HB2	1.97	0.47
1:C:1033:THR:HG23	1:C:1066:GLU:O	2.14	0.47
1:D:716:GLU:OE2	1:D:896:ARG:HD3	2.14	0.47
1:D:741:GLU:HG2	9:D:7119:HOH:O	2.14	0.47
1:A:925:GLU:OE1	1:A:943:ARG:NE	2.47	0.47
1:A:1141:TYR:HB2	1:A:1150:PRO:HG3	1.97	0.47
1:B:644:SER:OG	1:B:646:ILE:HG12	2.15	0.47
1:C:322:GLN:O	1:C:412:SER:HB3	2.15	0.47
1:C:352:ILE:CD1	1:C:407:ILE:HG12	2.44	0.47
1:D:571:GLU:CD	1:D:1058:PRO:HG3	2.35	0.47
1:A:1222:THR:HG22	1:A:1228:TYR:HB2	1.97	0.47
1:D:426:ARG:HD2	1:D:1232:ALA:HB2	1.96	0.47
1:D:1327:LYS:HD2	1:D:1328:PRO:O	2.14	0.47
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.80	0.47
1:A:714:LYS:HD2	1:A:896:ARG:NH1	2.30	0.47
1:B:668:ILE:HD13	1:B:688:ILE:HD13	1.96	0.47
1:B:1222:THR:HG22	1:B:1228:TYR:HB2	1.95	0.47
1:C:599:ARG:HH21	1:C:825:ARG:HD2	1.79	0.47
1:D:461:ASN:N	1:D:461:ASN:HD22	2.11	0.47
1:A:351:ASN:HD22	1:A:361:LEU:HB2	1.79	0.46
1:B:735:ILE:HD12	1:B:735:ILE:N	2.29	0.46
1:C:3:ALA:HA	1:C:227:LEU:HD22	1.96	0.46
1:C:656:PHE:HE2	1:C:815:LEU:HD23	1.79	0.46
1:D:740:GLN:HG2	1:D:912:PHE:CE2	2.50	0.46
1:D:1250:ASN:OD1	1:D:1252:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:HD2	1:A:745:LEU:HB3	1.81	0.46
1:B:623:THR:O	1:B:623:THR:CG2	2.64	0.46
1:C:124:MET:CE	1:C:127:LEU:HD23	2.44	0.46
1:C:467:LEU:O	1:C:471:GLN:HG2	2.15	0.46
1:C:1119:THR:O	1:C:1123:MET:HG2	2.15	0.46
1:A:505:VAL:HG23	1:A:506:ASP:N	2.30	0.46
1:B:257:LEU:O	5:B:3003:FAD:H2B	2.15	0.46
1:D:606:LEU:C	1:D:606:LEU:HD23	2.36	0.46
1:A:374:LEU:HD22	1:A:398:LEU:HD21	1.98	0.46
1:A:765:VAL:O	1:A:792:VAL:HG22	2.15	0.46
1:A:933:VAL:HG11	1:A:1280:ARG:NH2	2.30	0.46
1:B:314:ASP:O	1:B:318:LYS:HE2	2.15	0.46
1:B:987:LYS:O	1:B:991:GLU:HG3	2.16	0.46
1:B:1054:ALA:O	1:B:1099:LEU:HD11	2.14	0.46
1:C:881:ARG:HD2	1:C:915:PHE:O	2.16	0.46
1:C:1174:ASN:O	1:C:1237:PRO:HA	2.16	0.46
1:A:912:PHE:O	1:A:913:ARG:C	2.54	0.46
1:A:969:TRP:HZ3	1:A:1003:PRO:HD3	1.79	0.46
1:C:409:ILE:HA	1:C:410:PRO:HD3	1.74	0.46
1:D:498:PRO:HG2	1:D:1323:PRO:HD3	1.97	0.46
1:B:45:GLU:O	1:B:45:GLU:HG2	2.16	0.46
1:B:653:GLU:HB3	1:B:871:THR:HG21	1.97	0.46
1:C:304:PRO:O	1:C:307:ILE:HG13	2.16	0.46
1:C:735:ILE:CD1	1:C:845:ALA:HB3	2.45	0.46
1:D:304:PRO:HG2	1:D:307:ILE:HG23	1.96	0.46
1:A:97:ARG:HB2	1:A:97:ARG:HH11	1.81	0.46
1:A:166:ASP:O	1:A:167:GLY:C	2.53	0.46
1:A:552:LYS:HD3	1:A:552:LYS:N	2.31	0.46
1:A:641:VAL:O	1:A:641:VAL:HG23	2.14	0.46
1:A:1043:LEU:O	1:A:1047:MET:HG2	2.16	0.46
1:B:506:ASP:OD2	1:B:1320:THR:HG22	2.16	0.46
1:B:762:GLU:C	1:B:763:LEU:HD12	2.35	0.46
1:B:1300:PRO:HG2	1:B:1302:THR:HG23	1.96	0.46
1:C:117:THR:CG2	1:C:587:ALA:HA	2.45	0.46
1:C:218:ARG:HH11	1:C:218:ARG:CB	2.29	0.46
1:C:393:TYR:N	1:C:461:ASN:ND2	2.64	0.46
1:C:709:TYR:CE2	1:C:868:VAL:HG22	2.51	0.46
1:A:374:LEU:HD22	1:A:398:LEU:CD2	2.46	0.46
1:A:746:GLU:HB3	1:A:796:GLY:HA3	1.97	0.46
1:B:3:ALA:HB1	1:B:228:ARG:N	2.20	0.46
1:B:606:LEU:HD23	1:B:607:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:GLN:HG2	1:B:1134:TYR:CE1	2.51	0.46
1:C:152:GLY:HA2	1:C:1201:VAL:HG21	1.98	0.46
1:D:924:ALA:HA	1:D:927:TRP:NE1	2.30	0.46
1:D:989:ASN:OD1	1:D:996:LYS:HA	2.15	0.46
1:D:1050:VAL:HG13	1:D:1255:TYR:HE2	1.80	0.46
1:D:1262:GLU:N	1:D:1263:PRO:CD	2.79	0.46
1:A:754:PRO:HD3	1:A:817:ALA:HB1	1.98	0.46
1:B:829:ASP:HB2	1:B:832:GLU:HG3	1.97	0.46
1:B:1005:LYS:HG3	1:B:1156:TYR:CE1	2.50	0.46
1:C:393:TYR:N	1:C:461:ASN:HD21	2.12	0.46
1:C:890:TYR:OH	1:C:943:ARG:HD3	2.16	0.46
1:D:768:GLN:HG3	1:D:802:LYS:HB2	1.98	0.46
1:A:298:SER:HA	1:A:408:GLU:HA	1.97	0.46
1:A:482:LEU:O	1:A:486:VAL:HG23	2.15	0.46
1:A:506:ASP:OD2	1:A:1319:VAL:HA	2.16	0.46
1:B:309:GLU:HB2	1:B:334:LEU:HD13	1.97	0.46
1:B:662:THR:O	1:B:663:CYS:HB3	2.16	0.46
1:B:1320:THR:HG23	1:B:1321:GLY:N	2.31	0.46
1:C:147:LEU:HD13	1:C:1230:ILE:HD11	1.98	0.46
1:C:757:GLU:O	1:C:759:GLY:N	2.49	0.46
1:C:1263:PRO:HB2	1:C:1264:PRO:HD3	1.98	0.46
1:D:1109:ASN:ND2	1:D:1112:GLY:HA3	2.31	0.46
1:B:13:ARG:CB	1:B:13:ARG:HH11	2.29	0.45
1:B:857:VAL:HG21	1:B:892:ILE:HG12	1.99	0.45
1:C:3:ALA:HA	1:C:227:LEU:CD2	2.46	0.45
1:C:1319:VAL:HG23	1:C:1319:VAL:O	2.15	0.45
1:D:387:HIS:ND1	1:D:467:LEU:HD11	2.32	0.45
1:A:424:ALA:HB1	1:A:430:ASP:OD2	2.16	0.45
1:A:735:ILE:HD11	1:A:923:ILE:HG12	1.99	0.45
1:C:124:MET:HE2	1:C:128:LEU:HG	1.98	0.45
1:C:840:ARG:HB2	1:C:912:PHE:CD2	2.51	0.45
1:D:318:LYS:HD2	1:D:318:LYS:N	2.30	0.45
1:D:612:THR:O	1:D:613:ARG:HD3	2.16	0.45
1:A:375:VAL:HG12	1:A:380:ARG:HG3	1.97	0.45
1:A:550:PHE:HE2	1:A:552:LYS:HD2	1.80	0.45
1:B:236:TRP:CZ2	1:B:280:CYS:HB2	2.51	0.45
1:B:755:LYS:HE2	1:B:762:GLU:HB2	1.98	0.45
1:C:256:LYS:HG3	1:C:275:PHE:CD1	2.50	0.45
1:C:571:GLU:CD	1:C:1058:PRO:HG3	2.35	0.45
1:D:217:LEU:HD12	1:D:217:LEU:HA	1.77	0.45
1:D:649:ILE:HD11	1:D:804:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLN:HG3	1:A:64:LYS:HB2	1.99	0.45
1:A:372:LEU:HD23	1:A:407:ILE:HG13	1.97	0.45
1:D:997:ARG:HA	1:D:1163:VAL:O	2.16	0.45
1:D:1115:GLU:O	1:D:1119:THR:CG2	2.64	0.45
1:A:196:PHE:CE2	1:A:198:PRO:HG3	2.51	0.45
1:A:571:GLU:OE2	1:A:1058:PRO:HG3	2.17	0.45
1:A:1327:LYS:HD2	1:A:1327:LYS:C	2.37	0.45
1:A:1332:ARG:HG2	1:A:1332:ARG:NH1	2.30	0.45
1:B:768:GLN:HG3	1:B:802:LYS:HB2	1.97	0.45
1:C:399:SER:HB2	1:C:400:PRO:HD2	1.98	0.45
1:D:112:GLN:NE2	1:D:151:THR:HA	2.31	0.45
1:D:630:PRO:HD2	1:D:681:ARG:NH2	2.32	0.45
1:A:95:LYS:HG3	1:A:590:GLU:OE2	2.16	0.45
1:A:154:ARG:NH1	1:A:1197:GLU:OE1	2.50	0.45
1:A:442:PHE:HE1	1:A:478:TRP:HB2	1.82	0.45
1:B:195:LEU:HD22	1:B:1190:ALA:HA	1.99	0.45
1:C:97:ARG:CB	1:C:97:ARG:HH11	2.29	0.45
1:C:304:PRO:HG2	1:C:307:ILE:HG23	1.98	0.45
1:C:851:PHE:N	1:C:851:PHE:CD1	2.84	0.45
1:D:275:PHE:HA	1:D:276:PRO:HD2	1.82	0.45
1:D:422:LYS:HE3	1:D:432:ALA:HB2	1.99	0.45
1:D:1050:VAL:HG13	1:D:1255:TYR:CE2	2.52	0.45
1:A:98:LEU:HD21	1:A:588:SER:HB3	1.97	0.45
1:B:257:LEU:HD22	1:B:279:VAL:HG13	1.98	0.45
1:B:604:LEU:HD21	1:B:822:ARG:NH2	2.32	0.45
1:B:709:TYR:HE2	1:B:868:VAL:HG22	1.81	0.45
1:C:224:ARG:HD3	1:C:283:TRP:CE3	2.52	0.45
1:C:257:LEU:CD2	1:C:279:VAL:HG13	2.47	0.45
1:C:713:LEU:O	1:C:898:THR:HA	2.17	0.45
1:D:1327:LYS:HD2	1:D:1327:LYS:C	2.37	0.45
1:A:1216:PRO:HD2	1:A:1217:GLU:OE2	2.17	0.45
1:B:656:PHE:CD1	1:B:669:GLY:HA2	2.51	0.45
1:B:1199:ALA:HB3	1:B:1264:PRO:HB2	1.99	0.45
1:D:215:GLU:HG3	1:D:218:ARG:HH12	1.82	0.45
1:D:742:HIS:HA	1:D:912:PHE:CE2	2.52	0.45
1:A:530:GLU:O	1:A:531:ASN:HB2	2.16	0.45
1:A:578:LEU:HD12	1:A:579:PRO:HD2	1.98	0.45
1:A:927:TRP:O	1:A:931:VAL:HG23	2.17	0.45
1:A:981:ARG:NH1	1:A:1162:GLU:OE1	2.49	0.45
1:A:1289:ASN:O	1:A:1290:ASN:HB2	2.17	0.45
1:B:58:TYR:CZ	1:B:220:LYS:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1184:GLY:HA2	1:C:1248:CYS:O	2.16	0.45
1:B:96:THR:OG1	1:B:97:ARG:N	2.49	0.45
1:B:906:LEU:HD11	1:B:1333:VAL:HG22	1.99	0.45
1:C:640:ASP:HB3	1:C:819:LYS:HE3	1.99	0.45
1:D:1119:THR:O	1:D:1123:MET:HG2	2.17	0.45
1:A:924:ALA:HA	1:A:927:TRP:NE1	2.31	0.44
1:B:97:ARG:HB3	1:B:97:ARG:NH1	2.31	0.44
1:C:533:GLU:HG2	1:C:534:ASP:OD1	2.17	0.44
1:A:64:LYS:CE	1:A:65:ILE:H	2.28	0.44
1:B:439:ARG:NH2	1:B:451:GLU:OE1	2.50	0.44
1:B:607:ARG:HB3	1:B:679:THR:HB	1.99	0.44
1:C:257:LEU:HD23	1:C:279:VAL:HG13	1.98	0.44
1:D:224:ARG:HG2	1:D:224:ARG:HH11	1.83	0.44
1:D:1052:SER:HB2	1:D:1059:THR:HG22	1.98	0.44
1:D:1287:THR:OG1	1:D:1289:ASN:ND2	2.51	0.44
1:A:616:ALA:HB2	1:A:692:GLU:HA	1.99	0.44
1:B:1089:GLN:HG2	1:B:1134:TYR:CG	2.53	0.44
1:B:1302:THR:HB	1:B:1303:PRO:HD2	1.99	0.44
1:B:1332:ARG:HG2	1:B:1332:ARG:NH1	2.31	0.44
1:C:117:THR:HB	1:C:118:PRO:HD3	1.99	0.44
1:C:651:ASN:HD22	1:C:651:ASN:HA	1.59	0.44
1:C:1320:THR:CG2	1:C:1321:GLY:H	2.22	0.44
1:D:978:TYR:CE2	1:D:982:LYS:HD2	2.52	0.44
1:D:1022:LEU:HD23	1:D:1022:LEU:C	2.37	0.44
1:B:307:ILE:C	1:B:307:ILE:HD12	2.38	0.44
1:B:667:ILE:HD12	1:B:808:VAL:HG13	2.00	0.44
1:C:425:SER:HB2	1:C:1229:LYS:HG3	1.98	0.44
1:C:473:GLN:HE21	1:C:482:LEU:HG	1.82	0.44
1:D:97:ARG:CZ	1:D:98:LEU:H	2.30	0.44
1:D:623:THR:CG2	1:D:626:ALA:HB3	2.47	0.44
1:A:40:LYS:HB3	1:A:115:PHE:CZ	2.53	0.44
1:A:64:LYS:HE2	1:A:65:ILE:N	2.30	0.44
1:A:65:ILE:HD12	1:A:212:PHE:CE2	2.52	0.44
1:A:448:GLU:HG3	1:A:448:GLU:O	2.18	0.44
1:A:467:LEU:O	1:A:471:GLN:HG2	2.18	0.44
1:C:97:ARG:NH1	1:C:97:ARG:CB	2.78	0.44
1:C:1287:THR:CG2	1:C:1288:GLY:H	2.14	0.44
1:A:131:GLN:HE21	1:A:133:GLU:N	2.13	0.44
1:A:606:LEU:HD13	1:A:813:VAL:HA	1.98	0.44
1:A:996:LYS:NZ	1:A:1285:GLN:NE2	2.66	0.44
1:C:1262:GLU:N	1:C:1263:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:THR:HG22	1:D:51:CYS:HA	2.00	0.44
1:D:152:GLY:HA2	1:D:1201:VAL:HG21	2.00	0.44
1:D:164:ALA:C	1:D:166:ASP:N	2.65	0.44
1:D:1323:PRO:O	1:D:1324:GLU:C	2.56	0.44
1:A:117:THR:HG21	1:A:587:ALA:HA	1.99	0.44
1:A:1287:THR:O	1:A:1289:ASN:N	2.50	0.44
1:B:232:GLU:OE2	1:B:681:ARG:NH2	2.44	0.44
1:B:372:LEU:HD11	1:B:385:MET:HE3	1.99	0.44
1:B:1204:LEU:HD12	1:B:1204:LEU:C	2.38	0.44
1:C:333:GLN:OE1	1:C:333:GLN:HA	2.18	0.44
1:C:443:LYS:HD3	1:C:444:PRO:HD2	1.99	0.44
1:C:1200:PHE:CE1	1:C:1268:ALA:HA	2.53	0.44
1:D:1283:ARG:NH2	1:D:1293:GLU:OE2	2.50	0.44
1:A:117:THR:HB	1:A:118:PRO:HD3	1.99	0.44
1:A:256:LYS:HG3	1:A:275:PHE:CG	2.53	0.44
1:D:46:GLY:HA2	4:D:2002:FES:S1	2.58	0.44
1:A:443:LYS:HG2	1:A:450:GLN:HB2	2.00	0.43
1:A:1188:ASN:CG	1:A:1191:ILE:HG12	2.38	0.43
1:B:507:PHE:HB2	1:B:1304:GLU:HG3	1.99	0.43
1:C:58:TYR:OH	1:C:63:ASN:ND2	2.46	0.43
1:C:65:ILE:HD12	1:C:212:PHE:CD2	2.53	0.43
1:C:720:LEU:HD11	1:C:896:ARG:CB	2.48	0.43
1:C:1038:GLU:HB2	1:C:1044:HIS:CD2	2.53	0.43
1:A:97:ARG:HH11	1:A:97:ARG:CB	2.31	0.43
1:B:58:TYR:OH	1:B:63:ASN:ND2	2.52	0.43
1:C:310:LYS:HE2	1:C:310:LYS:CA	2.47	0.43
1:C:932:ALA:HA	1:C:942:VAL:HG21	2.00	0.43
1:D:196:PHE:O	1:D:198:PRO:HD3	2.19	0.43
1:A:298:SER:HA	1:A:407:ILE:O	2.18	0.43
1:A:602:ASN:O	1:A:822:ARG:HD2	2.17	0.43
1:B:3:ALA:HA	1:B:227:LEU:CD2	2.46	0.43
1:B:667:ILE:HD12	1:B:808:VAL:CG1	2.48	0.43
1:C:257:LEU:HD23	1:C:279:VAL:CG1	2.48	0.43
1:C:550:PHE:CE2	1:C:552:LYS:HG3	2.53	0.43
1:D:1302:THR:HB	1:D:1303:PRO:HD2	2.00	0.43
1:B:58:TYR:CE1	1:B:63:ASN:ND2	2.86	0.43
1:B:606:LEU:HD23	1:B:606:LEU:C	2.38	0.43
1:B:1183:VAL:HG22	9:B:7068:HOH:O	2.18	0.43
1:C:117:THR:O	1:C:121:VAL:HG23	2.19	0.43
1:C:267:GLU:HB3	1:C:273:MET:HG3	2.00	0.43
1:D:733:GLY:HA3	1:D:847:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1047:MET:SD	1:D:1088:GLY:HA2	2.59	0.43
1:A:616:ALA:CB	1:A:692:GLU:HA	2.48	0.43
1:A:1220:LEU:HD21	1:A:1222:THR:O	2.18	0.43
1:B:58:TYR:HE1	1:B:63:ASN:ND2	2.16	0.43
1:B:1320:THR:OG1	1:B:1321:GLY:N	2.49	0.43
1:C:154:ARG:N	1:C:155:PRO:HD2	2.33	0.43
1:D:298:SER:HA	1:D:408:GLU:HA	1.99	0.43
1:A:1009:SER:HA	1:A:1082:VAL:HG11	2.01	0.43
1:A:1083:SER:HB2	6:A:2004:MTE:O3P	2.19	0.43
1:A:1133:PHE:CG	1:B:1127:SER:HB2	2.53	0.43
1:B:888:ASN:ND2	1:B:925:GLU:OE2	2.51	0.43
1:B:1008:ILE:O	1:B:1009:SER:CB	2.66	0.43
1:A:197:LYS:HB2	1:A:200:GLU:HG3	2.01	0.43
1:C:131:GLN:O	1:C:134:PRO:HD3	2.19	0.43
1:C:490:LEU:HB2	1:C:513:LEU:CD2	2.49	0.43
1:D:87:THR:OG1	1:D:89:GLU:HG2	2.18	0.43
1:D:1323:PRO:O	1:D:1325:ASN:N	2.51	0.43
1:A:967:ARG:O	1:A:971:GLU:HB2	2.19	0.43
1:B:362:ASN:N	1:B:363:PRO:CD	2.82	0.43
1:B:1291:VAL:HG13	1:B:1292:LYS:HG3	2.00	0.43
1:C:506:ASP:OD1	1:C:1320:THR:N	2.52	0.43
1:C:1133:PHE:CG	1:D:1127:SER:HB2	2.54	0.43
1:D:1215:SER:HG	1:D:1217:GLU:HG2	1.83	0.43
1:A:443:LYS:HA	1:A:450:GLN:NE2	2.33	0.43
1:A:1222:THR:CG2	1:A:1228:TYR:HB2	2.49	0.43
1:C:656:PHE:CD1	1:C:669:GLY:HA2	2.54	0.43
1:C:1208:THR:C	1:C:1209:LEU:HD12	2.39	0.43
1:D:374:LEU:HD13	1:D:398:LEU:CD2	2.45	0.43
1:D:1089:GLN:HG2	1:D:1134:TYR:CE1	2.53	0.43
1:A:256:LYS:HG3	1:A:275:PHE:CD1	2.54	0.43
1:A:389:PHE:HA	1:A:397:LEU:CG	2.47	0.43
1:A:1034:HIS:HB2	1:A:1087:ASN:HD22	1.83	0.43
1:B:623:THR:HG23	1:B:626:ALA:HB3	2.01	0.43
1:C:28:ALA:CB	1:C:32:ARG:HH12	2.32	0.43
1:C:204:LEU:HG	1:C:206:PRO:HD3	2.01	0.43
1:C:912:PHE:O	1:C:913:ARG:C	2.57	0.43
1:C:1141:TYR:OH	1:C:1146:ASN:ND2	2.52	0.43
1:A:32:ARG:HD2	9:A:7112:HOH:O	2.18	0.42
1:A:582:ALA:O	1:A:586:GLN:HG3	2.19	0.42
1:A:734:GLU:O	1:A:735:ILE:HG23	2.19	0.42
1:B:758:ALA:O	1:B:787:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:646:ILE:O	1:D:646:ILE:HG13	2.19	0.42
1:A:96:THR:OG1	1:A:97:ARG:N	2.51	0.42
1:A:428:GLU:O	1:A:429:ASP:C	2.57	0.42
1:A:632:PHE:HE1	1:A:671:VAL:HG22	1.83	0.42
1:A:1279:ILE:HG21	1:A:1309:ALA:HB1	2.01	0.42
1:B:552:LYS:O	1:B:553:ASP:CB	2.65	0.42
1:B:859:ALA:HA	1:B:894:ASN:O	2.19	0.42
1:C:572:ASP:OD1	1:C:1053:ARG:HD3	2.19	0.42
1:C:869:GLY:HA3	1:C:908:SER:HA	2.01	0.42
1:A:428:GLU:OE2	1:A:1234:GLY:HA3	2.20	0.42
1:B:550:PHE:CE1	1:B:1173:LYS:HD3	2.53	0.42
1:B:558:VAL:HG21	1:B:1241:ARG:NH1	2.34	0.42
1:B:652:ASP:HB3	1:B:871:THR:HB	2.01	0.42
1:C:74:LEU:O	1:C:76:PRO:HD3	2.19	0.42
1:C:108:SER:O	1:C:109:HIS:HB2	2.20	0.42
1:C:357:PRO:HG3	1:C:461:ASN:O	2.18	0.42
1:C:550:PHE:HE2	1:C:552:LYS:HG3	1.83	0.42
1:A:97:ARG:HB2	1:A:97:ARG:CZ	2.49	0.42
1:A:419:SER:HB2	1:A:519:PHE:CD1	2.54	0.42
1:D:446:THR:HB	1:D:535:LYS:HZ2	1.83	0.42
1:D:661:VAL:HA	1:D:666:HIS:ND1	2.34	0.42
1:A:425:SER:HB2	1:A:1229:LYS:HG3	2.02	0.42
1:A:562:GLN:HG3	1:A:1246:ARG:NH2	2.35	0.42
1:A:977:GLN:O	1:A:981:ARG:HG3	2.18	0.42
1:B:55:LEU:CD2	1:B:85:VAL:HG22	2.50	0.42
1:B:346:ALA:HB1	5:B:3003:FAD:H4'	2.00	0.42
1:B:835:LEU:HD22	1:B:1223:ARG:NH1	2.35	0.42
1:C:363:PRO:HG3	1:C:463:THR:HG23	2.01	0.42
1:C:735:ILE:HG21	1:C:926:CYS:SG	2.59	0.42
1:D:117:THR:CG2	1:D:587:ALA:HA	2.50	0.42
1:D:592:VAL:HG13	1:D:596:ASP:HB2	2.02	0.42
1:D:641:VAL:O	1:D:641:VAL:HG23	2.19	0.42
1:D:1034:HIS:NE2	1:D:1047:MET:HG3	2.35	0.42
1:A:498:PRO:HG3	1:A:1320:THR:OG1	2.20	0.42
1:A:532:LEU:C	1:A:534:ASP:H	2.23	0.42
1:B:642:PRO:HG2	1:B:781:LEU:HA	2.00	0.42
1:B:1109:ASN:N	1:B:1110:PRO:HD3	2.35	0.42
1:D:136:MET:CE	1:D:167:GLY:HA2	2.49	0.42
1:D:1079:ALA:HB1	7:D:5005:MOM:OM1	2.19	0.42
1:A:112:GLN:NE2	1:A:151:THR:HA	2.34	0.42
1:A:742:HIS:HA	1:A:912:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:TYR:CE1	1:B:33:LYS:HG2	2.54	0.42
1:B:886:MET:SD	1:B:897:GLY:HA3	2.59	0.42
1:B:1141:TYR:HE1	1:B:1146:ASN:HD22	1.68	0.42
1:C:217:LEU:HD12	1:C:217:LEU:HA	1.92	0.42
1:C:950:GLU:OE2	1:C:961:GLU:HA	2.19	0.42
1:C:1019:GLY:HA2	1:C:1132:GLY:O	2.20	0.42
1:D:613:ARG:NH1	1:D:692:GLU:HG3	2.34	0.42
1:D:649:ILE:HD13	1:D:873:ASP:OD1	2.19	0.42
1:A:68:PHE:HD2	1:A:344:SER:HB3	1.84	0.42
1:B:735:ILE:HD11	1:B:847:TYR:HD1	1.85	0.42
1:B:787:ARG:HG2	1:B:787:ARG:HH11	1.85	0.42
1:C:399:SER:OG	1:C:402:GLU:HG3	2.19	0.42
1:D:307:ILE:HG13	1:D:308:VAL:N	2.35	0.42
1:D:841:HIS:CE1	1:D:878:ILE:HD12	2.55	0.42
1:A:749:CYS:HA	1:A:826:CYS:O	2.20	0.42
1:A:1113:SER:O	1:A:1116:ASP:HB2	2.20	0.42
1:A:1149:ASN:HA	1:A:1150:PRO:HD3	1.85	0.42
1:B:500:ALA:HA	1:B:501:PRO:HD3	1.93	0.42
1:C:1105:TYR:CD1	1:C:1105:TYR:N	2.88	0.42
1:D:124:MET:HE2	1:D:128:LEU:HD11	2.02	0.42
1:D:558:VAL:HG13	1:D:1241:ARG:HG2	2.01	0.42
1:D:650:CYS:HB2	1:D:652:ASP:HB2	2.01	0.42
1:D:860:LEU:HD22	1:D:927:TRP:CZ2	2.54	0.42
1:A:640:ASP:OD1	1:A:819:LYS:HE3	2.20	0.42
1:A:1105:TYR:CD1	1:A:1105:TYR:N	2.88	0.42
1:B:572:ASP:OD2	1:B:1053:ARG:HD2	2.20	0.42
1:C:786:ASN:ND2	1:D:1029:SER:HB2	2.35	0.42
1:C:1260:VAL:HG22	1:C:1260:VAL:O	2.19	0.42
1:A:257:LEU:HD13	1:A:279:VAL:HG13	2.02	0.41
1:A:443:LYS:HA	1:A:450:GLN:HE21	1.85	0.41
1:A:1210:GLU:O	1:A:1300:PRO:HG3	2.19	0.41
1:B:233:ARG:HD3	1:B:681:ARG:CZ	2.50	0.41
1:C:1089:GLN:HG2	1:C:1134:TYR:CE1	2.55	0.41
1:A:10:VAL:HG21	1:A:34:LEU:HD11	2.01	0.41
1:B:212:PHE:CD1	1:B:213:PRO:HD2	2.54	0.41
1:B:233:ARG:HD3	1:B:681:ARG:NH1	2.35	0.41
1:C:242:LEU:O	1:C:246:LEU:HG	2.20	0.41
1:C:924:ALA:HA	1:C:927:TRP:NE1	2.35	0.41
1:C:933:VAL:CG1	1:C:1280:ARG:HH21	2.29	0.41
1:C:953:LEU:HD23	1:C:959:LYS:HA	2.03	0.41
1:D:561:PHE:HB2	9:D:7144:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:566:LYS:HD3	1:D:566:LYS:C	2.41	0.41
1:A:225:LYS:HE2	1:A:226:GLN:O	2.19	0.41
1:B:552:LYS:H	1:B:552:LYS:HG2	1.44	0.41
1:B:752:ALA:HB3	1:B:813:VAL:HG12	2.03	0.41
1:B:927:TRP:O	1:B:931:VAL:HG23	2.20	0.41
1:C:87:THR:OG1	1:C:89:GLU:HG2	2.21	0.41
1:C:152:GLY:O	1:C:1236:ILE:HG21	2.20	0.41
1:C:1135:ARG:HD2	1:C:1135:ARG:O	2.21	0.41
1:D:741:GLU:CG	1:D:834:MET:HG2	2.40	0.41
1:A:143:PHE:HB3	1:A:1233:PHE:CE1	2.55	0.41
1:A:650:CYS:O	1:A:651:ASN:C	2.57	0.41
1:A:1176:ARG:HH21	1:A:1241:ARG:CD	2.33	0.41
1:B:671:VAL:HG11	1:B:682:ALA:HB3	2.03	0.41
1:C:573:MET:HA	1:C:576:ARG:HD2	2.02	0.41
1:D:3:ALA:HA	1:D:227:LEU:HD22	2.02	0.41
1:D:441:LEU:HB3	1:D:451:GLU:HB2	2.02	0.41
1:D:1107:LYS:HB3	1:D:1107:LYS:HE2	1.85	0.41
1:B:549:LEU:O	1:B:551:GLN:HG2	2.20	0.41
1:B:1103:GLU:O	1:B:1107:LYS:HG3	2.20	0.41
1:C:218:ARG:HB2	1:C:218:ARG:NH1	2.35	0.41
1:C:303:CYS:SG	1:C:307:ILE:HD11	2.60	0.41
1:C:607:ARG:HB3	1:C:671:VAL:HG12	2.03	0.41
1:C:632:PHE:HE1	1:C:671:VAL:HG22	1.86	0.41
1:C:722:LYS:HD3	1:C:726:GLU:OE2	2.19	0.41
1:D:584:ASP:HB2	9:D:7063:HOH:O	2.21	0.41
1:D:750:THR:HG23	1:D:765:VAL:HG22	2.01	0.41
1:D:860:LEU:HD12	1:D:861:GLU:N	2.34	0.41
1:A:154:ARG:CD	1:A:1197:GLU:OE2	2.67	0.41
1:A:619:LYS:HD2	1:A:691:GLU:HB2	2.01	0.41
1:C:650:CYS:O	1:C:651:ASN:C	2.58	0.41
1:C:1084:ALA:HB3	9:C:7132:HOH:O	2.21	0.41
1:D:560:LEU:O	1:D:1243:SER:HA	2.20	0.41
1:D:614:ALA:O	1:D:905:ASN:HB3	2.21	0.41
1:D:1106:LYS:HE3	1:D:1117:TRP:CH2	2.56	0.41
1:A:254:ASP:O	1:A:255:ALA:C	2.59	0.41
1:A:1317:LEU:N	1:A:1317:LEU:HD22	2.35	0.41
1:B:224:ARG:HG2	1:B:224:ARG:NH1	2.36	0.41
1:B:236:TRP:CD1	1:B:236:TRP:C	2.94	0.41
1:B:303:CYS:HA	1:B:304:PRO:HD2	1.96	0.41
1:B:747:THR:HG23	9:B:7032:HOH:O	2.20	0.41
1:C:829:ASP:O	1:C:830:ARG:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1092:TYR:O	1:C:1096:GLN:HG2	2.21	0.41
1:C:1236:ILE:HB	1:C:1237:PRO:HD2	2.02	0.41
1:D:56:SER:HA	1:D:66:VAL:O	2.20	0.41
1:D:562:GLN:HG3	1:D:1246:ARG:NH1	2.36	0.41
1:D:1253:ALA:HB3	1:D:1257:SER:O	2.21	0.41
1:A:59:ASP:OD1	1:A:62:GLN:HB3	2.21	0.41
1:A:68:PHE:CD2	1:A:344:SER:HB3	2.56	0.41
1:A:315:ALA:O	1:A:319:LEU:HG	2.20	0.41
1:A:1253:ALA:HB3	1:A:1257:SER:O	2.21	0.41
1:B:351:ASN:HB2	5:B:3003:FAD:O4'	2.21	0.41
1:B:504:MET:HG2	1:B:1304:GLU:OE2	2.20	0.41
1:B:568:GLN:HG2	1:B:572:ASP:HB3	2.03	0.41
1:C:3:ALA:HB2	1:C:225:LYS:HE3	2.01	0.41
1:C:357:PRO:HA	1:C:462:ARG:HA	2.02	0.41
1:C:732:SER:HA	1:C:847:TYR:O	2.20	0.41
1:C:1210:GLU:O	1:C:1300:PRO:HG3	2.21	0.41
1:D:303:CYS:HB3	1:D:307:ILE:HD11	2.03	0.41
1:D:1039:MET:HG3	6:D:5004:MTE:C4	2.50	0.41
1:A:334:LEU:HA	1:A:337:PHE:HB2	2.02	0.41
1:A:606:LEU:HD23	1:A:607:ARG:N	2.35	0.41
1:A:1174:ASN:HB3	9:A:7076:HOH:O	2.19	0.41
1:B:215:GLU:O	1:B:218:ARG:HB3	2.20	0.41
1:B:430:ASP:CG	1:B:1229:LYS:HE2	2.41	0.41
1:B:758:ALA:HB1	1:B:787:ARG:HE	1.86	0.41
1:C:192:SER:N	1:C:193:PRO:HD3	2.35	0.41
1:C:1140:GLY:O	1:C:1148:GLY:HA3	2.21	0.41
1:C:1193:ILE:O	1:C:1197:GLU:HG3	2.20	0.41
1:D:97:ARG:HA	1:D:97:ARG:NH1	2.36	0.41
1:D:165:ARG:O	1:D:166:ASP:O	2.39	0.41
1:A:384:GLN:HG3	1:A:384:GLN:O	2.21	0.41
1:A:418:PHE:HD1	1:A:439:ARG:HB2	1.86	0.41
1:A:742:HIS:CE1	1:A:839:GLY:HA2	2.56	0.41
1:A:1022:LEU:HD23	1:A:1032:LEU:HD13	2.03	0.41
1:B:9:PHE:CE2	1:B:14:LYS:HB2	2.55	0.41
1:B:117:THR:CG2	1:B:587:ALA:HA	2.51	0.41
1:B:154:ARG:HD2	9:B:7076:HOH:O	2.21	0.41
1:B:205:ASP:HA	1:B:206:PRO:HD2	1.91	0.41
1:B:477:LEU:HB3	1:B:479:LYS:HG2	2.03	0.41
1:B:645:ASN:O	1:B:654:THR:HA	2.21	0.41
1:B:646:ILE:HG13	1:B:779:LYS:NZ	2.36	0.41
1:B:740:GLN:HG2	1:B:912:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:981:ARG:O	1:B:985:VAL:HG23	2.20	0.41
1:B:1036:GLY:HA3	1:B:1043:LEU:HD21	2.03	0.41
1:C:298:SER:HA	1:C:407:ILE:O	2.21	0.41
1:A:647:THR:HG21	9:A:7205:HOH:O	2.20	0.40
1:A:886:MET:SD	1:A:897:GLY:HA3	2.61	0.40
1:A:1159:ALA:HA	1:A:1178:ASP:O	2.21	0.40
1:B:301:ALA:O	1:B:347:SER:HB2	2.21	0.40
1:B:981:ARG:CZ	1:B:1176:ARG:HD3	2.52	0.40
1:C:234:VAL:HG12	1:C:235:THR:N	2.37	0.40
1:C:443:LYS:HD3	1:C:450:GLN:NE2	2.37	0.40
1:C:780:MET:SD	1:C:780:MET:C	3.00	0.40
1:C:1327:LYS:C	1:C:1327:LYS:HD2	2.42	0.40
1:D:56:SER:HB2	1:D:84:ALA:HB3	2.03	0.40
1:A:6:LEU:HB3	1:A:17:GLU:HB3	2.03	0.40
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.92	0.40
1:C:735:ILE:CD1	1:C:923:ILE:HG12	2.52	0.40
1:A:74:LEU:O	1:A:76:PRO:HD3	2.21	0.40
1:B:154:ARG:CD	1:B:1197:GLU:OE2	2.69	0.40
1:B:709:TYR:CE2	1:B:868:VAL:CG2	3.04	0.40
1:C:328:ARG:HH11	1:C:328:ARG:CG	2.35	0.40
1:D:29:TYR:O	1:D:33:LYS:HB3	2.21	0.40
1:D:362:ASN:N	1:D:363:PRO:CD	2.85	0.40
1:D:418:PHE:HD1	1:D:439:ARG:HB2	1.85	0.40
1:D:1199:ALA:HB3	1:D:1264:PRO:HB2	2.03	0.40
1:A:218:ARG:HB2	1:A:218:ARG:NH1	2.37	0.40
1:A:263:GLU:HB3	5:A:2003:FAD:H52A	2.03	0.40
1:A:400:PRO:HG2	1:A:401:GLU:CD	2.42	0.40
1:A:840:ARG:HG3	2:A:6001:BCT:O1	2.21	0.40
1:A:1107:LYS:HE2	1:A:1107:LYS:HB3	1.90	0.40
1:B:442:PHE:CE2	1:B:527:LEU:HD21	2.56	0.40
1:B:480:GLU:O	1:B:483:LEU:HB3	2.21	0.40
1:B:1032:LEU:O	1:B:1064:ILE:HG12	2.22	0.40
1:B:1200:PHE:CE1	1:B:1268:ALA:HA	2.56	0.40
1:C:750:THR:HG23	1:C:765:VAL:HG22	2.04	0.40
1:C:860:LEU:HD22	1:C:892:ILE:HD13	2.03	0.40
1:A:242:LEU:O	1:A:246:LEU:HG	2.21	0.40
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.79	0.40
1:B:965:LEU:N	1:B:966:PRO:CD	2.84	0.40
1:C:1122:TYR:HD1	9:D:7164:HOH:O	2.04	0.40
1:D:332:GLU:O	1:D:335:ARG:HB3	2.22	0.40
1:D:500:ALA:HA	1:D:501:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:VAL:HG23	1:D:506:ASP:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1303/1333 (98%)	1225 (94%)	64 (5%)	14 (1%)	14	30
1	B	1303/1333 (98%)	1228 (94%)	65 (5%)	10 (1%)	19	39
1	C	1303/1333 (98%)	1228 (94%)	69 (5%)	6 (0%)	29	52
1	D	1303/1333 (98%)	1223 (94%)	64 (5%)	16 (1%)	13	27
All	All	5212/5332 (98%)	4904 (94%)	262 (5%)	46 (1%)	17	35

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1009	SER
1	A	1290	ASN
1	B	553	ASP
1	B	1009	SER
1	C	758	ALA
1	C	1009	SER
1	C	1320	THR
1	D	166	ASP
1	D	1009	SER
1	D	1324	GLU
1	D	1325	ASN
1	D	377	ARG
1	D	391	PRO
1	D	758	ALA

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Mol	Chain	Res	Type
1	D	798	GLY
1	D	1319	VAL
1	D	1320	THR
1	A	429	ASP
1	A	1288	GLY
1	B	552	LYS
1	B	798	GLY
1	D	1290	ASN
1	A	4	ASP
1	A	533	GLU
1	A	624	SER
1	A	798	GLY
1	A	913	ARG
1	B	4	ASP
1	B	913	ARG
1	D	429	ASP
1	D	1323	PRO
1	B	1323	PRO
1	C	798	GLY
1	C	1289	ASN
1	D	978	TYR
1	A	1247	ASP
1	A	1319	VAL
1	B	213	PRO
1	B	1081	SER
1	A	1260	VAL
1	A	1322	VAL
1	A	1323	PRO
1	B	1321	GLY
1	C	1003	PRO
1	D	1003	PRO
1	D	213	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	1104/1126 (98%)	1066 (97%)	38 (3%)	37	63
1	B	1104/1126 (98%)	1063 (96%)	41 (4%)	34	60
1	C	1104/1126 (98%)	1070 (97%)	34 (3%)	40	66
1	D	1104/1126 (98%)	1060 (96%)	44 (4%)	31	57
All	All	4416/4504 (98%)	4259 (96%)	157 (4%)	35	61

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	60	ARG
1	A	62	GLN
1	A	64	LYS
1	A	89	GLU
1	A	129	ARG
1	A	154	ARG
1	A	202	THR
1	A	209	GLU
1	A	220	LYS
1	A	254	ASP
1	A	257	LEU
1	A	313	VAL
1	A	328	ARG
1	A	462	ARG
1	A	529	GLN
1	A	552	LYS
1	A	619	LYS
1	A	649	ILE
1	A	652	ASP
1	A	671	VAL
1	A	741	GLU
1	A	744	TYR
1	A	753	VAL
1	A	857	VAL
1	A	868	VAL
1	A	912	PHE
1	A	947	LEU
1	A	970	GLU
1	A	1033	THR
1	A	1053	ARG
1	A	1100	LYS
1	A	1146	ASN

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Mol	Chain	Res	Type
1	A	1240	PHE
1	A	1280	ARG
1	A	1291	VAL
1	A	1319	VAL
1	A	1327	LYS
1	B	13	ARG
1	B	62	GLN
1	B	64	LYS
1	B	89	GLU
1	B	100	PRO
1	B	129	ARG
1	B	144	GLN
1	B	154	ARG
1	B	209	GLU
1	B	254	ASP
1	B	277	MET
1	B	328	ARG
1	B	462	ARG
1	B	468	LYS
1	B	477	LEU
1	B	534	ASP
1	B	552	LYS
1	B	553	ASP
1	B	619	LYS
1	B	641	VAL
1	B	652	ASP
1	B	671	VAL
1	B	735	ILE
1	B	744	TYR
1	B	789	VAL
1	B	857	VAL
1	B	912	PHE
1	B	940	GLU
1	B	965	LEU
1	B	970	GLU
1	B	1032	LEU
1	B	1033	THR
1	B	1053	ARG
1	B	1073	PRO
1	B	1119	THR
1	B	1135	ARG
1	B	1146	ASN

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Mol	Chain	Res	Type
1	B	1204	LEU
1	B	1240	PHE
1	B	1327	LYS
1	B	1333	VAL
1	C	62	GLN
1	C	89	GLU
1	C	100	PRO
1	C	129	ARG
1	C	154	ARG
1	C	199	GLU
1	C	202	THR
1	C	209	GLU
1	C	310	LYS
1	C	322	GLN
1	C	328	ARG
1	C	433	LYS
1	C	462	ARG
1	C	529	GLN
1	C	553	ASP
1	C	599	ARG
1	C	607	ARG
1	C	652	ASP
1	C	671	VAL
1	C	722	LYS
1	C	744	TYR
1	C	789	VAL
1	C	853	LYS
1	C	1003	PRO
1	C	1032	LEU
1	C	1033	THR
1	C	1053	ARG
1	C	1073	PRO
1	C	1119	THR
1	C	1146	ASN
1	C	1217	GLU
1	C	1240	PHE
1	C	1317	LEU
1	C	1327	LYS
1	D	32	ARG
1	D	89	GLU
1	D	97	ARG
1	D	100	PRO

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Mol	Chain	Res	Type
1	D	133	GLU
1	D	154	ARG
1	D	166	ASP
1	D	209	GLU
1	D	254	ASP
1	D	310	LYS
1	D	312	LEU
1	D	328	ARG
1	D	380	ARG
1	D	461	ASN
1	D	462	ARG
1	D	468	LYS
1	D	513	LEU
1	D	532	LEU
1	D	533	GLU
1	D	558	VAL
1	D	566	LYS
1	D	620	SER
1	D	646	ILE
1	D	741	GLU
1	D	744	TYR
1	D	753	VAL
1	D	789	VAL
1	D	808	VAL
1	D	857	VAL
1	D	868	VAL
1	D	912	PHE
1	D	970	GLU
1	D	971	GLU
1	D	1003	PRO
1	D	1073	PRO
1	D	1119	THR
1	D	1135	ARG
1	D	1146	ASN
1	D	1217	GLU
1	D	1222	THR
1	D	1240	PHE
1	D	1277	ASP
1	D	1325	ASN
1	D	1327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	71	ASN
1	A	131	GLN
1	A	351	ASN
1	A	450	GLN
1	A	473	GLN
1	A	531	ASN
1	A	551	GLN
1	A	586	GLN
1	A	651	ASN
1	A	1087	ASN
1	A	1146	ASN
1	A	1285	GLN
1	A	1290	ASN
1	B	63	ASN
1	B	131	GLN
1	B	351	ASN
1	B	450	GLN
1	B	473	GLN
1	B	531	ASN
1	B	651	ASN
1	B	748	HIS
1	B	1087	ASN
1	B	1109	ASN
1	B	1146	ASN
1	B	1285	GLN
1	B	1289	ASN
1	B	1325	ASN
1	C	63	ASN
1	C	131	GLN
1	C	322	GLN
1	C	351	ASN
1	C	450	GLN
1	C	461	ASN
1	C	473	GLN
1	C	484	GLN
1	C	529	GLN
1	C	586	GLN
1	C	651	ASN
1	C	684	GLN
1	C	876	GLN
1	C	1087	ASN
1	C	1109	ASN

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Mol	Chain	Res	Type
1	C	1146	ASN
1	C	1285	GLN
1	D	62	GLN
1	D	63	ASN
1	D	131	GLN
1	D	450	GLN
1	D	461	ASN
1	D	471	GLN
1	D	473	GLN
1	D	529	GLN
1	D	586	GLN
1	D	841	HIS
1	D	1087	ASN
1	D	1146	ASN
1	D	1285	GLN
1	D	1289	ASN
1	D	1290	ASN
1	D	1325	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FES	C	2002	1	0,4,4	-	-	-		
4	FES	A	2002	1	0,4,4	-	-	-		
2	BCT	C	6003	-	0,3,3	-	-	0,3,3	-	-
4	FES	B	2002	1	0,4,4	-	-	-		
5	FAD	D	5003	-	51,58,58	2.85	20 (39%)	60,89,89	2.90	25 (41%)
8	SAL	A	2006	-	8,10,10	1.94	4 (50%)	9,13,13	1.22	1 (11%)
4	FES	D	2002	1	0,4,4	-	-	-		
2	BCT	B	6002	-	0,3,3	-	-	0,3,3	-	-
2	BCT	D	6004	-	0,3,3	-	-	0,3,3	-	-
7	MOM	C	4005	6	0,3,3	-	-	-		
4	FES	B	2001	1	0,4,4	-	-	-		
6	MTE	D	5004	7	21,26,26	7.01	14 (66%)	21,40,40	5.69	9 (42%)
6	MTE	A	2004	7	21,26,26	7.11	12 (57%)	21,40,40	3.10	10 (47%)
6	MTE	C	4004	7	21,26,26	7.07	13 (61%)	21,40,40	6.20	10 (47%)
4	FES	C	2001	1	0,4,4	-	-	-		
6	MTE	B	3004	7	21,26,26	6.62	13 (61%)	21,40,40	4.09	9 (42%)
5	FAD	C	4003	-	51,58,58	2.93	22 (43%)	60,89,89	2.91	24 (40%)
8	SAL	C	4006	-	8,10,10	2.11	4 (50%)	9,13,13	1.18	0
5	FAD	B	3003	-	51,58,58	2.96	22 (43%)	60,89,89	2.92	23 (38%)
7	MOM	A	2005	6	0,3,3	-	-	-		
7	MOM	D	5005	6	0,3,3	-	-	-		
8	SAL	D	5006	-	8,10,10	2.15	4 (50%)	9,13,13	1.19	0
7	MOM	B	3005	6	0,3,3	-	-	-		
5	FAD	A	2003	-	51,58,58	2.93	21 (41%)	60,89,89	2.93	24 (40%)
4	FES	A	2001	1	0,4,4	-	-	-		
4	FES	D	2001	1	0,4,4	-	-	-		
2	BCT	A	6001	-	0,3,3	-	-	0,3,3	-	-
8	SAL	B	3006	-	8,10,10	2.00	4 (50%)	9,13,13	1.20	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	C	2002	1	-	-	0/1/1/1
4	FES	A	2002	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	B	2002	1	-	-	0/1/1/1
8	SAL	A	2006	-	-	0/0/4/4	0/1/1/1
5	FAD	D	5003	-	-	5/30/50/50	0/6/6/6
4	FES	D	2002	1	-	-	0/1/1/1
4	FES	B	2001	1	-	-	0/1/1/1
6	MTE	D	5004	7	-	2/6/34/34	0/3/3/3
6	MTE	A	2004	7	-	3/6/34/34	0/3/3/3
6	MTE	C	4004	7	-	6/6/34/34	0/3/3/3
4	FES	C	2001	1	-	-	0/1/1/1
6	MTE	B	3004	7	-	3/6/34/34	0/3/3/3
5	FAD	C	4003	-	-	4/30/50/50	0/6/6/6
8	SAL	C	4006	-	-	0/0/4/4	0/1/1/1
5	FAD	B	3003	-	-	5/30/50/50	0/6/6/6
8	SAL	D	5006	-	-	0/0/4/4	0/1/1/1
5	FAD	A	2003	-	-	5/30/50/50	0/6/6/6
4	FES	A	2001	1	-	-	0/1/1/1
4	FES	D	2001	1	-	-	0/1/1/1
8	SAL	B	3006	-	-	0/0/4/4	0/1/1/1

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	5004	MTE	C7-C6	18.61	1.68	1.53
6	A	2004	MTE	C7-C6	18.49	1.68	1.53
6	B	3004	MTE	C7-C6	18.07	1.68	1.53
6	C	4004	MTE	C7-C6	17.81	1.67	1.53
6	B	3004	MTE	C4'-C3'	-15.35	1.31	1.52
6	C	4004	MTE	C9-N5	14.92	1.68	1.38
6	A	2004	MTE	C9-N5	14.77	1.68	1.38
6	A	2004	MTE	C6-N5	13.00	1.63	1.45
6	D	5004	MTE	C4'-C3'	-12.99	1.34	1.52
6	C	4004	MTE	C4'-C3'	-12.17	1.35	1.52
6	A	2004	MTE	C9-C10	11.47	1.63	1.41
6	D	5004	MTE	C9-N5	11.32	1.61	1.38
6	C	4004	MTE	C9-C10	11.27	1.62	1.41
6	B	3004	MTE	C9-C10	11.25	1.62	1.41
6	D	5004	MTE	C9-C10	11.22	1.62	1.41
5	B	3003	FAD	C10-N1	9.85	1.45	1.33
5	A	2003	FAD	C10-N1	9.30	1.45	1.33
5	C	4003	FAD	C10-N1	8.91	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5003	FAD	C10-N1	8.69	1.44	1.33
6	C	4004	MTE	O4'-C4'	-8.54	1.11	1.44
6	D	5004	MTE	O4'-C4'	-8.32	1.12	1.44
5	C	4003	FAD	C9A-N10	7.96	1.49	1.38
6	A	2004	MTE	C4'-C3'	-7.77	1.41	1.52
5	A	2003	FAD	C9A-N10	7.76	1.49	1.38
5	A	2003	FAD	C4X-C10	7.72	1.46	1.38
5	C	4003	FAD	C4X-C10	7.56	1.46	1.38
5	D	5003	FAD	C9A-N10	7.51	1.48	1.38
5	B	3003	FAD	C9A-N10	7.51	1.48	1.38
5	D	5003	FAD	C4X-C10	7.49	1.46	1.38
6	B	3004	MTE	C6-N5	7.47	1.55	1.45
5	B	3003	FAD	C4X-C10	7.43	1.46	1.38
6	B	3004	MTE	P-O4'	-6.79	1.38	1.60
6	C	4004	MTE	P-O4'	-6.65	1.38	1.60
5	B	3003	FAD	C4-N3	6.61	1.44	1.33
5	C	4003	FAD	C4-N3	6.56	1.44	1.33
6	D	5004	MTE	C6-N5	6.52	1.54	1.45
6	D	5004	MTE	P-O4'	-6.51	1.39	1.60
5	A	2003	FAD	C4-N3	6.45	1.44	1.33
6	A	2004	MTE	P-O4'	-6.45	1.39	1.60
5	D	5003	FAD	C4-N3	6.13	1.43	1.33
6	D	5004	MTE	C4-C9	5.80	1.49	1.41
6	B	3004	MTE	C4-C9	5.44	1.48	1.41
5	C	4003	FAD	C1'-N10	5.42	1.53	1.48
6	A	2004	MTE	C4-C9	5.38	1.48	1.41
5	D	5003	FAD	C1'-N10	5.20	1.53	1.48
5	B	3003	FAD	C1'-N10	5.06	1.53	1.48
6	C	4004	MTE	C6-N5	-4.94	1.38	1.45
6	C	4004	MTE	C4-C9	4.93	1.48	1.41
5	A	2003	FAD	C1'-N10	4.85	1.53	1.48
6	B	3004	MTE	C4-N3	4.83	1.41	1.33
6	C	4004	MTE	P-O3P	-4.72	1.36	1.54
6	D	5004	MTE	C4-N3	4.64	1.41	1.33
6	A	2004	MTE	P-O3P	-4.63	1.37	1.54
6	D	5004	MTE	P-O3P	-4.63	1.37	1.54
5	A	2003	FAD	C4X-N5	4.43	1.39	1.33
6	B	3004	MTE	P-O3P	-4.41	1.37	1.54
5	D	5003	FAD	C4X-N5	4.36	1.39	1.33
5	B	3003	FAD	C4X-N5	4.21	1.39	1.33
6	C	4004	MTE	C4-N3	4.18	1.40	1.33
5	C	4003	FAD	C4X-N5	4.11	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2004	MTE	C4-N3	4.04	1.40	1.33
6	B	3004	MTE	C9-N5	3.93	1.46	1.38
5	C	4003	FAD	C4A-N3A	3.70	1.40	1.35
5	D	5003	FAD	C4A-N3A	3.60	1.40	1.35
5	A	2003	FAD	C4A-N3A	3.57	1.40	1.35
5	B	3003	FAD	C4A-N3A	3.55	1.40	1.35
5	B	3003	FAD	C2A-N3A	3.55	1.37	1.32
5	A	2003	FAD	O4B-C1B	3.52	1.46	1.41
5	C	4003	FAD	O4B-C1B	3.44	1.45	1.41
8	C	4006	SAL	C1-C1'	-3.42	1.44	1.47
5	D	5003	FAD	C2A-N3A	3.37	1.37	1.32
6	A	2004	MTE	C2-N1	3.37	1.41	1.35
8	D	5006	SAL	C1-C1'	-3.31	1.44	1.47
5	B	3003	FAD	C9-C9A	3.30	1.47	1.40
5	C	4003	FAD	C2A-N3A	3.26	1.37	1.32
5	D	5003	FAD	O4B-C1B	3.23	1.45	1.41
6	B	3004	MTE	C2-N1	3.20	1.41	1.35
5	A	2003	FAD	C2A-N3A	3.17	1.37	1.32
5	A	2003	FAD	C9A-C5X	3.17	1.48	1.42
5	A	2003	FAD	C9-C9A	3.16	1.47	1.40
8	B	3006	SAL	C1-C1'	-3.08	1.44	1.47
5	C	4003	FAD	C9-C9A	3.07	1.46	1.40
5	C	4003	FAD	C9A-C5X	3.06	1.48	1.42
5	D	5003	FAD	C9-C9A	2.93	1.46	1.40
6	B	3004	MTE	O4-C4	2.93	1.31	1.24
8	A	2006	SAL	C5-C6	2.92	1.45	1.38
5	C	4003	FAD	C5'-C4'	2.91	1.55	1.51
6	D	5004	MTE	O4-C4	2.90	1.31	1.24
5	D	5003	FAD	C9A-C5X	2.90	1.48	1.42
5	C	4003	FAD	C8-C7	2.88	1.48	1.40
5	A	2003	FAD	C5'-C4'	2.87	1.55	1.51
8	D	5006	SAL	C5-C6	2.86	1.45	1.38
5	B	3003	FAD	C6-C7	2.85	1.45	1.37
5	B	3003	FAD	C9A-C5X	2.85	1.48	1.42
5	B	3003	FAD	O4B-C1B	2.82	1.45	1.41
5	D	5003	FAD	C6-C7	2.81	1.44	1.37
8	A	2006	SAL	C6-C1	2.81	1.44	1.40
5	A	2003	FAD	C8-C7	2.81	1.47	1.40
5	A	2003	FAD	C6-C7	2.80	1.44	1.37
8	D	5006	SAL	C6-C1	2.78	1.44	1.40
5	D	5003	FAD	C8-C7	2.78	1.47	1.40
6	C	4004	MTE	C2-N1	2.76	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	3006	SAL	C5-C6	2.75	1.44	1.38
5	B	3003	FAD	C2A-N1A	2.73	1.39	1.33
5	B	3003	FAD	C8-C7	2.73	1.47	1.40
8	C	4006	SAL	C5-C6	2.71	1.44	1.38
5	B	3003	FAD	C2-N3	2.69	1.43	1.38
5	A	2003	FAD	C5X-N5	2.68	1.39	1.35
5	D	5003	FAD	C2A-N1A	2.64	1.38	1.33
8	C	4006	SAL	C6-C1	2.64	1.44	1.40
6	A	2004	MTE	O4-C4	2.58	1.31	1.24
6	D	5004	MTE	C2-N1	2.55	1.39	1.35
6	C	4004	MTE	O4-C4	2.53	1.30	1.24
5	D	5003	FAD	C4'-C3'	2.52	1.58	1.53
5	C	4003	FAD	C2A-N1A	2.49	1.38	1.33
5	C	4003	FAD	C4'-C3'	2.47	1.58	1.53
5	C	4003	FAD	C6-C7	2.47	1.44	1.37
5	A	2003	FAD	C2A-N1A	2.47	1.38	1.33
8	A	2006	SAL	C3-C2	2.47	1.43	1.39
5	A	2003	FAD	P-O1P	2.46	1.59	1.50
8	B	3006	SAL	C6-C1	2.45	1.43	1.40
6	D	5004	MTE	P-O1P	2.44	1.58	1.50
5	B	3003	FAD	C4'-C3'	2.41	1.58	1.53
5	C	4003	FAD	C5X-N5	2.40	1.39	1.35
8	B	3006	SAL	C3-C2	2.39	1.43	1.39
5	D	5003	FAD	C2-N3	2.38	1.42	1.38
6	B	3004	MTE	O3'-C3'	2.37	1.46	1.43
5	D	5003	FAD	PA-O1A	2.37	1.59	1.50
5	D	5003	FAD	C5'-C4'	2.36	1.55	1.51
8	D	5006	SAL	C3-C2	2.36	1.43	1.39
8	C	4006	SAL	C3-C2	2.34	1.43	1.39
5	A	2003	FAD	PA-O1A	2.32	1.59	1.50
5	C	4003	FAD	P-O1P	2.32	1.59	1.50
5	B	3003	FAD	C5'-C4'	2.32	1.55	1.51
5	B	3003	FAD	P-O1P	2.32	1.59	1.50
5	B	3003	FAD	C5X-N5	2.31	1.39	1.35
5	C	4003	FAD	C2-N3	2.29	1.42	1.38
5	D	5003	FAD	P-O1P	2.28	1.59	1.50
5	B	3003	FAD	PA-O1A	2.27	1.59	1.50
5	C	4003	FAD	PA-O1A	2.23	1.58	1.50
5	A	2003	FAD	C6-C5X	2.21	1.45	1.41
5	D	5003	FAD	C5X-N5	2.21	1.39	1.35
5	B	3003	FAD	C9-C8	2.18	1.43	1.37
5	C	4003	FAD	C2'-C3'	2.13	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2003	FAD	C2-N3	2.10	1.42	1.38
6	A	2004	MTE	C2'-C1'	2.06	1.48	1.35
5	C	4003	FAD	C9-C8	2.06	1.42	1.37
6	C	4004	MTE	C2'-C1'	2.05	1.48	1.35
5	B	3003	FAD	C5A-N7A	-2.05	1.32	1.39
6	B	3004	MTE	C2'-C1'	2.04	1.48	1.35
8	A	2006	SAL	C1-C1'	-2.04	1.45	1.47
6	D	5004	MTE	C2'-C1'	2.02	1.48	1.35
5	A	2003	FAD	C9-C8	2.00	1.42	1.37

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	5004	MTE	P-O4'-C4'	20.58	174.99	118.30
6	C	4004	MTE	P-O4'-C4'	19.50	172.01	118.30
6	C	4004	MTE	C4-C9-N5	17.45	133.76	119.12
6	B	3004	MTE	C4-C9-N5	14.09	130.95	119.12
5	A	2003	FAD	C1'-N10-C9A	11.72	127.52	118.29
6	D	5004	MTE	C4-C9-N5	11.58	128.84	119.12
5	D	5003	FAD	C1'-N10-C9A	11.56	127.39	118.29
5	C	4003	FAD	C1'-N10-C9A	11.49	127.33	118.29
5	B	3003	FAD	C1'-N10-C9A	11.19	127.10	118.29
5	B	3003	FAD	C4X-N5-C5X	8.44	125.21	116.77
6	A	2004	MTE	C4-C9-N5	8.33	126.11	119.12
5	C	4003	FAD	C4X-N5-C5X	8.29	125.05	116.77
5	D	5003	FAD	C4X-N5-C5X	8.06	124.83	116.77
5	A	2003	FAD	C4X-N5-C5X	7.97	124.73	116.77
5	A	2003	FAD	C4-N3-C2	7.68	121.62	115.14
5	B	3003	FAD	C4-N3-C2	7.55	121.51	115.14
5	C	4003	FAD	C4-N3-C2	7.33	121.33	115.14
5	D	5003	FAD	C4-N3-C2	7.24	121.25	115.14
5	C	4003	FAD	N3A-C2A-N1A	-6.99	117.75	128.68
5	A	2003	FAD	N3A-C2A-N1A	-6.98	117.77	128.68
5	B	3003	FAD	N3A-C2A-N1A	-6.90	117.89	128.68
5	D	5003	FAD	N3A-C2A-N1A	-6.88	117.92	128.68
6	D	5004	MTE	C2-N1-C10	5.99	127.97	114.54
6	B	3004	MTE	C2-N1-C10	5.98	127.95	114.54
5	A	2003	FAD	C1'-N10-C10	-5.88	113.14	118.41
6	A	2004	MTE	C2-N1-C10	5.83	127.60	114.54
6	C	4004	MTE	C2-N1-C10	5.81	127.56	114.54
5	D	5003	FAD	C1'-N10-C10	-5.68	113.32	118.41
5	C	4003	FAD	C1'-N10-C10	-5.55	113.44	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3003	FAD	C1'-N10-C10	-5.51	113.47	118.41
6	B	3004	MTE	P-O4'-C4'	5.38	133.12	118.30
6	D	5004	MTE	N2-C2-N3	4.54	124.31	117.25
6	B	3004	MTE	C4-N3-C2	4.45	123.00	115.93
6	C	4004	MTE	C4-N3-C2	4.39	122.91	115.93
6	C	4004	MTE	N2-C2-N3	4.39	124.08	117.25
6	A	2004	MTE	C4-N3-C2	4.37	122.87	115.93
6	B	3004	MTE	N2-C2-N3	4.36	124.04	117.25
6	D	5004	MTE	C4-N3-C2	4.35	122.85	115.93
5	B	3003	FAD	O4'-C4'-C3'	4.35	119.68	109.10
6	A	2004	MTE	N2-C2-N3	4.35	124.02	117.25
5	C	4003	FAD	O4'-C4'-C3'	4.25	119.43	109.10
5	D	5003	FAD	O4'-C4'-C3'	4.22	119.36	109.10
5	A	2003	FAD	O4'-C4'-C3'	4.06	118.97	109.10
6	B	3004	MTE	N3-C2-N1	-3.92	119.27	125.42
5	B	3003	FAD	C3B-C2B-C1B	3.87	106.81	100.98
6	C	4004	MTE	N3-C2-N1	-3.78	119.49	125.42
6	D	5004	MTE	N3-C2-N1	-3.77	119.50	125.42
6	A	2004	MTE	N3-C2-N1	-3.75	119.54	125.42
6	C	4004	MTE	O3'-C7-C6	-3.68	106.51	108.96
6	B	3004	MTE	O3'-C7-C6	-3.57	106.58	108.96
6	A	2004	MTE	O3'-C7-C6	-3.41	106.69	108.96
5	A	2003	FAD	C5'-C4'-C3'	-3.29	105.84	112.20
6	D	5004	MTE	O3'-C7-N8	-3.27	105.20	108.57
5	C	4003	FAD	C3B-C2B-C1B	3.25	105.87	100.98
5	B	3003	FAD	O3'-C3'-C4'	3.18	116.50	108.81
5	A	2003	FAD	C4-C4X-N5	3.18	122.23	118.60
5	D	5003	FAD	C5'-C4'-C3'	-3.18	106.06	112.20
5	A	2003	FAD	C3B-C2B-C1B	3.17	105.75	100.98
5	C	4003	FAD	C4-C4X-N5	3.12	122.16	118.60
5	B	3003	FAD	C5'-C4'-C3'	-3.11	106.19	112.20
5	D	5003	FAD	C4-C4X-N5	3.11	122.15	118.60
5	C	4003	FAD	C5'-C4'-C3'	-3.02	106.37	112.20
6	C	4004	MTE	O3'-C7-N8	-3.02	105.47	108.57
5	B	3003	FAD	C4-C4X-N5	2.99	122.01	118.60
5	D	5003	FAD	O3'-C3'-C4'	2.96	115.97	108.81
5	B	3003	FAD	C10-C4X-N5	-2.83	119.30	121.26
6	A	2004	MTE	O3'-C7-N8	-2.82	105.66	108.57
5	C	4003	FAD	O3'-C3'-C4'	2.80	115.59	108.81
5	D	5003	FAD	C3B-C2B-C1B	2.77	105.15	100.98
5	B	3003	FAD	O2B-C2B-C3B	2.77	120.78	111.82
5	D	5003	FAD	O2B-C2B-C3B	2.76	120.77	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	FAD	O3'-C3'-C4'	2.75	115.45	108.81
5	C	4003	FAD	O3B-C3B-C4B	-2.68	103.31	111.05
5	A	2003	FAD	O3B-C3B-C4B	-2.67	103.34	111.05
5	D	5003	FAD	C10-C4X-N5	-2.66	119.42	121.26
5	A	2003	FAD	C10-C4X-N5	-2.66	119.42	121.26
5	B	3003	FAD	O3B-C3B-C4B	-2.63	103.43	111.05
5	C	4003	FAD	C10-C4X-N5	-2.62	119.45	121.26
5	A	2003	FAD	O2B-C2B-C3B	2.56	120.09	111.82
6	D	5004	MTE	C9-C10-N8	2.55	120.47	118.13
5	C	4003	FAD	O2B-C2B-C3B	2.55	120.07	111.82
6	A	2004	MTE	P-O4'-C4'	2.54	125.30	118.30
5	A	2003	FAD	C2A-N1A-C6A	2.54	123.10	118.75
5	A	2003	FAD	O5B-PA-O1A	2.51	118.86	109.07
5	D	5003	FAD	O3B-C3B-C4B	-2.48	103.87	111.05
5	C	4003	FAD	C4X-C4-N3	-2.48	120.04	123.43
5	D	5003	FAD	O5B-PA-O1A	2.47	118.72	109.07
5	C	4003	FAD	C2A-N1A-C6A	2.46	122.96	118.75
5	D	5003	FAD	O2'-C2'-C1'	2.45	115.49	109.59
6	A	2004	MTE	C9-N5-C6	-2.44	111.16	120.00
5	C	4003	FAD	O5B-PA-O1A	2.43	118.54	109.07
5	A	2003	FAD	C4-C4X-C10	-2.42	118.35	119.95
5	D	5003	FAD	C2A-N1A-C6A	2.42	122.89	118.75
5	B	3003	FAD	O2'-C2'-C1'	2.38	115.33	109.59
5	D	5003	FAD	C8M-C8-C7	2.38	125.61	120.74
6	A	2004	MTE	C9-C10-N8	2.37	120.30	118.13
5	C	4003	FAD	C4-C4X-C10	-2.36	118.39	119.95
5	B	3003	FAD	O5B-PA-O1A	2.36	118.28	109.07
5	B	3003	FAD	C4X-C4-N3	-2.34	120.22	123.43
5	D	5003	FAD	C4X-C4-N3	-2.34	120.22	123.43
5	D	5003	FAD	C8M-C8-C9	-2.34	114.75	120.34
5	A	2003	FAD	C4X-C4-N3	-2.33	120.24	123.43
5	D	5003	FAD	C4-C4X-C10	-2.30	118.43	119.95
5	A	2003	FAD	C8M-C8-C7	2.30	125.44	120.74
5	B	3003	FAD	C2A-N1A-C6A	2.29	122.68	118.75
5	C	4003	FAD	C8M-C8-C7	2.29	125.43	120.74
5	C	4003	FAD	C7M-C7-C6	-2.28	114.89	120.34
6	B	3004	MTE	O3'-C7-N8	-2.28	106.23	108.57
5	B	3003	FAD	C8M-C8-C7	2.27	125.39	120.74
5	A	2003	FAD	C8M-C8-C9	-2.26	114.93	120.34
5	C	4003	FAD	C8M-C8-C9	-2.25	114.95	120.34
5	D	5003	FAD	O4B-C1B-C2B	-2.25	103.64	106.93
5	A	2003	FAD	O5'-P-O1P	2.22	117.72	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	FAD	C7M-C7-C6	-2.21	115.05	120.34
6	B	3004	MTE	C9-C10-N8	2.20	120.14	118.13
6	D	5004	MTE	O2P-P-O4'	2.18	112.54	106.73
5	B	3003	FAD	C8M-C8-C9	-2.18	115.13	120.34
5	B	3003	FAD	C9A-C5X-N5	-2.15	118.99	122.36
5	D	5003	FAD	C9A-C5X-N5	-2.14	119.02	122.36
8	A	2006	SAL	C3-C2-C1	2.13	123.66	120.37
5	C	4003	FAD	O5'-P-O1P	2.12	117.35	109.07
5	D	5003	FAD	O5'-P-O1P	2.12	117.35	109.07
8	B	3006	SAL	C3-C2-C1	2.12	123.64	120.37
5	A	2003	FAD	C4'-C3'-C2'	-2.11	108.96	113.36
5	B	3003	FAD	C7M-C7-C6	-2.11	115.31	120.34
5	A	2003	FAD	C9A-C5X-N5	-2.10	119.07	122.36
5	C	4003	FAD	C9A-C5X-N5	-2.09	119.09	122.36
5	D	5003	FAD	C7M-C7-C6	-2.08	115.36	120.34
5	B	3003	FAD	C4'-C3'-C2'	-2.08	109.04	113.36
6	C	4004	MTE	C9-C10-N8	2.07	120.02	118.13
5	A	2003	FAD	O2'-C2'-C1'	2.06	114.55	109.59
6	C	4004	MTE	O2P-P-O4'	2.06	112.21	106.73
5	D	5003	FAD	C9A-N10-C10	-2.06	119.22	121.91
5	C	4003	FAD	C9A-N10-C10	-2.05	119.22	121.91
5	B	3003	FAD	O5'-P-O1P	2.03	117.01	109.07
5	C	4003	FAD	O2'-C2'-C1'	2.03	114.48	109.59

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2003	FAD	N10-C1'-C2'-O2'
5	A	2003	FAD	N10-C1'-C2'-C3'
5	B	3003	FAD	N10-C1'-C2'-O2'
5	B	3003	FAD	N10-C1'-C2'-C3'
5	C	4003	FAD	N10-C1'-C2'-O2'
5	C	4003	FAD	N10-C1'-C2'-C3'
5	D	5003	FAD	N10-C1'-C2'-O2'
5	D	5003	FAD	N10-C1'-C2'-C3'
6	A	2004	MTE	C4'-O4'-P-O2P
6	A	2004	MTE	C4'-O4'-P-O3P
6	B	3004	MTE	C4'-O4'-P-O1P
6	B	3004	MTE	C4'-O4'-P-O2P
6	B	3004	MTE	C4'-O4'-P-O3P
6	C	4004	MTE	C4'-O4'-P-O1P

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Mol	Chain	Res	Type	Atoms
6	C	4004	MTE	C4'-O4'-P-O2P
6	C	4004	MTE	C4'-O4'-P-O3P
6	D	5004	MTE	C2'-C3'-C4'-O4'
5	B	3003	FAD	C2'-C3'-C4'-O4'
5	A	2003	FAD	C2'-C3'-C4'-O4'
5	C	4003	FAD	C2'-C3'-C4'-O4'
6	A	2004	MTE	C3'-C4'-O4'-P
5	B	3003	FAD	O3'-C3'-C4'-O4'
6	C	4004	MTE	C2'-C3'-C4'-O4'
5	D	5003	FAD	C2'-C3'-C4'-O4'
5	A	2003	FAD	O3'-C3'-C4'-O4'
5	C	4003	FAD	O3'-C3'-C4'-O4'
6	C	4004	MTE	O3'-C3'-C4'-O4'
6	D	5004	MTE	O3'-C3'-C4'-O4'
5	D	5003	FAD	O3'-C3'-C4'-O4'
5	B	3003	FAD	C2'-C3'-C4'-C5'
6	C	4004	MTE	C3'-C4'-O4'-P
5	A	2003	FAD	O4'-C4'-C5'-O5'
5	D	5003	FAD	O4'-C4'-C5'-O5'

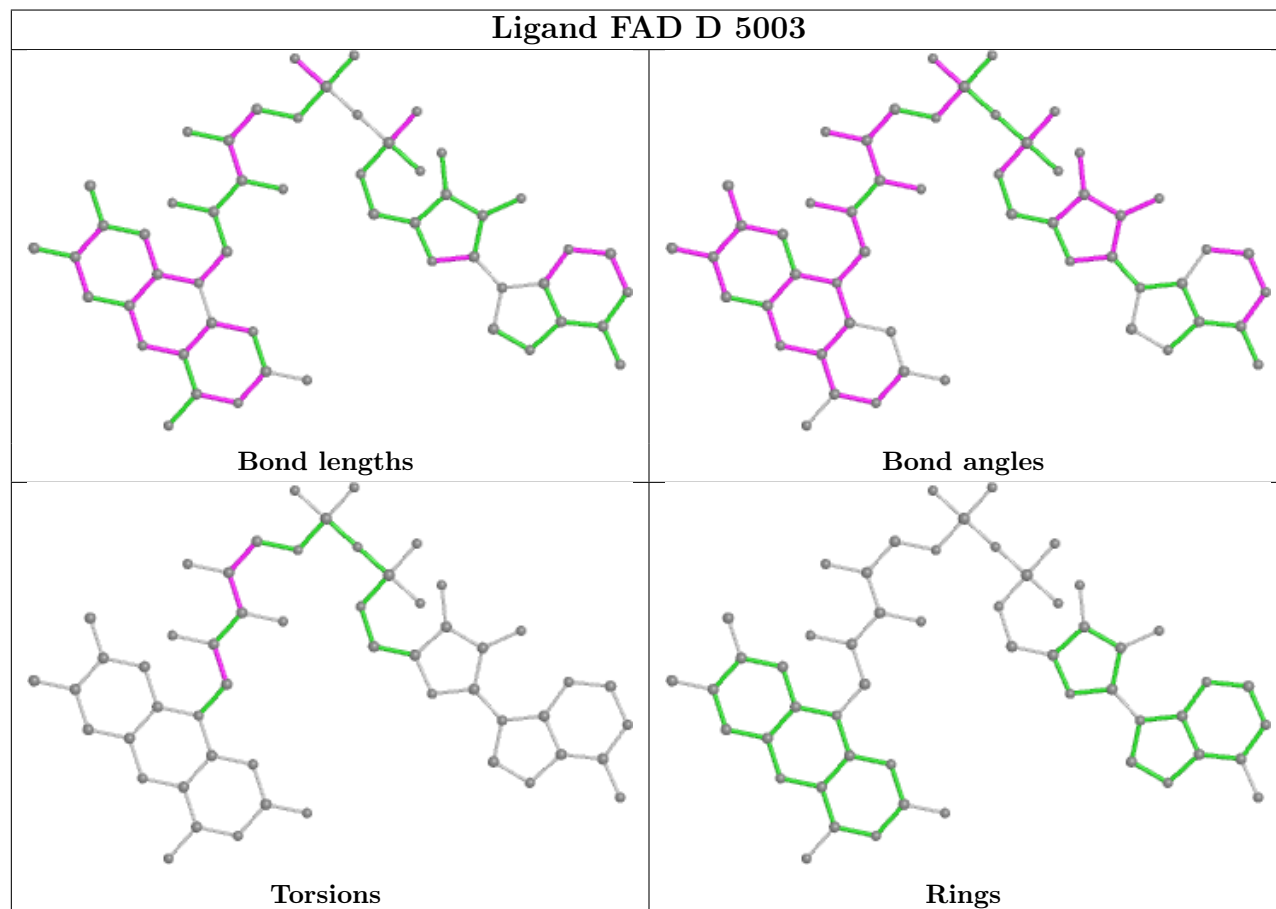
There are no ring outliers.

15 monomers are involved in 32 short contacts:

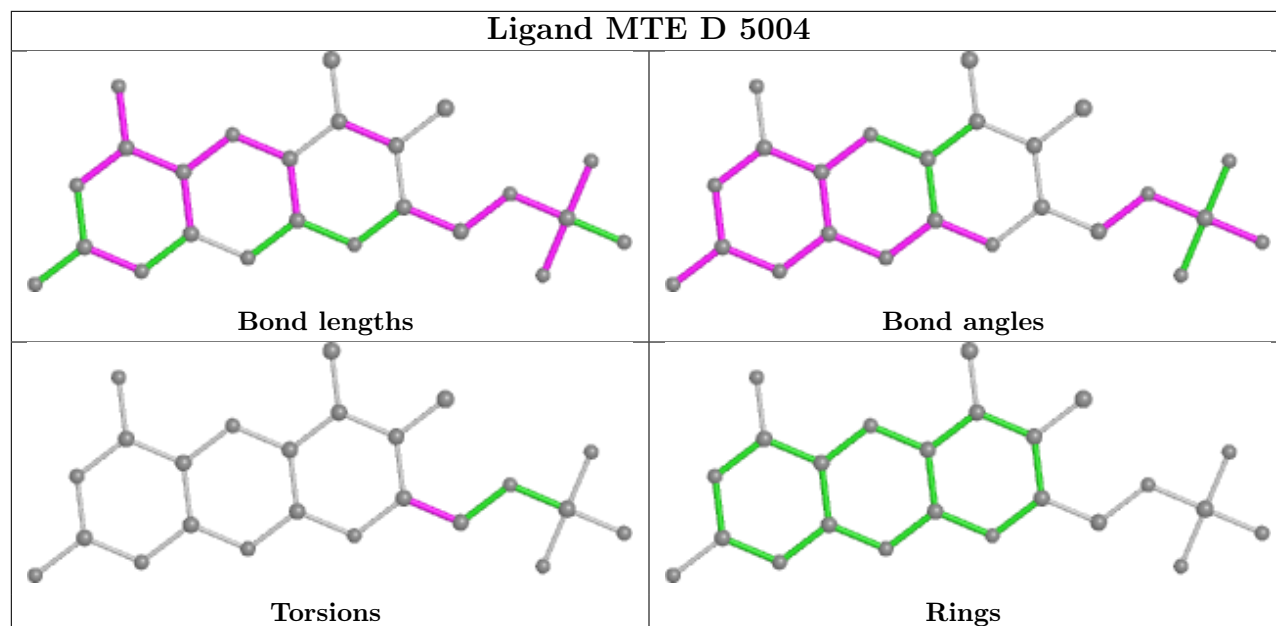
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5003	FAD	3	0
4	D	2002	FES	1	0
2	B	6002	BCT	1	0
7	C	4005	MOM	2	0
6	D	5004	MTE	2	0
6	A	2004	MTE	4	0
6	C	4004	MTE	2	0
6	B	3004	MTE	2	0
5	C	4003	FAD	2	0
5	B	3003	FAD	3	0
7	A	2005	MOM	2	0
7	D	5005	MOM	3	0
7	B	3005	MOM	2	0
5	A	2003	FAD	2	0
2	A	6001	BCT	1	0

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

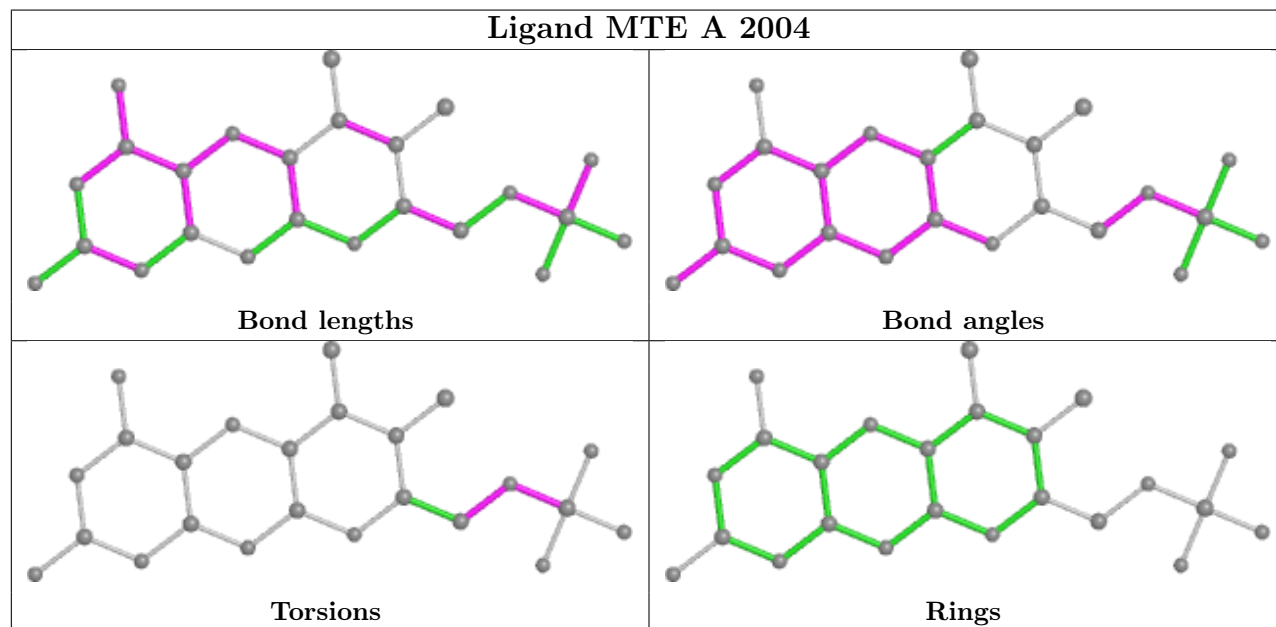
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



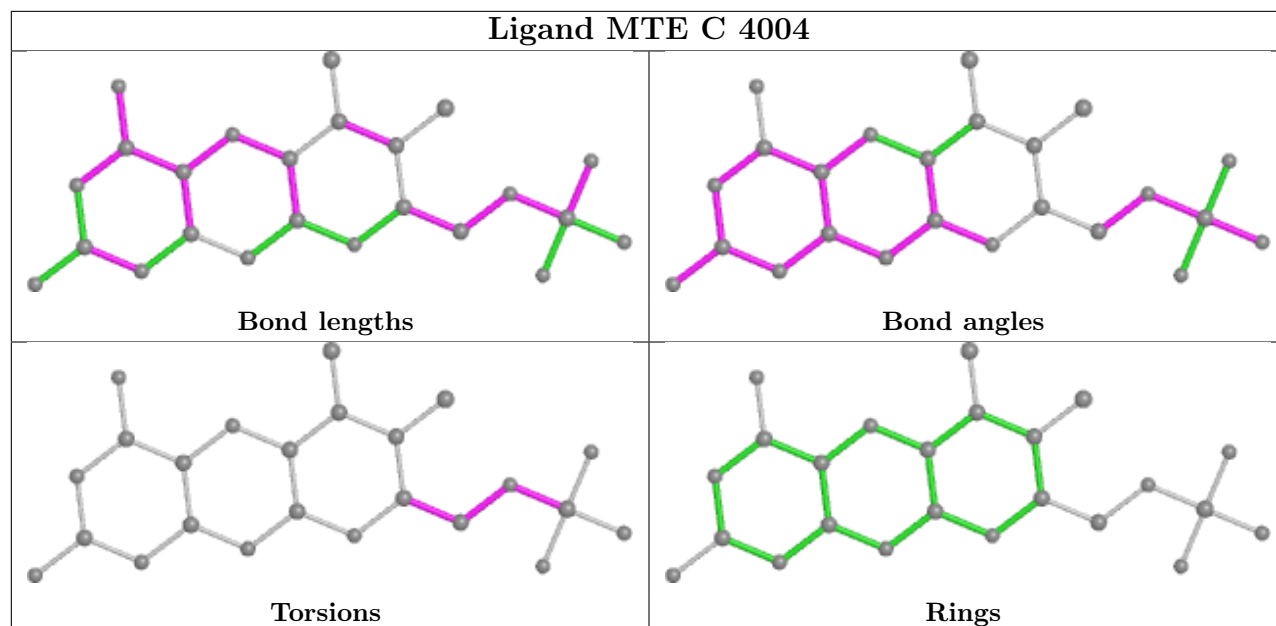
Ligand MTE D 5004



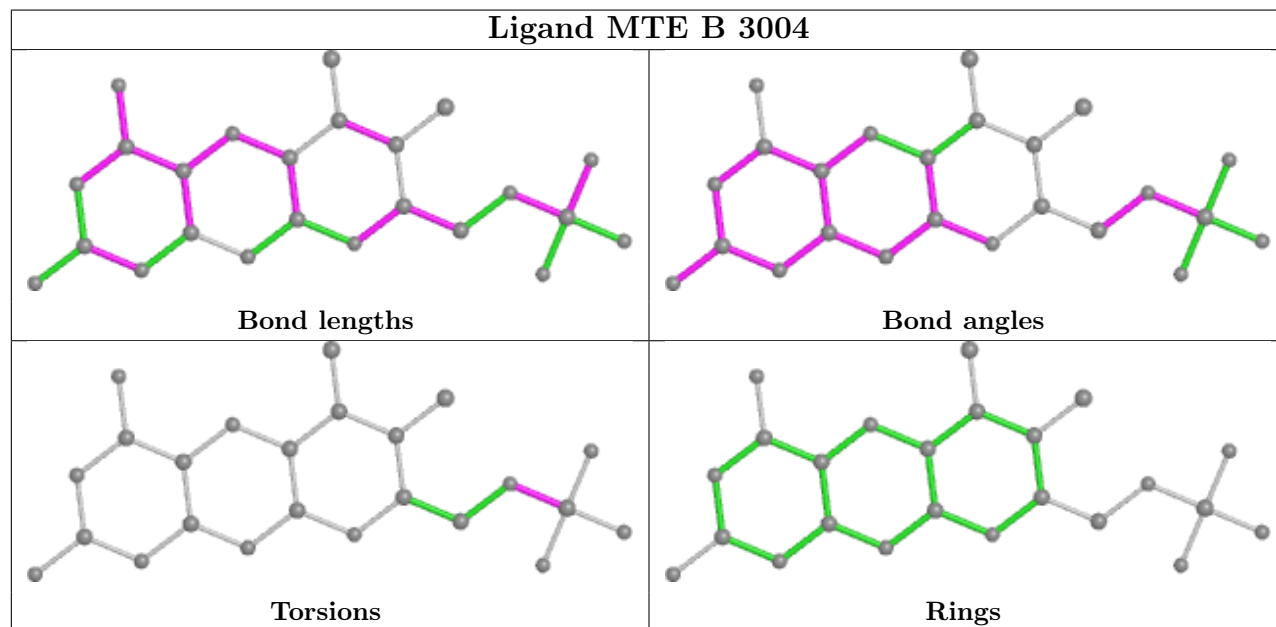
Ligand MTE A 2004

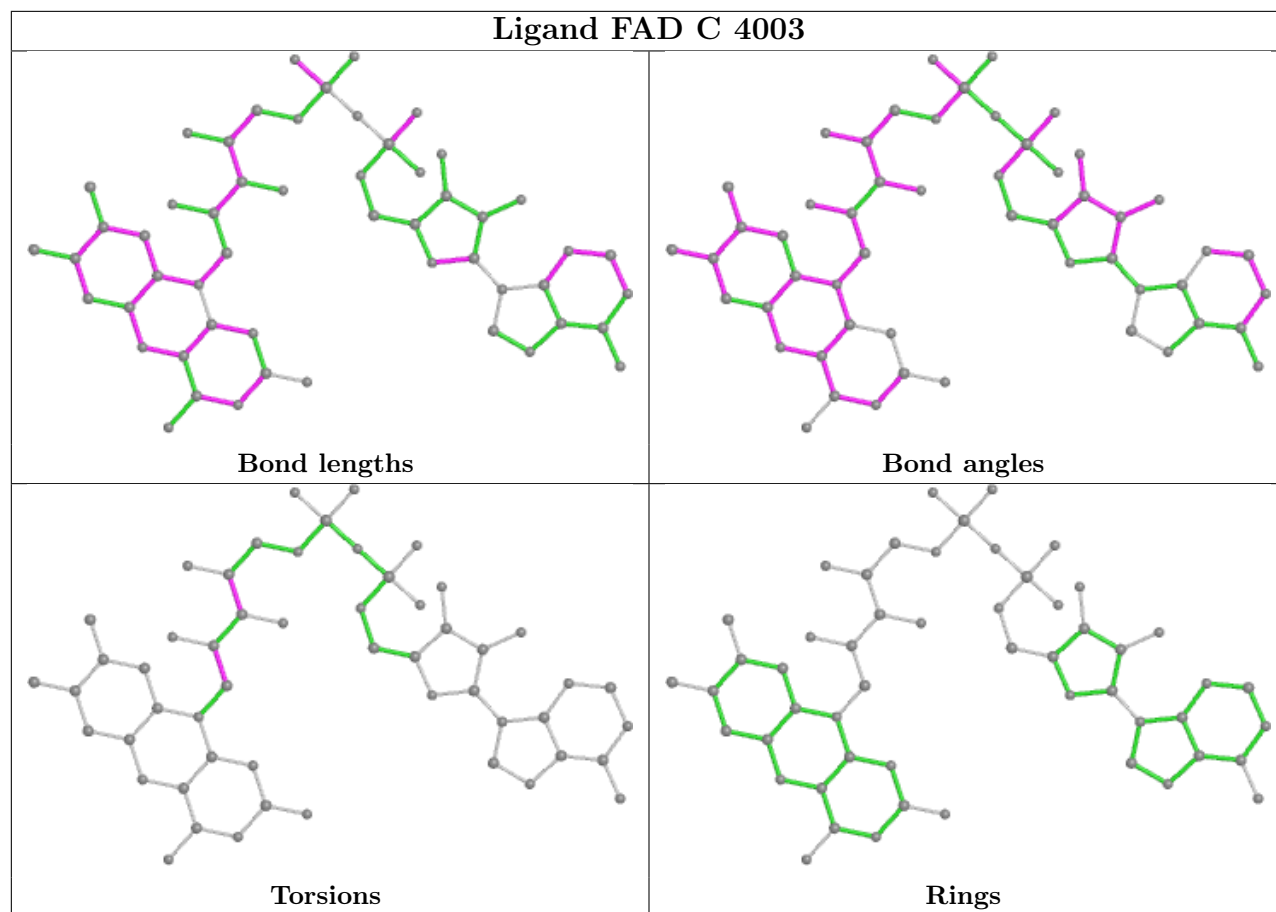


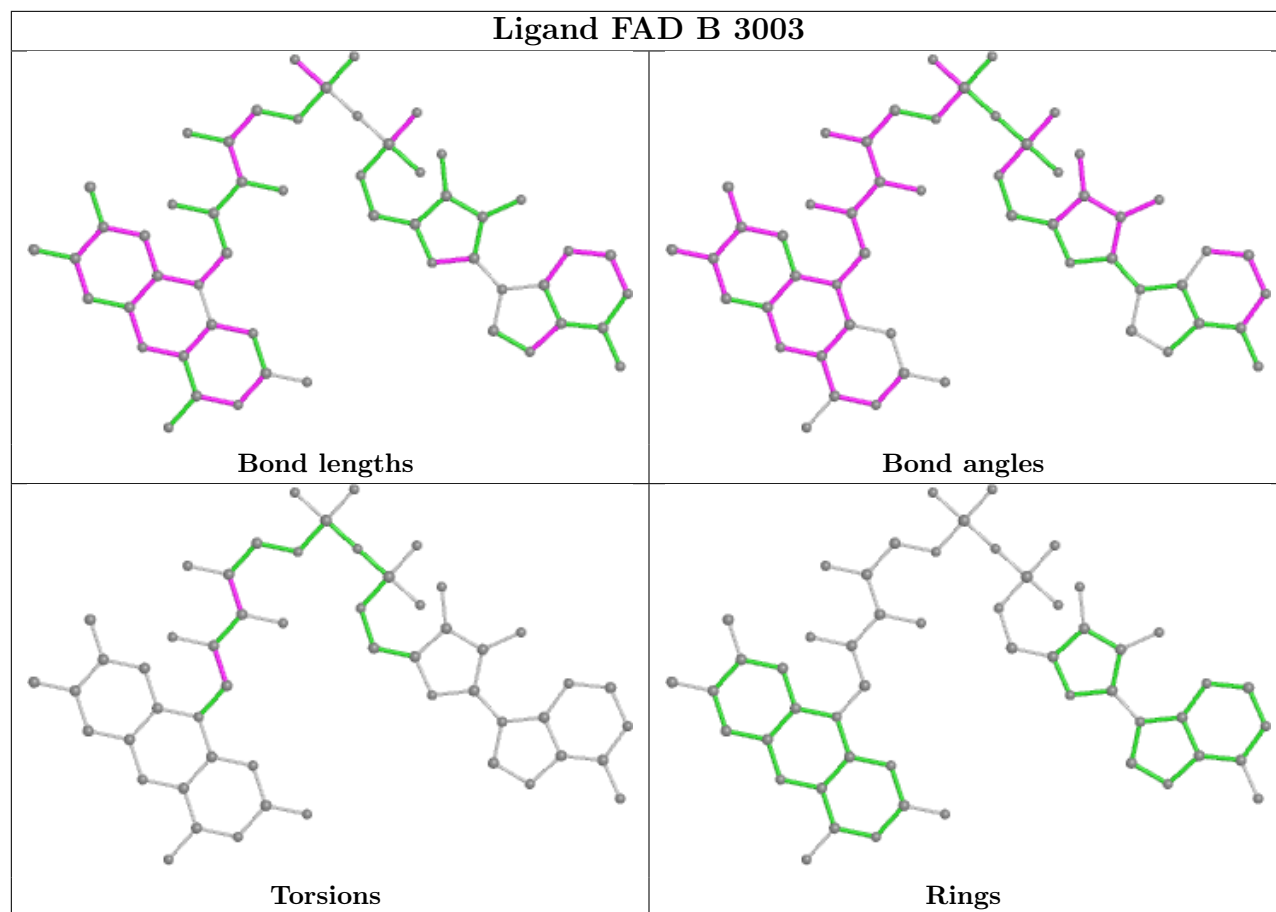
Ligand MTE C 4004

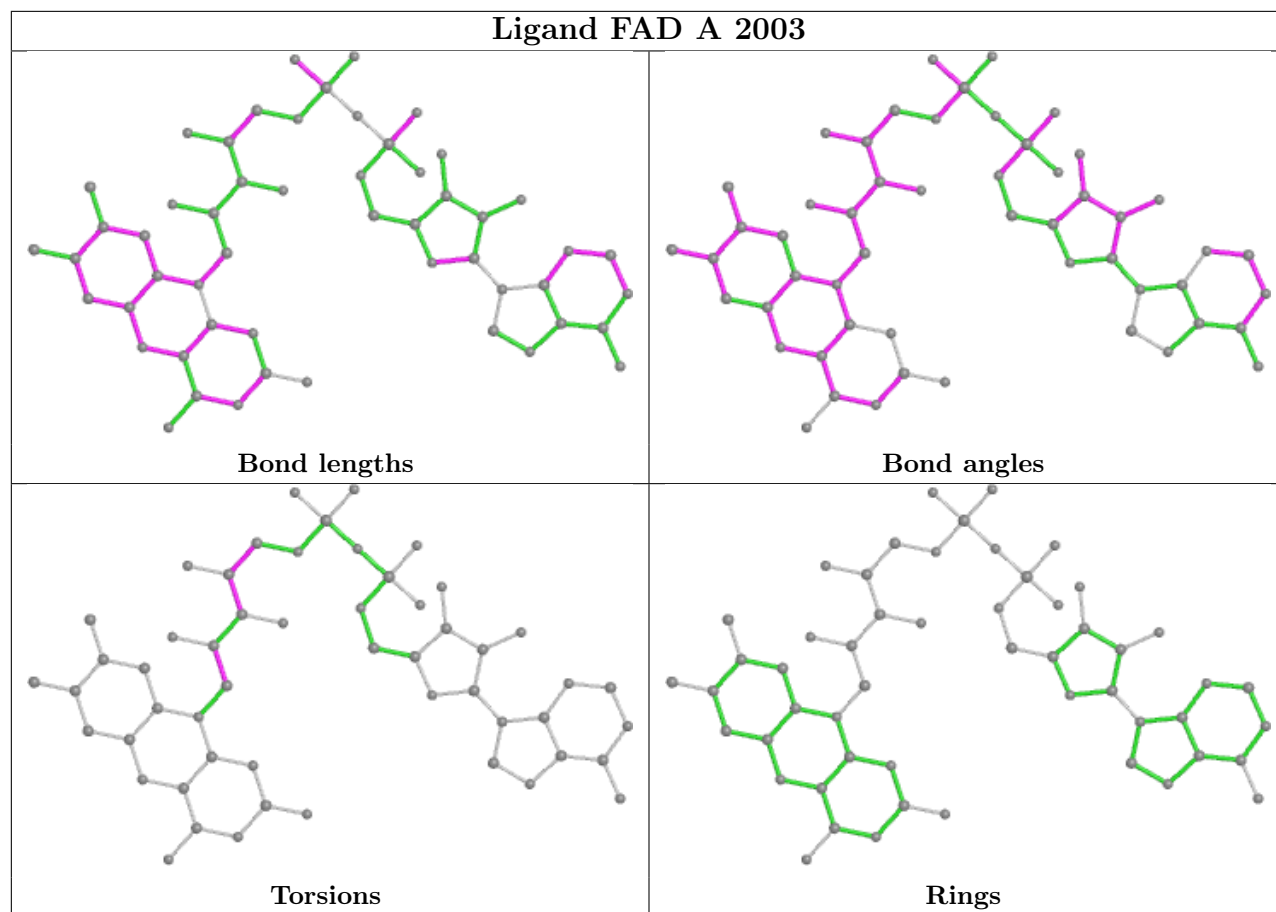


Ligand MTE B 3004









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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1307/1333 (98%)	-0.39	11 (0%) 86 84	10, 27, 56, 169	0
1	B	1307/1333 (98%)	-0.47	5 (0%) 92 91	10, 25, 52, 166	0
1	C	1307/1333 (98%)	-0.43	7 (0%) 91 89	9, 26, 54, 156	0
1	D	1307/1333 (98%)	-0.46	9 (0%) 87 86	8, 25, 55, 150	0
All	All	5228/5332 (98%)	-0.44	32 (0%) 89 88	8, 26, 55, 169	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1321	GLY	4.9
1	B	1325	ASN	4.8
1	C	1289	ASN	4.7
1	D	1325	ASN	4.5
1	B	566	LYS	4.1
1	A	538	LYS	3.8
1	B	1324	GLU	3.8
1	A	1288	GLY	3.4
1	D	566	LYS	3.3
1	D	167	GLY	3.1
1	C	1112	GLY	3.1
1	D	1324	GLU	2.9
1	C	1111	SER	2.8
1	C	60	ARG	2.8
1	A	1289	ASN	2.7
1	C	566	LYS	2.6
1	A	566	LYS	2.6
1	D	3	ALA	2.6
1	A	219	LEU	2.5
1	D	1323	PRO	2.5
1	A	3	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1323	PRO	2.3
1	A	223	PRO	2.3
1	A	1325	ASN	2.2
1	C	167	GLY	2.2
1	A	1111	SER	2.1
1	C	472	ARG	2.1
1	A	192	SER	2.1
1	D	1332	ARG	2.1
1	A	1110	PRO	2.0
1	D	1322	VAL	2.0
1	D	377	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	B	7003	1/1	0.91	0.20	20,20,20,20	0
8	SAL	C	4006	10/10	0.91	0.19	36,37,37,38	0
8	SAL	B	3006	10/10	0.92	0.19	41,42,42,43	0
8	SAL	D	5006	10/10	0.92	0.20	41,42,42,43	0
8	SAL	A	2006	10/10	0.93	0.18	36,37,37,38	0
2	BCT	C	6003	4/4	0.94	0.20	17,18,19,19	0
6	MTE	D	5004	24/24	0.94	0.13	19,23,28,30	0
2	BCT	D	6004	4/4	0.94	0.17	17,18,19,19	0
2	BCT	A	6001	4/4	0.95	0.17	17,18,19,19	0
6	MTE	B	3004	24/24	0.95	0.12	19,23,28,30	0
6	MTE	C	4004	24/24	0.95	0.12	20,24,28,30	0
3	CA	A	7001	1/1	0.95	0.18	20,20,20,20	0

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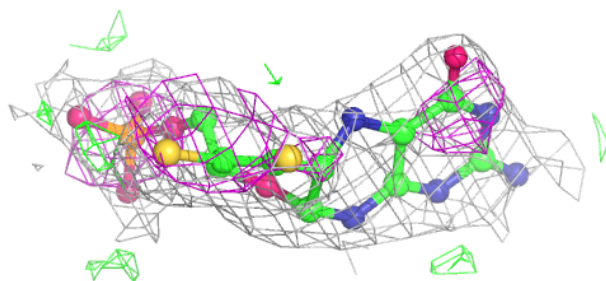
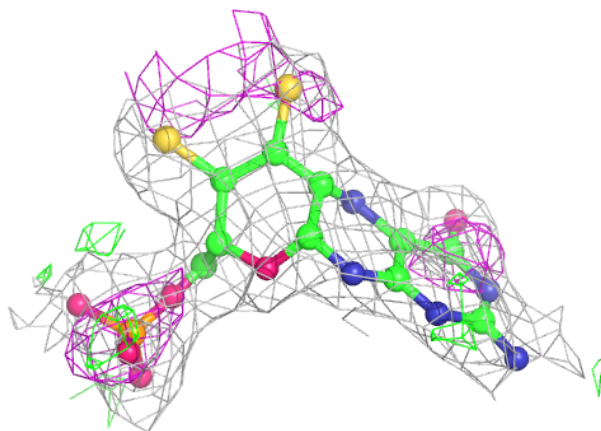
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FES	A	2001	4/4	0.96	0.12	14,14,14,33	0
5	FAD	B	3003	53/53	0.96	0.16	26,34,47,49	0
5	FAD	C	4003	53/53	0.96	0.17	26,36,47,49	0
5	FAD	D	5003	53/53	0.96	0.16	26,35,45,47	0
6	MTE	A	2004	24/24	0.96	0.12	20,24,28,30	0
3	CA	D	7007	1/1	0.96	0.17	20,20,20,20	0
3	CA	C	7005	1/1	0.97	0.14	20,20,20,20	0
3	CA	A	7002	1/1	0.97	0.38	18,18,18,18	0
2	BCT	B	6002	4/4	0.97	0.12	17,18,19,19	0
5	FAD	A	2003	53/53	0.97	0.15	26,36,46,48	0
3	CA	B	7004	1/1	0.97	0.38	18,18,18,18	0
3	CA	D	7008	1/1	0.98	0.26	23,23,23,23	0
3	CA	C	7006	1/1	0.98	0.36	18,18,18,18	0
4	FES	D	2001	4/4	0.99	0.09	14,14,14,14	0
4	FES	D	2002	4/4	0.99	0.08	14,14,14,14	0
4	FES	A	2002	4/4	0.99	0.08	14,14,14,14	0
7	MOM	A	2005	4/4	0.99	0.14	28,29,30,31	0
7	MOM	B	3005	4/4	0.99	0.13	27,28,28,29	0
7	MOM	C	4005	4/4	0.99	0.14	28,29,30,31	0
7	MOM	D	5005	4/4	0.99	0.14	27,28,28,29	0
4	FES	B	2001	4/4	0.99	0.10	14,14,14,14	0
4	FES	B	2002	4/4	0.99	0.09	14,14,14,14	0
4	FES	C	2001	4/4	0.99	0.09	14,14,14,14	0
4	FES	C	2002	4/4	0.99	0.09	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

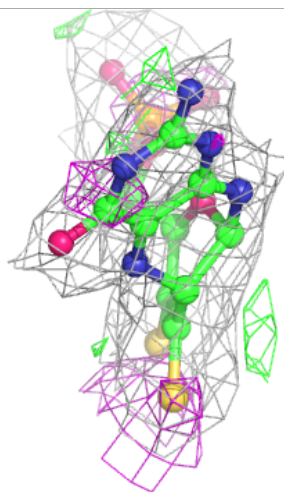
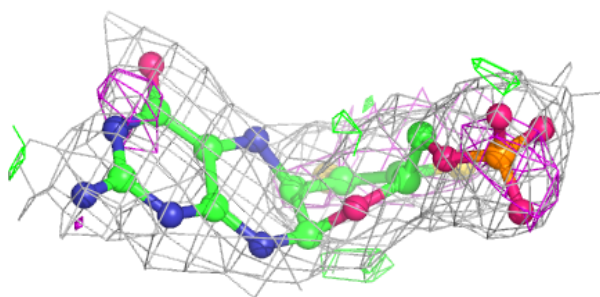
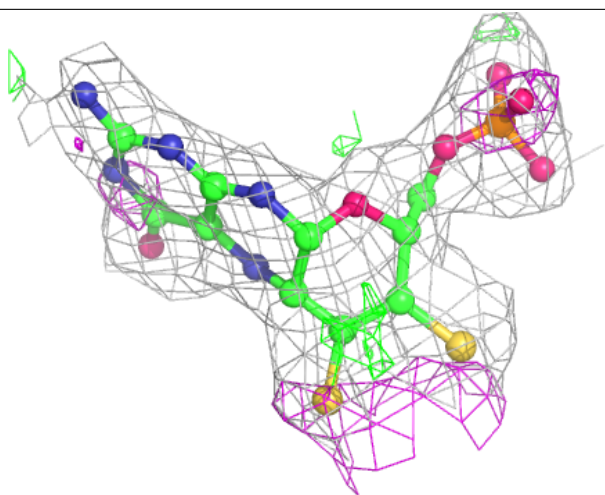
Electron density around MTE D 5004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



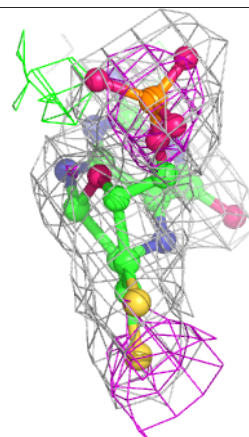
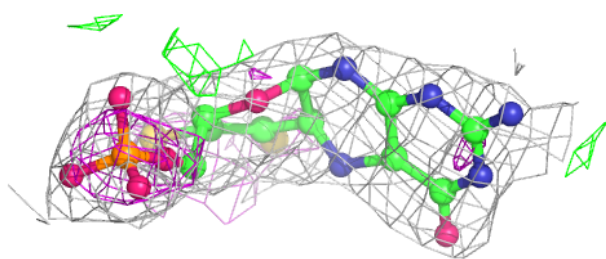
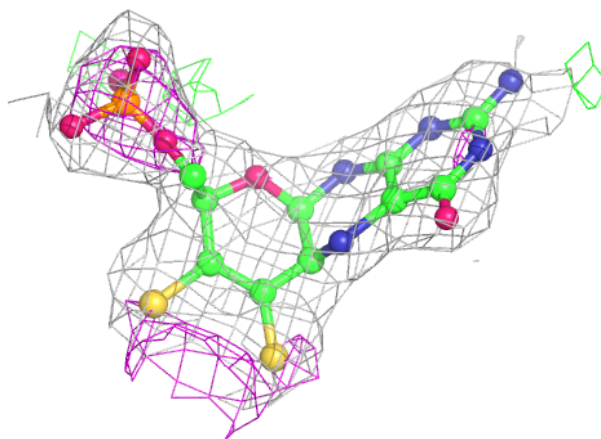
Electron density around MTE B 3004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

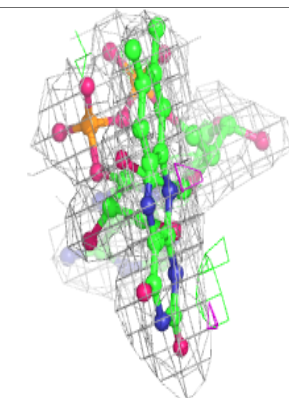
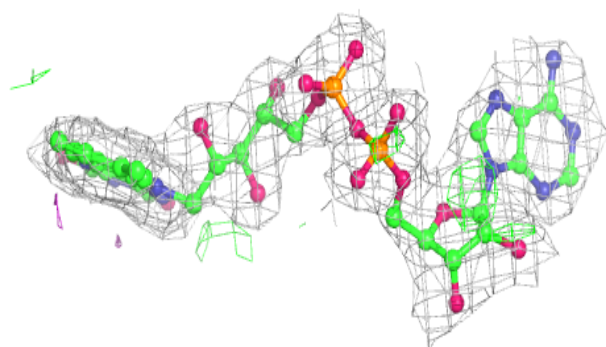
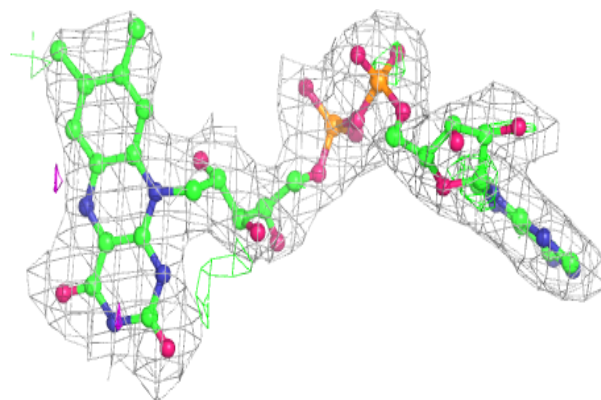


Electron density around MTE C 4004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

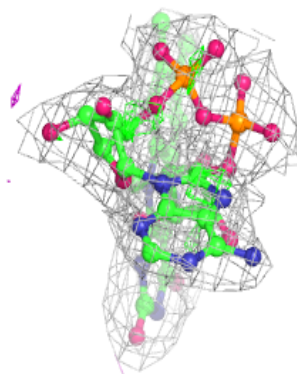
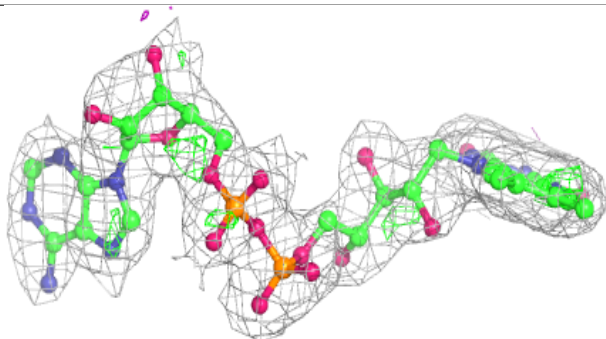
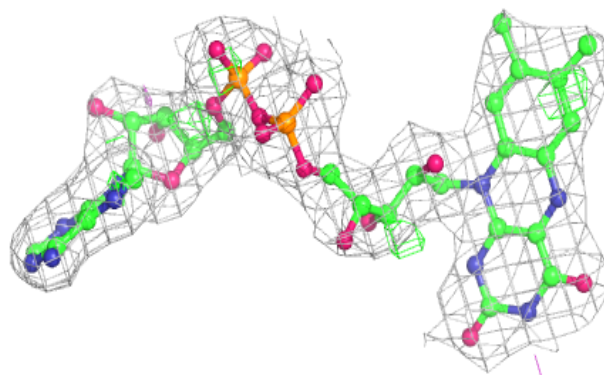
**Electron density around FAD B 3003:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

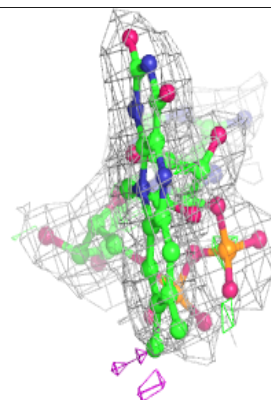
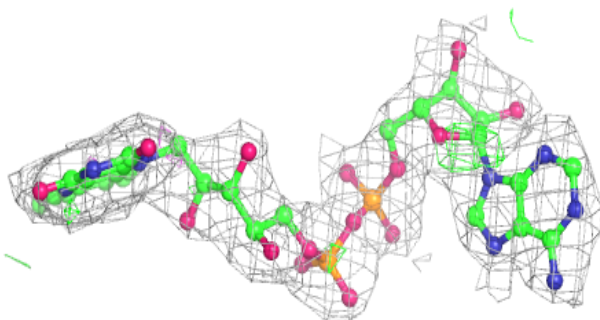
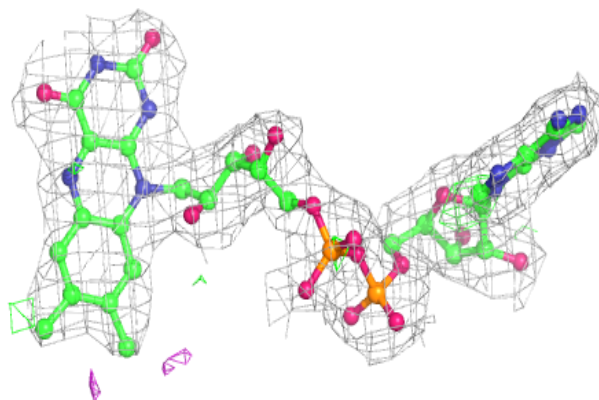


Electron density around FAD C 4003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

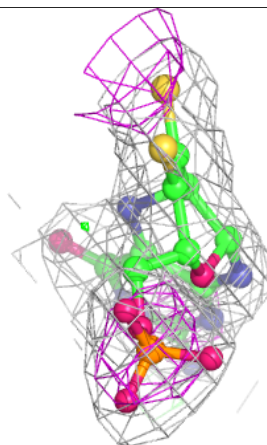
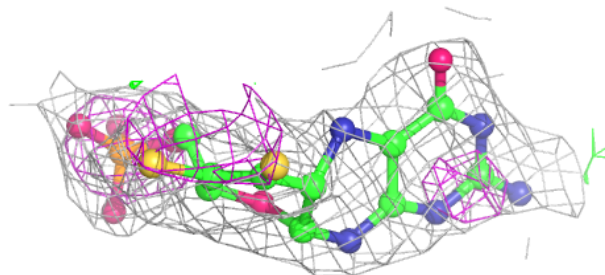
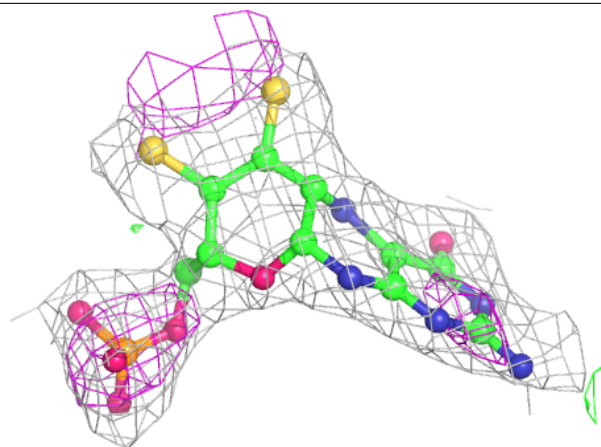
**Electron density around FAD D 5003:**

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and green (positive)

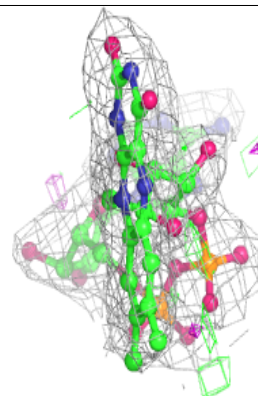
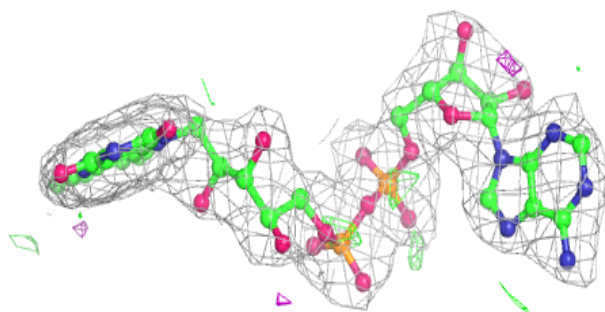
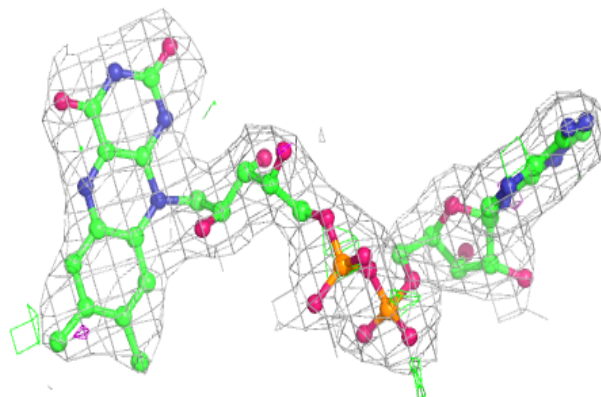


Electron density around MTE A 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD A 2003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.