



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2021 – 02:44 pm BST

PDB ID : 7B04
Title : Structure of Nitrite oxidoreductase (Nxr) from the anammox bacterium *Kuenenia stuttgartiensis*.
Authors : Moreno-Chicano, T.; Dietl, A.; Akram, M.; Barends, T.R.M.
Deposited on : 2020-11-18
Resolution : 2.97 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 : 2.22
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) : 2.22

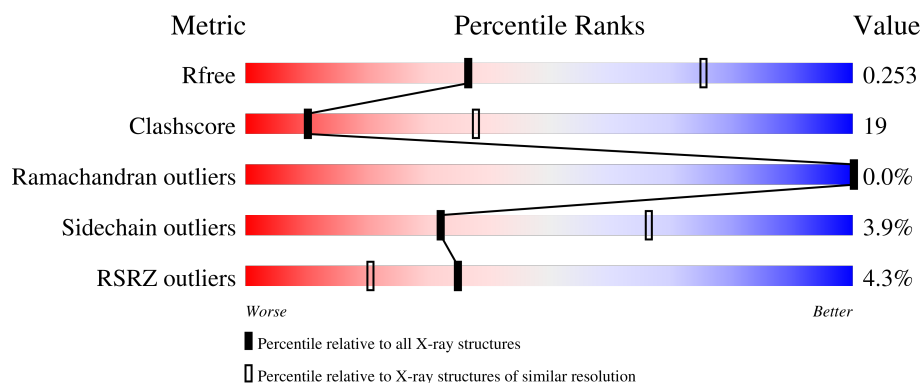
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	410	<div> <div></div> <div>74%</div> <div>25%</div> <div>.</div> </div>
1	D	410	<div> <div>26%</div> <div>65%</div> <div>32%</div> <div>.</div> </div>
1	G	410	<div> <div>74%</div> <div>25%</div> <div>.</div> </div>
1	J	410	<div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	M	410	<div> <div>64%</div> <div>34%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	410	
1	S	410	
1	V	410	
2	B	1148	
2	E	1148	
2	H	1148	
2	K	1148	
2	N	1148	
2	Q	1148	
2	T	1148	
2	W	1148	
3	C	322	
3	F	322	
3	I	322	
3	L	322	
3	O	322	
3	R	322	
3	U	322	
3	X	322	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	D	501	-	-	X	-
4	SF4	D	502	-	-	X	-
4	SF4	G	503	-	-	X	-
4	SF4	J	503	-	-	X	-
4	SF4	M	503	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	N	5804	-	-	X	-
4	SF4	P	503	-	-	X	-
4	SF4	Q	5804	-	-	X	-
4	SF4	S	503	-	-	X	-
4	SF4	T	5804	-	-	X	-
4	SF4	V	501	-	-	X	-
4	SF4	V	503	-	-	X	-
4	SF4	W	5804	-	-	X	-
5	F3S	D	504	-	-	X	-
5	F3S	M	504	-	-	X	-
5	F3S	V	504	-	-	X	-
6	MD1	E	5801	X	-	-	-
8	HEM	F	401	-	-	X	-
8	HEM	I	401	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 115931 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 Nitrite oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3349	2138	579	606	26			
1	D	408	Total	C	N	O	S	0	0	0
			2872	1805	508	534	25			
1	G	409	Total	C	N	O	S	0	0	0
			3344	2138	578	602	26			
1	J	409	Total	C	N	O	S	0	0	0
			3361	2147	580	608	26			
1	M	409	Total	C	N	O	S	0	0	0
			3309	2114	572	597	26			
1	P	409	Total	C	N	O	S	0	0	0
			3321	2121	573	601	26			
1	S	409	Total	C	N	O	S	0	0	0
			3333	2131	577	599	26			
1	V	409	Total	C	N	O	S	0	0	0
			3239	2063	556	594	26			

- Molecule 2 is a protein called Nitrite oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1120	Total	C	N	O	S	0	1	0
			9003	5748	1551	1662	42			
2	E	1111	Total	C	N	O	S	0	1	0
			6871	4264	1247	1334	26			
2	H	1118	Total	C	N	O	S	0	1	0
			9028	5760	1561	1665	42			
2	K	1119	Total	C	N	O	S	0	1	0
			9046	5777	1559	1668	42			
2	N	1117	Total	C	N	O	S	0	3	0
			9052	5773	1564	1672	43			
2	Q	1116	Total	C	N	O	S	0	1	0
			8902	5678	1533	1649	42			

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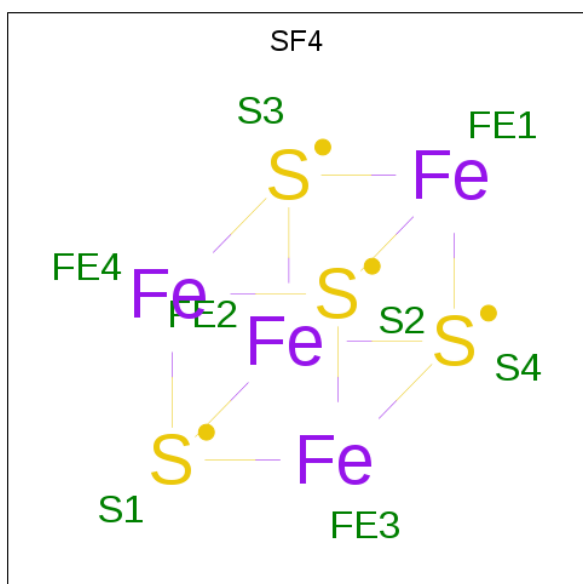
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	1119	Total	C	N	O	S	0	0	0
			9034	5766	1555	1671	42			
2	W	1118	Total	C	N	O	S	0	1	0
			8920	5688	1532	1658	42			

- Molecule 3 is a protein called Nitrite oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	1	0
			2281	1435	400	438	8			
3	F	292	Total	C	N	O	S	0	0	0
			2068	1305	358	398	7			
3	I	292	Total	C	N	O	S	0	0	0
			2216	1401	385	422	8			
3	L	292	Total	C	N	O	S	0	1	0
			2274	1431	396	439	8			
3	O	291	Total	C	N	O	S	0	0	0
			2124	1337	369	410	8			
3	R	291	Total	C	N	O	S	0	0	0
			2261	1423	392	438	8			
3	U	292	Total	C	N	O	S	0	0	0
			2267	1428	393	438	8			
3	X	292	Total	C	N	O	S	0	0	0
			2225	1401	387	429	8			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



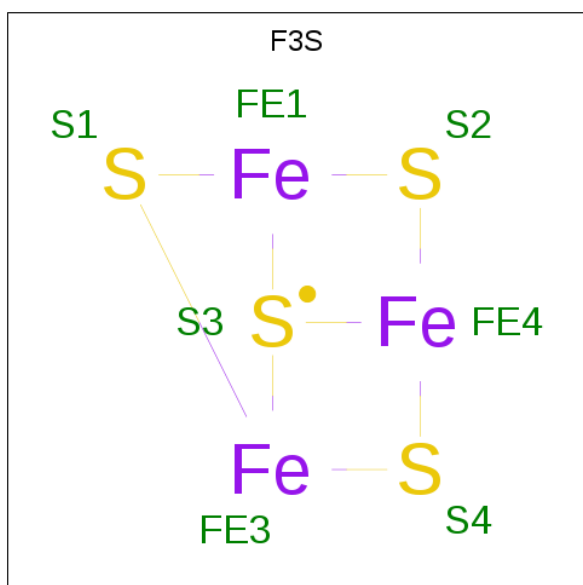
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	Fe 4	S 4	0	0
4	A	1	Total 8	Fe 4	S 4	0	0
4	A	1	Total 8	Fe 4	S 4	0	0
4	B	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	E	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	H	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	K	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	N	1	Total 8	Fe 4	S 4	0	0
4	P	1	Total 8	Fe 4	S 4	0	0
4	P	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	Fe	S	0	0
			8	4	4		
4	Q	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	T	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	W	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



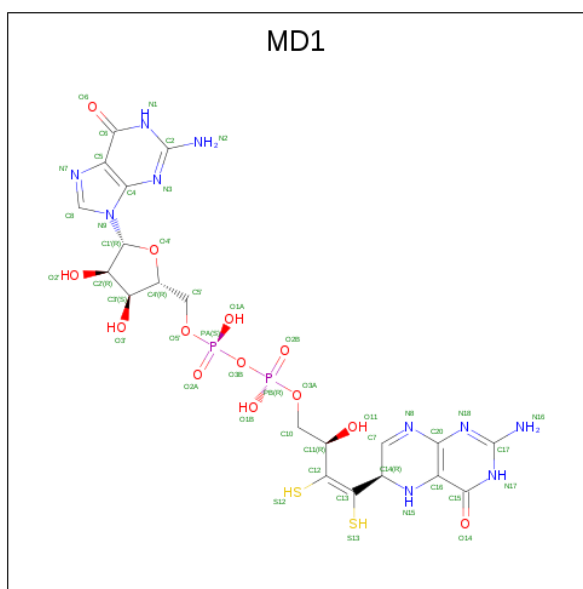
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			7	3	4		
5	G	1	Total	Fe	S	0	0
			7	3	4		
5	J	1	Total	Fe	S	0	0
			7	3	4		
5	M	1	Total	Fe	S	0	0
			7	3	4		
5	P	1	Total	Fe	S	0	0
			7	3	4		
5	S	1	Total	Fe	S	0	0
			7	3	4		
5	V	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTERIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 7 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

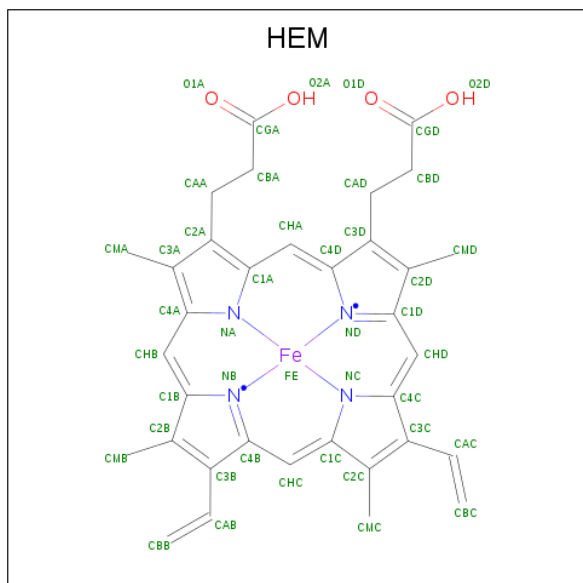
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Mo 1	0	0
7	E	1	Total 1	Mo 1	0	0
7	H	1	Total 1	Mo 1	0	0
7	K	1	Total 1	Mo 1	0	0
7	N	1	Total 1	Mo 1	0	0
7	Q	1	Total 1	Mo 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	1	Total	Mo	0	0
			1	1		
7	W	1	Total	Mo	0	0
			1	1		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	2	Total 2 Ca 2	0	0
9	F	2	Total 2 Ca 2	0	0
9	I	2	Total 2 Ca 2	0	0
9	L	2	Total 2 Ca 2	0	0
9	O	2	Total 2 Ca 2	0	0
9	R	2	Total 2 Ca 2	0	0
9	U	2	Total 2 Ca 2	0	0
9	X	2	Total 2 Ca 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	37	Total 37 O 37	0	0
10	B	72	Total 72 O 72	0	0
10	C	35	Total 35 O 35	0	0
10	D	6	Total 6 O 6	0	0
10	E	13	Total 13 O 13	0	0
10	F	8	Total 8 O 8	0	0
10	G	25	Total 25 O 25	0	0
10	H	83	Total 83 O 83	0	0
10	I	20	Total 20 O 20	0	0
10	J	28	Total 28 O 28	0	0
10	K	74	Total 74 O 74	0	0
10	L	30	Total 30 O 30	0	0

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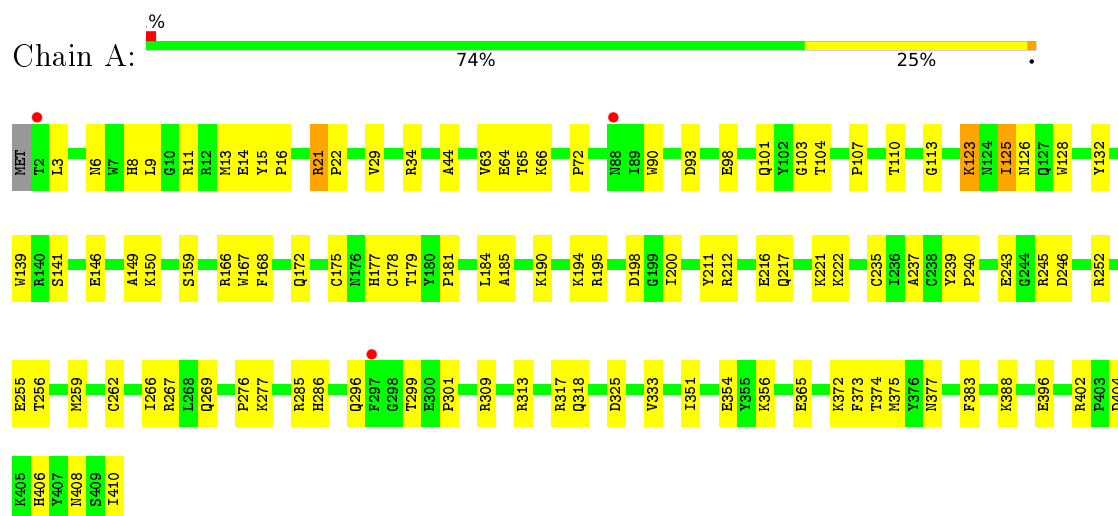
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	10	Total 10	O 10	0	0
10	N	76	Total 76	O 76	0	0
10	O	17	Total 17	O 17	0	0
10	P	16	Total 16	O 16	0	0
10	Q	43	Total 43	O 43	0	0
10	R	22	Total 22	O 22	0	0
10	S	20	Total 20	O 20	0	0
10	T	62	Total 62	O 62	0	0
10	U	25	Total 25	O 25	0	0
10	V	12	Total 12	O 12	0	0
10	W	41	Total 41	O 41	0	0
10	X	24	Total 24	O 24	0	0

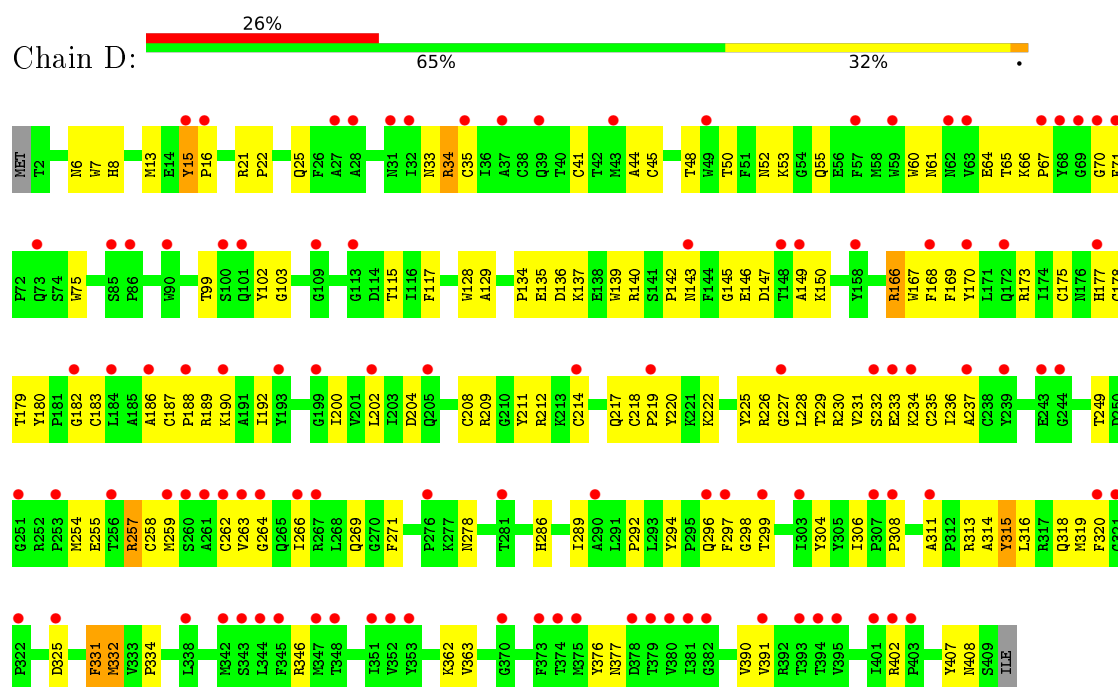
3 Residue-property plots [i](#)

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

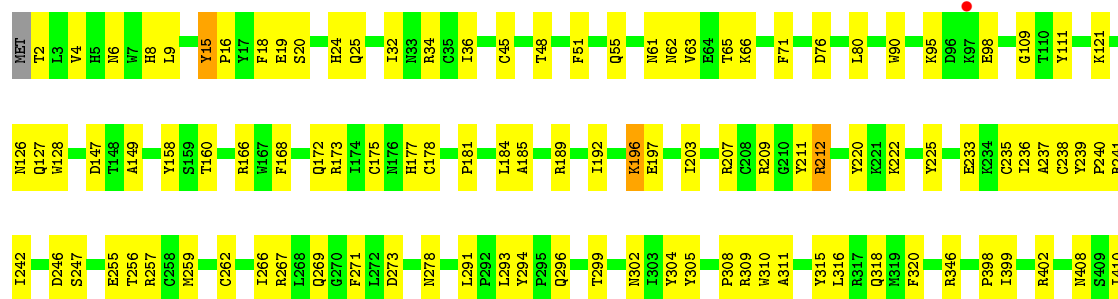


• Molecule 1: Nitrite oxidoreductase subunit B




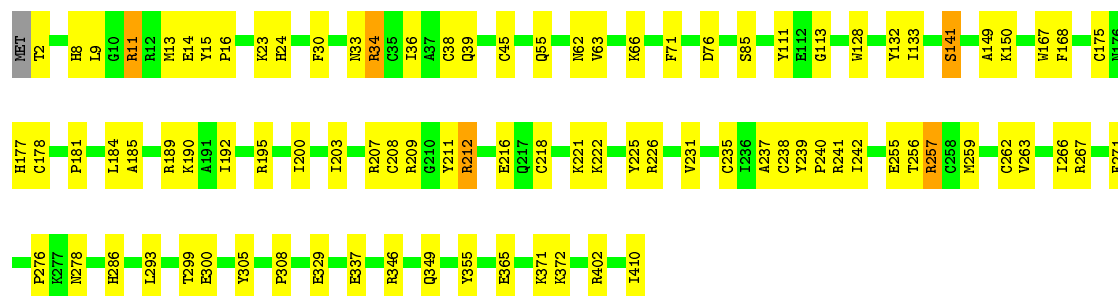
• Molecule 1: Nitrite oxidoreductase subunit B

Chain G:  74% 25% .



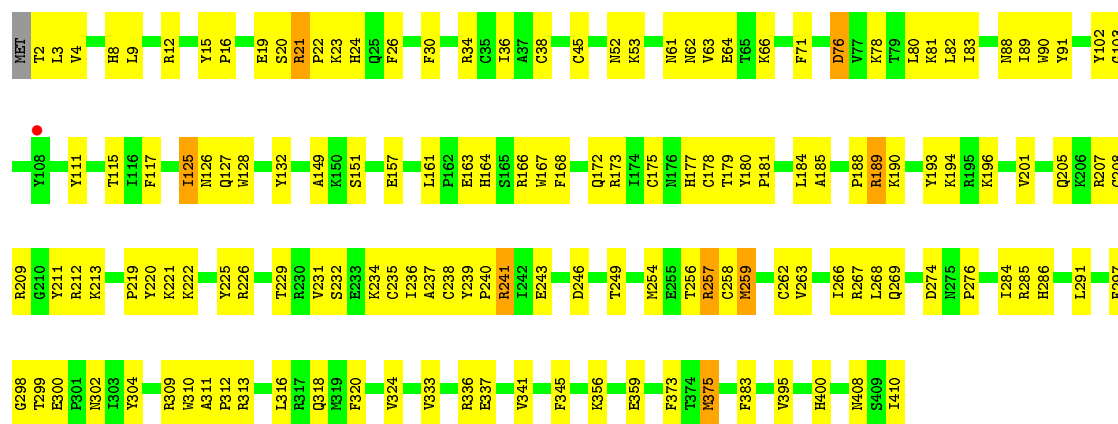
• Molecule 1: Nitrite oxidoreductase subunit B

Chain J:  77% 21% .



• Molecule 1: Nitrite oxidoreductase subunit B

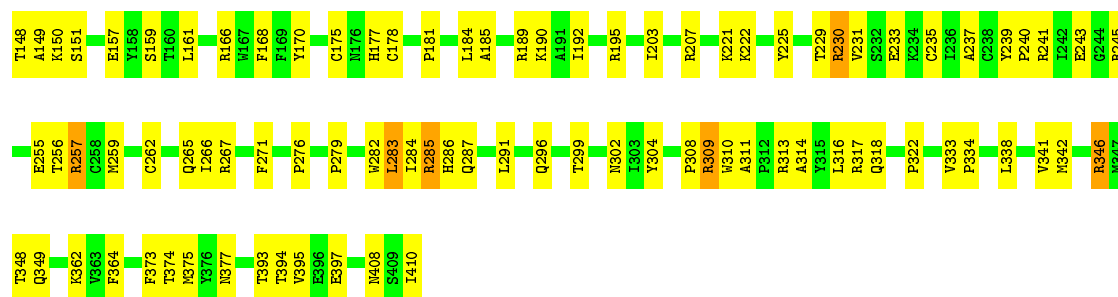
Chain M:  64% 34% .



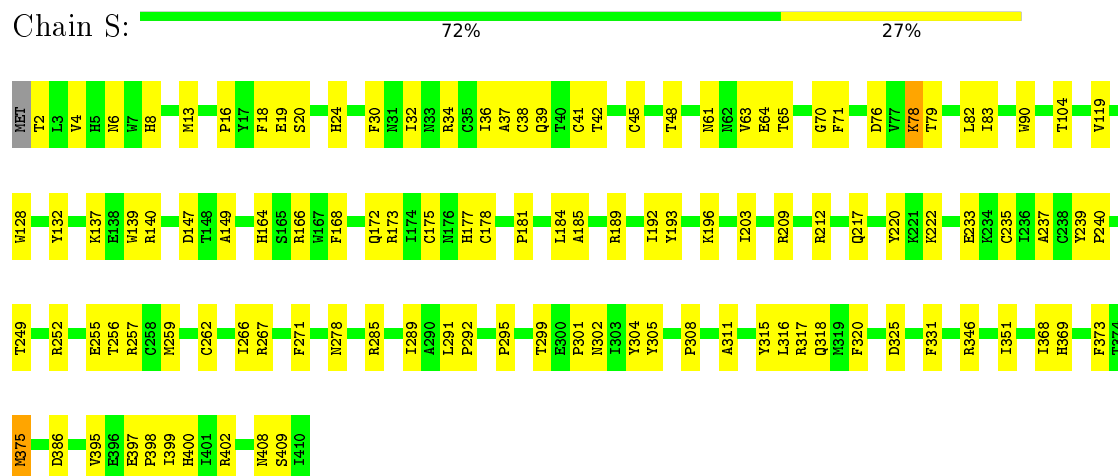
• Molecule 1: Nitrite oxidoreductase subunit B

Chain P:  70% 28% .

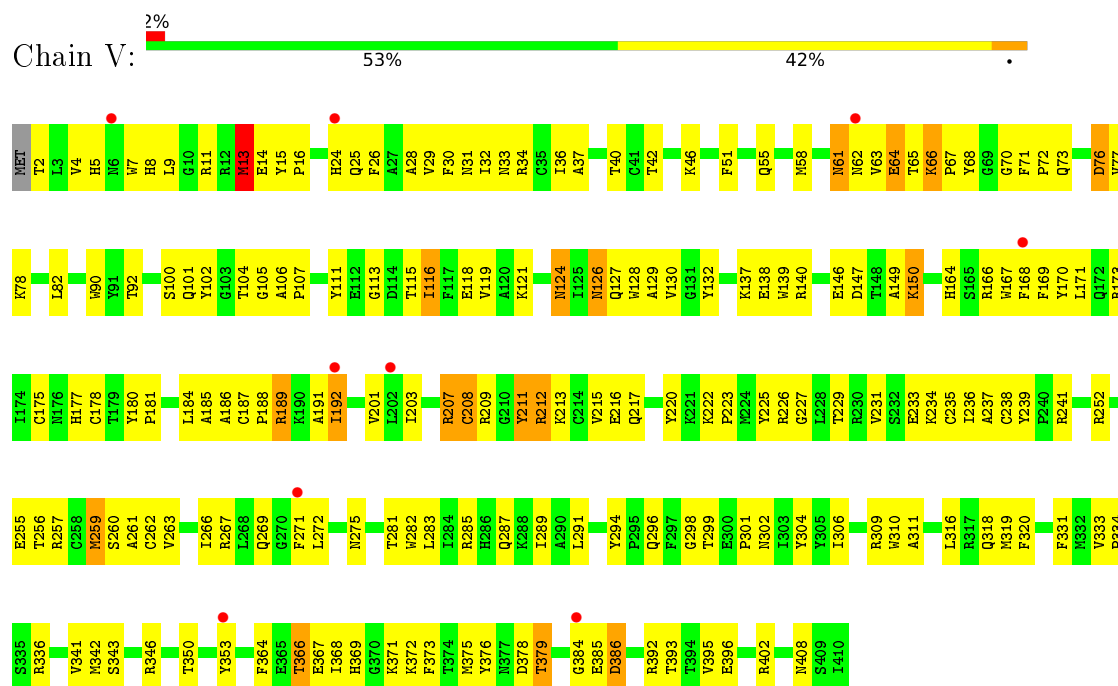




• Molecule 1: Nitrite oxidoreductase subunit B

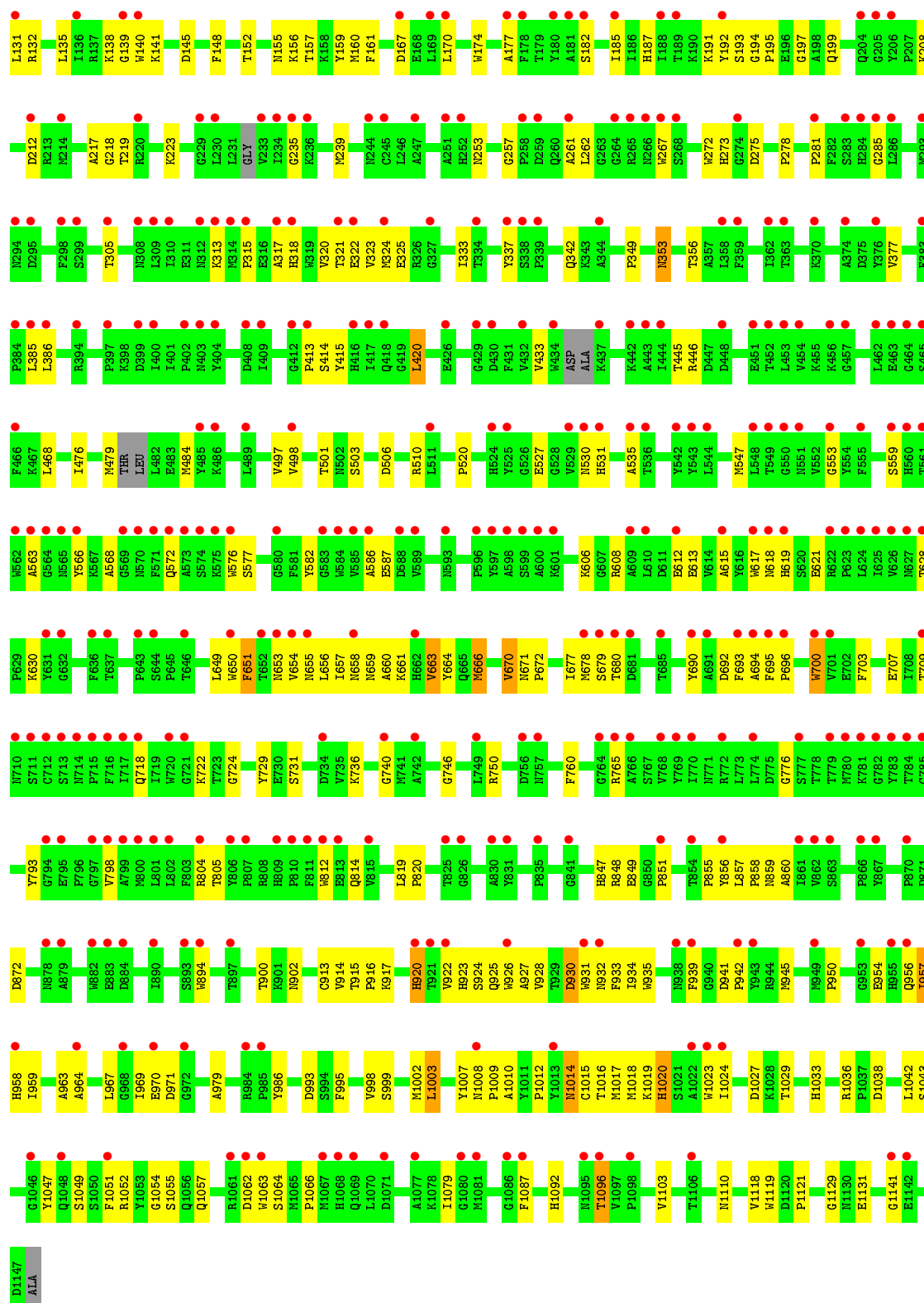


• Molecule 1: Nitrite oxidoreductase subunit B



• Molecule 2: Nitrite oxidoreductase subunit A





• Molecule 2: Nitrite oxidoreductase subunit A

Chain H:

69%

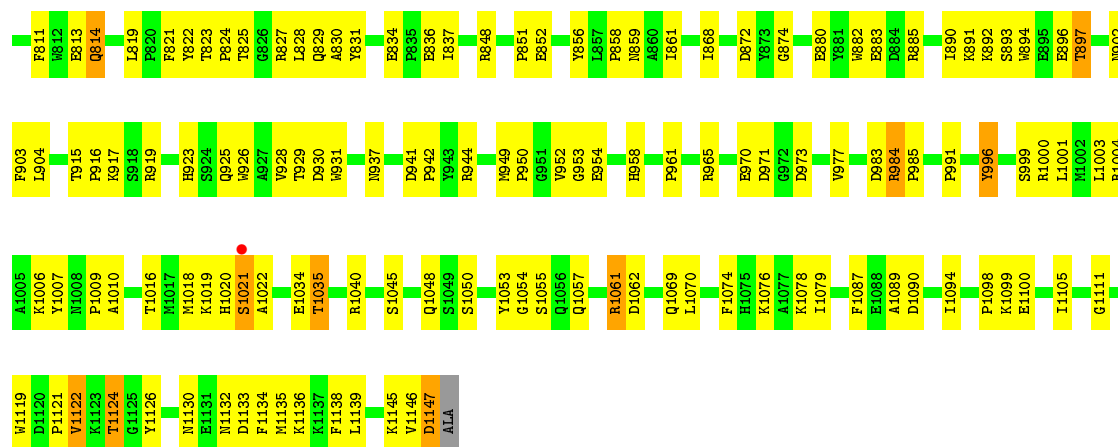
27%

MET	LYS	LEU	THR	ARG	ARG	ALA	PHE	LEU	GLN	VAL	ALA	GLY	ALA	THR	LEU	THR	LEU	ALA	LYS	ASN	ALA	MET	ALA	PHE	ARG	L30	L31	K32	P33	V36	P40	L41	D42	T43	Y44	R47	R48	W49	V52	Y53	R54	T55	Q56	Y57	Q58	Y59	D60	R61	C67	S68	P69
N70	D71	H72	H73	R76	I77	V81	R88	V89	E90	Q91	N92	Y93	D100	G103	N104	P112	R113	M114	K117	F121	H122	R123	R124	V125	R130	L135	K138	G139	W140	L151	T152	P153	E154	N155	K156	Y159	M160	R164	G165	N166	L170	G184	P89								
K190	S193	L201	R213	A217	G218	T219	R220	K223	G224	R225	G226	G227	M228	G232	K236	Y237	D250	A251	H252	N253	R254	A261	L262	W267	Y270	T271	W272	D275	Q276	A277	P278	H284	G285	L286	Q287	N294	D295	V296	R297	F298	L301	N308	L309								
I310	E311	N312	P315	E316	T321	E322	N324	I330	F331	V332	E336	P339	A344	D345	Y346	I350	R351	T354	N353	G361	D375	I376	K379	F380	T381	D382	F383	P384	L385	R388	T389	D390	V395	L286	Q418	Q424	R425	I428	G429	D430	W434	D435									
S438	P441	T444	R446	D447	V449	O450	K456	V461	L462	F466	K467	L468	V478	M479	T480	E483	W484	K486	H488	V497	V498	T501	P504	K505	D506	L507	R510	L511	A512	K513	I515	A516	T517	I518	V521	Y525	G526	E527	G528	H531											
F532	F533	T536	L537	Y543	G550	Y554	S559	H560	T561	A563	F571	Q572	S577	I708	F581	D585	R608	K609	L610	D611	E612	E613	V614	N618	L625	R633	K634	V635	T640	P645	V648	H653	V654	N658	K661	H662	V663	M666													
V670	N673	I674	E675	O676	I677	N678	D681	T683	R684	F683	A694	S699	W700	V701	E702	F706	E707	I708	T709	W714	Q718	I719	W720	G721	K722	D734	D751	K752	F759	R760	E763	G764	W765	Y769	R773	G776	N790	F803	R804	T805	T806	R808									
F811	H812	E813	O814	W815	L819	P820	T823	R824	R827	L828	O829	E834	I837	F844	I845	W846	H847	R848	P858	N859	A860	I861	Y867	I868	R869	P870	H882	E883	R888	K891	A903	I1024	R1040	A1041	L1042	Q1048	Y1052	Y1053	G1054	S1055	Q1056	Q1057	T1060								
W926	D930	W931	K947	R948	P949	P950	E954	H955	A964	I969	E970	D971	G972	D973	Y974	G1101	L1001	W1119	D1120	P1121	N1132	V1135	M1135	I1144	K1145	V1146	D1147	ALA	T1016	M1017	M1018	K1019	H1020	S1021	A1022	W1023	R1040	A1041	L1042	Q1048	Y1052	Y1053	G1054	S1055	Q1056	Q1057	T1060				
R1061	D1062	H1068	F1074	K1078	I1079	F1085	G1086	F1087	E1088	A1089	C1093	I1094	N1095	P1098	K1099	E1100	I1105	G1111	G1112	W1119	D1120	P1121	N1132	V1135	M1135	I1144	K1145	V1146	D1147	ALA	T1016	M1017	M1018	K1019	H1020	S1021	A1022	W1023	R1040	A1041	L1042	Q1048	Y1052	Y1053	G1054	S1055	Q1056	Q1057	T1060		

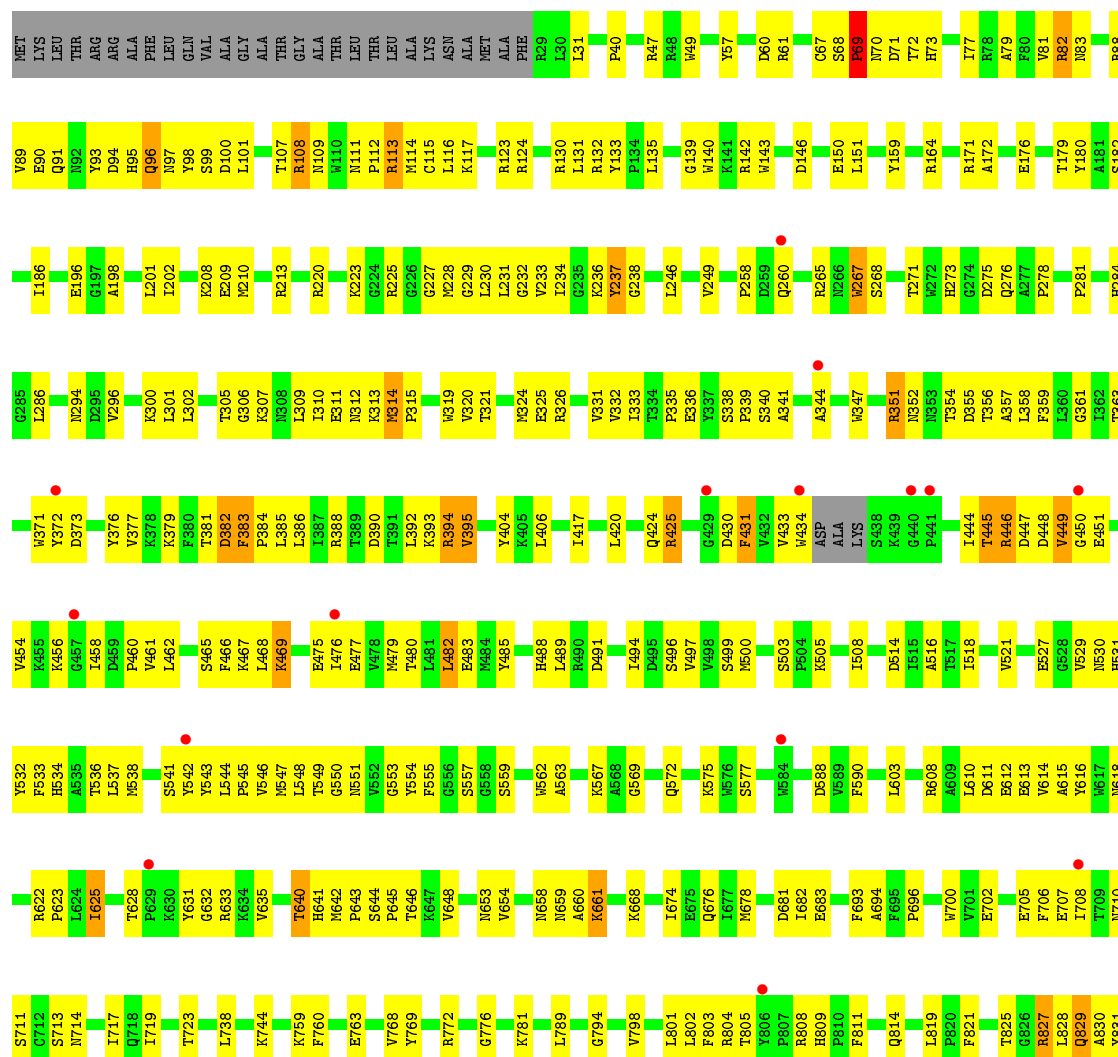
• Molecule 2: Nitrite oxidoreductase subunit A

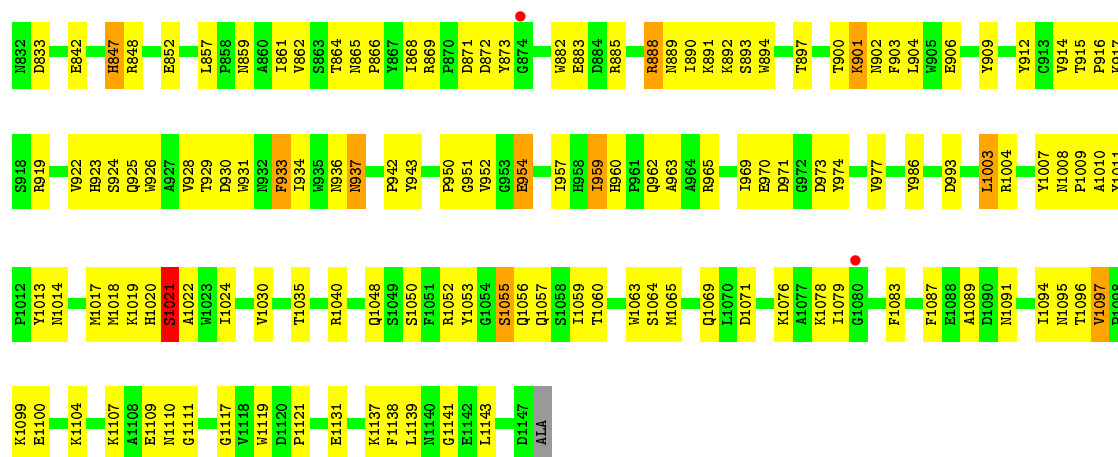
Chain K:  66% 30%

MET	LYS	LEU	THR	ARG	ARG	ALA	PHE	LEU	GLN	VAL	ALA	GLY	ALA	THR	LEU	THR	LEU	ALA	LYS	ASN	ALA	MET	ALA	PHE	R29	L30	L31	K32	P33	A34	V35	V36	V37	P40	Y44	P69	N70	D71	H72	H73	E90	Q91	R92	Y93	D94	H95	Q96	N97	Y98	S99	D100	L101																																				
	K105	W110	H111	P112	R113	M114	C115	L116	K117	G118	Y119	T120	H121	H122	R123	R124	Y133	P134	L135	K138	K141	R142	W143	P149	E150	L151	K152	T152	N155	K158	R164	L170	R171	W174	D175	T179	Y180	K190	S193	E196	E209	R213	C218	R219	T220	F222	R225	G226	G227	G228	G229	L230	L231	G232	R236	Y237	R241	D250	R254	A261	R265	M269	Y270	T271	W272	H273	G274	D275	Q276	H284	G285	L286	Q287	D290	D295	V296	R297	L301	L302	L303	K307	I310	N311	N312	K313	M314	P315	E316
	T219	R220	T221	F222	R225	G226	G227	G228	G229	L230	L231	G232	R236	Y237	R241	D250	R254	A261	R265	M269	Y270	T271	W272	H273	G274	D275	Q276	H284	G285	L286	Q287	D290	D295	V296	R297	L301	L302	L303	K307	I310	N311	N312	K313	M314	P315	E316																																										
	V320	T321	E322	V323	K324	I330	V331	V332	I333	T334	P335	E336	Q342	K343	A344	D345	T346	W347	I348	N353	T354	D355	L358	F359	L360	Y376	K379	D382	F383	P384	L385	R388	T389	D390	T391	L392	K393	R394	V395	S396	P397	R403	Y404	K405	D408	I409	S410	Y415																																								
	V320	T321	E322	V323	K324	I330	V331	V332	I333	T334	P335	E336	Q342	K343	A344	D345	T346	W347	I348	N353	T354	D355	L358	F359	L360	Y376	K379	D382	F383	P384	L385	R388	T389	D390	T391	L392	K393	R394	V395	S396	P397	R403	Y404	K405	D408	I409	S410	Y415																																								
	V320	T321	E322	V323	K324	I330	V331	V332	I333	T334	P335	E336	Q342	K343	A344	D345	T346	W347	I348	N353	T354	D355	L358	F359	L360	Y376	K379	D382	F383	P384	L385	R388	T389	D390	T391	L392	K393	R394	V395	S396	P397	R403	Y404	K405	D408	I409	S410	Y415																																								
	V320	T321	E322	V323	K324	I330	V331	V332	I333	T334	P335	E336	Q342	K343	A344	D345	T346	W347	I348	N353	T354	D355	L358	F359	L360	Y376	K379	D382	F383	P384	L385	R388	T389	D390	T391	L392	K393	R394	V395	S396	P397	R403	Y404	K405	D408	I409	S410	Y415																																								
	V320	T321	E322	V323	K324	I330	V331	V332	I333	T334	P335	E336	Q342	K343	A344	D345	T346	W347	I348	N353	T354	D355	L358	F359	L360	Y376	K379	D382	F383	P384	L385	R388	T389	D390	T391	L392	K393	R394	V395	S396	P397	R403	Y404	K405	D408	I409	S410	Y415																																								
	V320	T321	E322	V323	K324	I330	V331	V332	I333	T334	P335	E336	Q342	K343	A344	D345	T346	W347	I348	N353	T354	D355	L358	F359	L360	Y376	K379	D382	F383	P384	L385	R388	T389	D390	T391	L392	K393	R394	V395	S396	P397	R403	Y404	K405	D408	I409	S410	Y415																																								
	V320	T321	E322	V323	K324	I330	V331	V332	I333	T334	P335	E336	Q342	K343	A344	D345	T346	W347	I348	N353	T354	D355	L358	F359	L360	Y376	K379	D382	F383	P384	L385	R388	T389	D390	T391	L392	K393	R394	V395	S396	P397	R403	Y404	K405	D408	I409	S410	Y415																																								



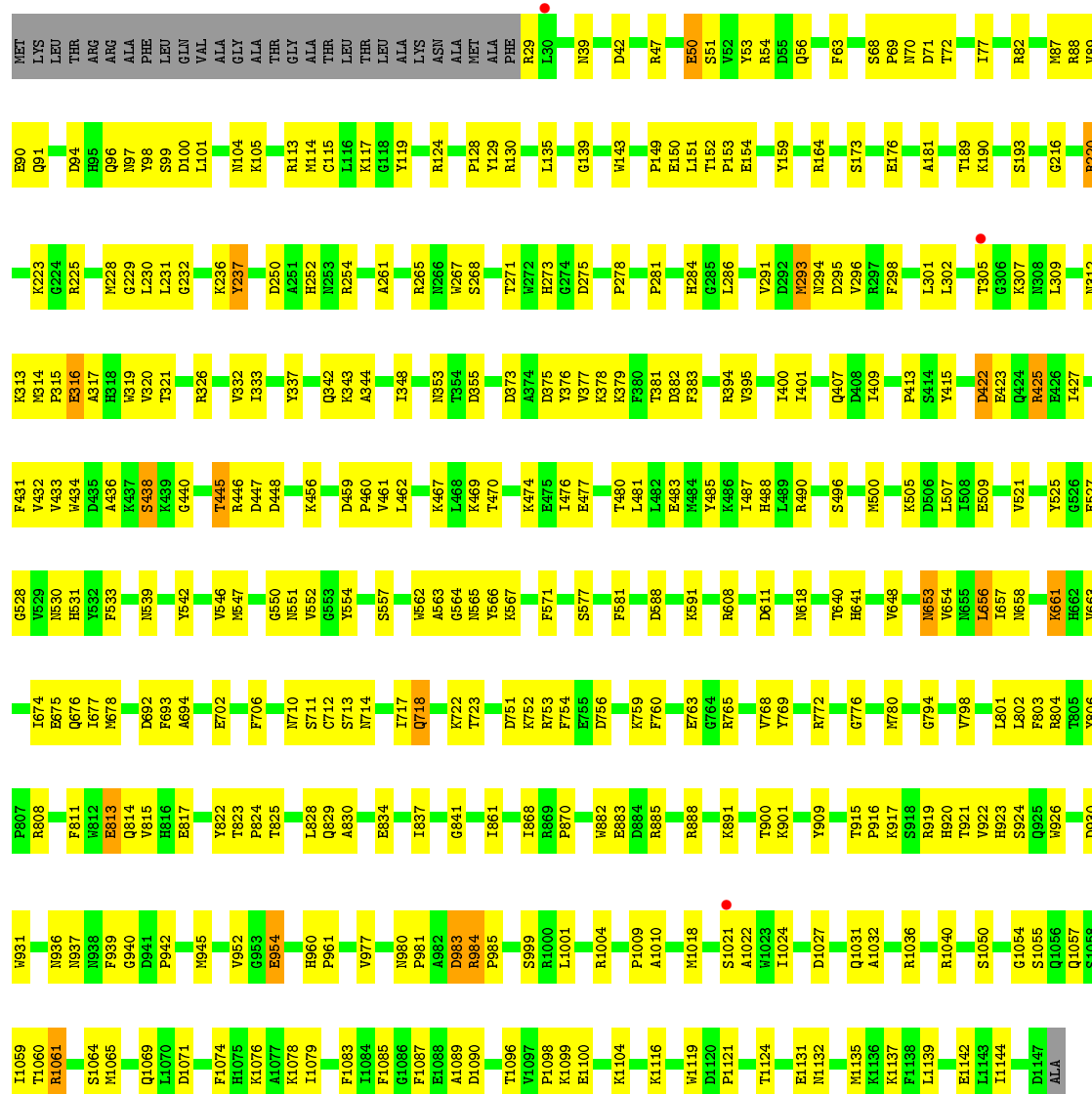
• Molecule 2: Nitrite oxidoreductase subunit A



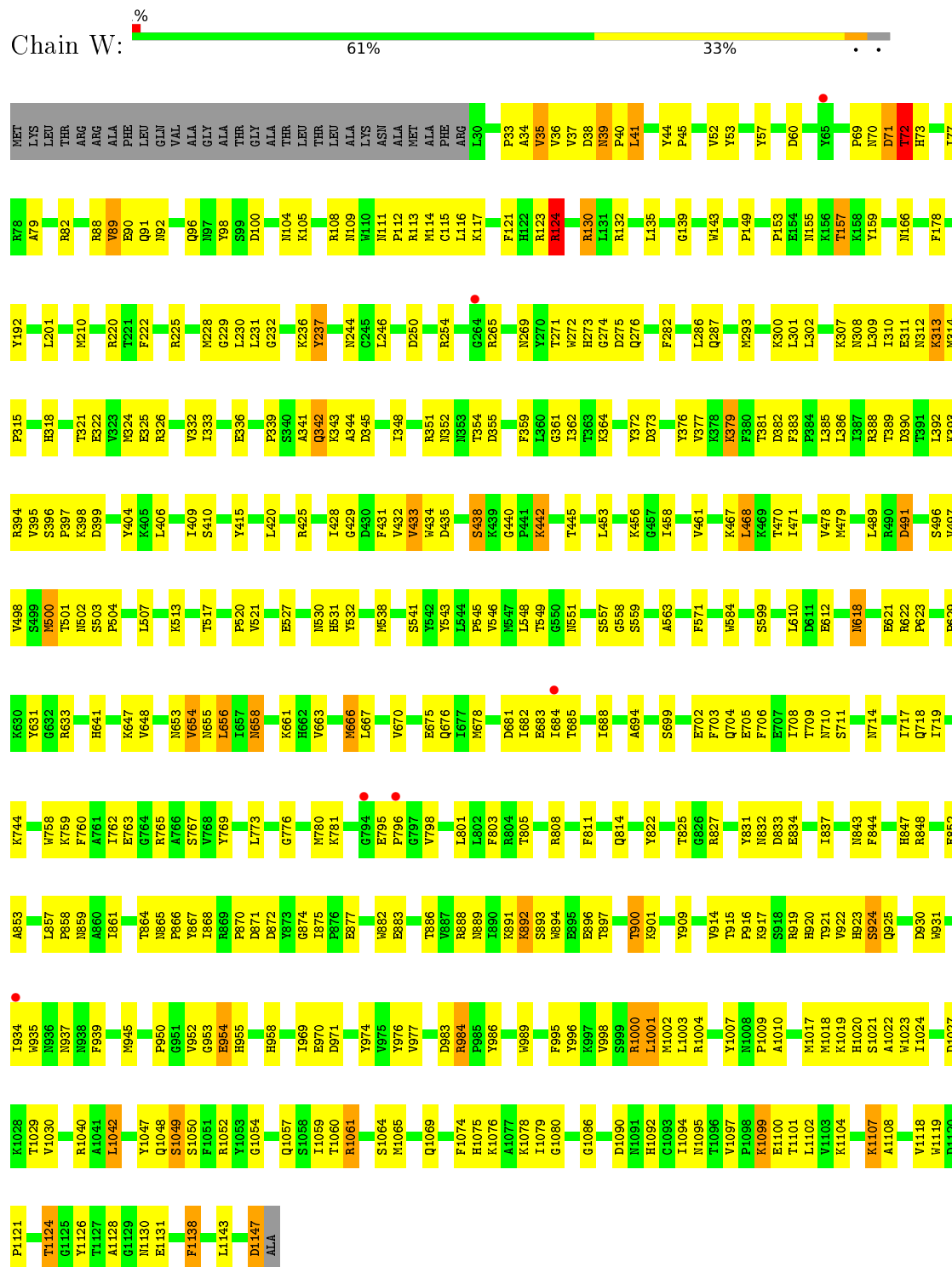


• Molecule 2: Nitrite oxidoreductase subunit A

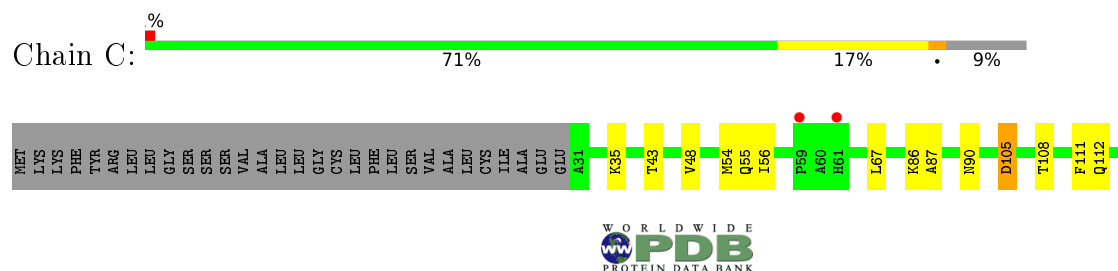
Chain T: 67% 29%

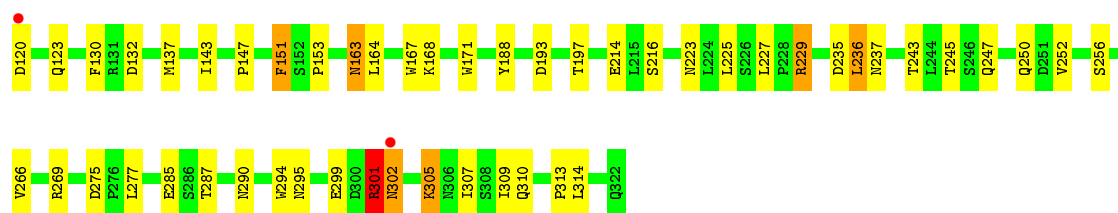


- Molecule 2: Nitrite oxidoreductase subunit A

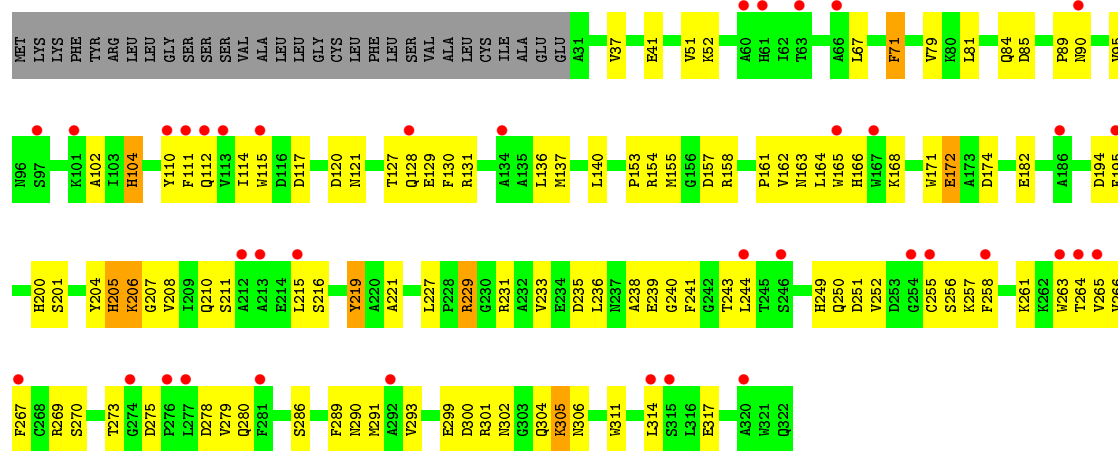


- Molecule 3: Nitrite oxidoreductase subunit C

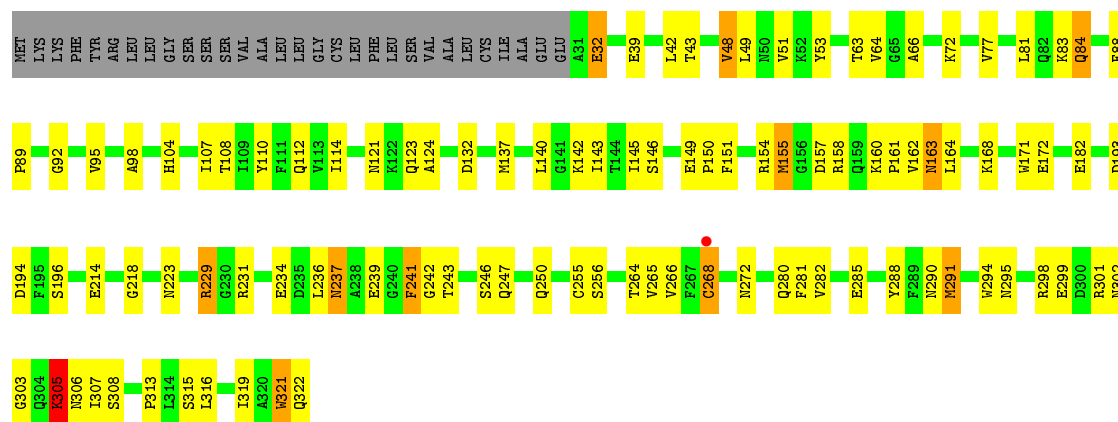




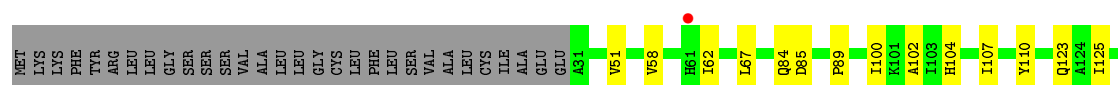
• Molecule 3: Nitrite oxidoreductase subunit C

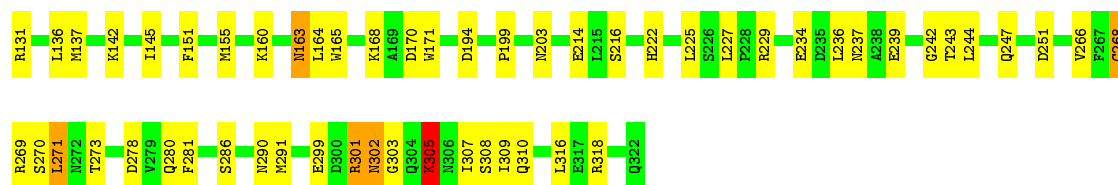


• Molecule 3: Nitrite oxidoreductase subunit C

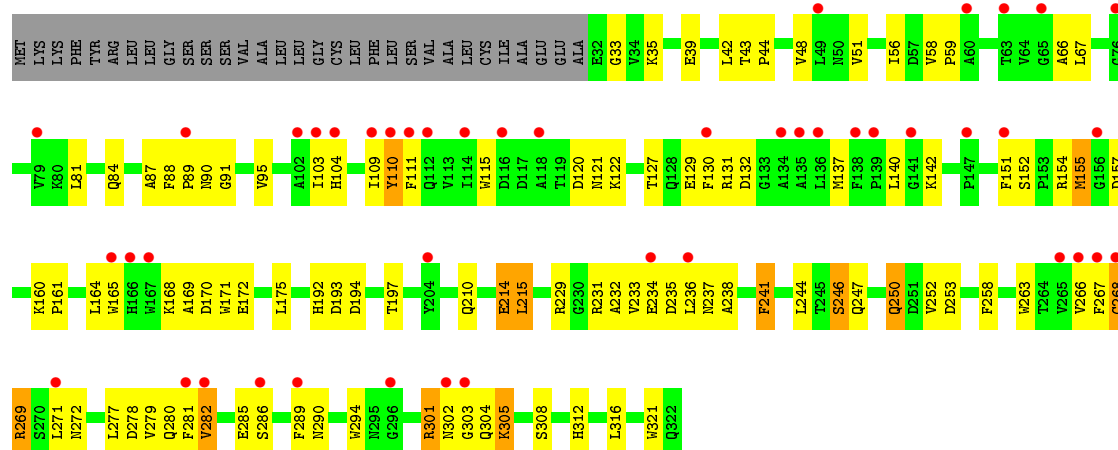


• Molecule 3: Nitrite oxidoreductase subunit C

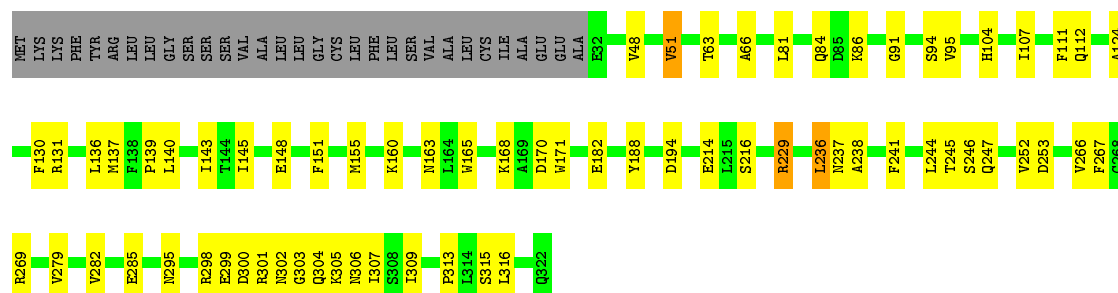




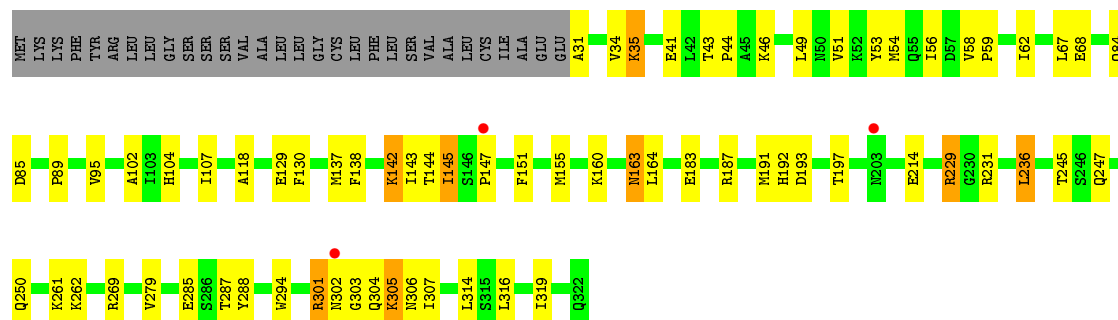
• Molecule 3: Nitrite oxidoreductase subunit C



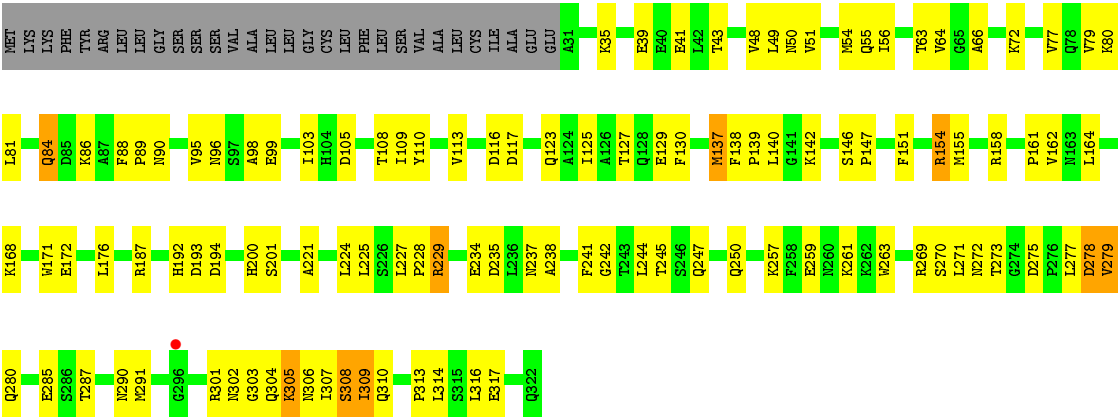
• Molecule 3: Nitrite oxidoreductase subunit C



• Molecule 3: Nitrite oxidoreductase subunit C



● Molecule 3: Nitrite oxidoreductase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	177.63Å 206.47Å 527.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	192.25 – 2.97 192.25 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.4 (192.25-2.97) 95.4 (192.25-2.97)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.96Å)	Xtriage
Refinement program	PHENIX v1.14rc1	Depositor
R, R_{free}	0.223 , 0.255 0.222 , 0.253	Depositor DCC
R_{free} test set	21282 reflections (5.64%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	115931	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: MD1, F3S, HEM, SF4, MO, 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	0.36	0/3450	0.52	0/4676
1	D	0.33	0/2957	0.53	0/4058
1	G	0.29	0/3445	0.49	0/4670
1	J	0.33	0/3462	0.49	0/4690
1	M	0.34	0/3410	0.56	1/4632 (0.0%)
1	P	0.39	0/3422	0.57	0/4646
1	S	0.31	2/3434 (0.1%)	0.49	0/4657
1	V	0.50	1/3339 (0.0%)	0.68	4/4545 (0.1%)
2	B	0.41	1/9267 (0.0%)	0.59	2/12591 (0.0%)
2	E	0.44	1/7024 (0.0%)	0.69	1/9696 (0.0%)
2	H	0.37	1/9292 (0.0%)	0.57	3/12617 (0.0%)
2	K	0.37	0/9313	0.55	0/12642
2	N	0.39	1/9319 (0.0%)	0.57	2/12649 (0.0%)
2	Q	0.48	1/9165 (0.0%)	0.67	4/12465 (0.0%)
2	T	0.39	3/9298 (0.0%)	0.55	2/12625 (0.0%)
2	W	0.43	1/9187 (0.0%)	0.61	1/12501 (0.0%)
3	C	0.42	2/2338 (0.1%)	0.64	3/3175 (0.1%)
3	F	0.43	0/2123	0.68	0/2911
3	I	0.40	0/2272	0.68	1/3093 (0.0%)
3	L	0.49	3/2331 (0.1%)	0.60	1/3169 (0.0%)
3	O	0.47	1/2179 (0.0%)	0.69	1/2983 (0.0%)
3	R	0.44	1/2318 (0.0%)	0.57	0/3151
3	U	0.39	0/2324	0.58	1/3158 (0.0%)
3	X	0.41	0/2282	0.63	0/3104
All	All	0.40	19/116951 (0.0%)	0.59	27/159104 (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
2	B	0	1
2	H	0	1
2	K	0	2
2	W	0	3
All	All	0	7

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	663	VAL	C-N	15.00	1.68	1.34
2	Q	1097	VAL	CB-CG2	-9.56	1.32	1.52
3	C	214	GLU	CD-OE1	-6.92	1.18	1.25
3	C	214	GLU	CD-OE2	-6.58	1.18	1.25
2	T	954	GLU	CD-OE1	-6.28	1.18	1.25
3	L	214	GLU	CD-OE2	-6.24	1.18	1.25
2	N	813	GLU	CD-OE1	-6.22	1.18	1.25
2	T	954	GLU	CD-OE2	-6.10	1.19	1.25
1	S	233	GLU	CD-OE1	-5.82	1.19	1.25
3	L	214	GLU	CD-OE1	-5.79	1.19	1.25
1	S	233	GLU	CD-OE2	-5.66	1.19	1.25
2	B	1088	GLU	CD-OE2	-5.58	1.19	1.25
3	R	214	GLU	CD-OE1	-5.51	1.19	1.25
2	H	232	GLY	C-O	-5.35	1.15	1.23
3	L	299	GLU	CD-OE2	-5.17	1.20	1.25
1	V	208	CYS	CB-SG	-5.16	1.73	1.81
2	W	954	GLU	CD-OE1	-5.10	1.20	1.25
3	O	214	GLU	CD-OE1	-5.07	1.20	1.25
2	T	981	PRO	C-O	-5.01	1.13	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	954	GLU	O-C-N	-16.77	95.87	122.70
3	I	305	LYS	CB-CA-C	13.42	137.23	110.40
2	Q	954	GLU	CB-CA-C	9.42	129.23	110.40
2	E	663	VAL	C-N-CA	-9.22	98.64	121.70
2	Q	69	PRO	N-CA-CB	-8.98	92.53	103.30
1	V	211	TYR	CB-CA-C	6.75	123.89	110.40
3	C	302	ASN	CB-CA-C	6.58	123.55	110.40
2	N	115	CYS	CB-CA-C	6.35	123.10	110.40
3	L	305	LYS	CB-CA-C	6.24	122.89	110.40
2	N	1124	THR	CB-CA-C	-6.22	94.80	111.60
1	M	257	ARG	CB-CA-C	-6.10	98.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	50	GLU	CB-CA-C	-6.09	98.22	110.40
2	T	71	ASP	CB-CG-OD2	5.99	123.69	118.30
1	V	124	ASN	CB-CA-C	5.95	122.29	110.40
3	U	304	GLN	N-CA-C	-5.73	95.54	111.00
1	V	287	GLN	CA-CB-CG	-5.58	101.13	113.40
3	O	155	MET	CA-CB-CG	5.58	122.78	113.30
2	H	653	ASN	CB-CA-C	5.52	121.44	110.40
2	B	425	ARG	CG-CD-NE	-5.49	100.26	111.80
2	Q	936	ASN	CB-CA-C	5.34	121.08	110.40
1	V	13	MET	CB-CA-C	-5.22	99.96	110.40
2	Q	653	ASN	CB-CA-C	5.22	120.83	110.40
3	C	302	ASN	C-N-CA	5.19	133.19	122.30
2	B	984	ARG	CG-CD-NE	5.12	122.56	111.80
2	W	900	THR	CA-CB-OG1	-5.11	98.28	109.00
3	C	301	ARG	CG-CD-NE	5.05	122.42	111.80
2	H	43	THR	CB-CA-C	-5.00	98.10	111.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	446	ARG	Sidechain
2	H	954	GLU	Mainchain
2	K	1021	SER	Mainchain
2	K	446	ARG	Sidechain
2	W	1020	HIS	Peptide
2	W	111	ASN	Peptide
2	W	124	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3349	0	3216	88	0
1	D	2872	0	2267	142	0
1	G	3344	0	3208	92	0
1	J	3361	0	3242	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3309	0	3136	155	0
1	P	3321	0	3149	117	0
1	S	3333	0	3198	92	0
1	V	3239	0	2948	264	0
2	B	9003	0	8576	356	0
2	E	6871	0	4598	311	0
2	H	9028	0	8644	244	0
2	K	9046	0	8683	294	0
2	N	9052	0	8682	316	0
2	Q	8902	0	8343	440	0
2	T	9034	0	8643	270	0
2	W	8920	0	8364	432	0
3	C	2281	0	2171	60	0
3	F	2068	0	1752	149	0
3	I	2216	0	2068	149	0
3	L	2274	0	2151	62	0
3	O	2124	0	1863	123	0
3	R	2261	0	2134	59	0
3	U	2267	0	2146	53	0
3	X	2225	0	2060	134	0
4	A	24	0	0	1	0
4	B	8	0	0	0	0
4	D	24	0	0	7	0
4	E	8	0	0	0	0
4	G	24	0	0	3	0
4	H	8	0	0	0	0
4	J	24	0	0	5	0
4	K	8	0	0	1	0
4	M	24	0	0	3	0
4	N	8	0	0	3	0
4	P	24	0	0	3	0
4	Q	8	0	0	3	0
4	S	24	0	0	3	0
4	T	8	0	0	3	0
4	V	24	0	0	6	0
4	W	8	0	0	2	0
5	A	7	0	0	0	0
5	D	7	0	0	3	0
5	G	7	0	0	0	0
5	J	7	0	0	0	0
5	M	7	0	0	2	0
5	P	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	7	0	0	0	0
5	V	7	0	0	5	0
6	B	94	0	43	12	0
6	E	94	0	41	19	0
6	H	94	0	42	13	0
6	K	94	0	43	14	0
6	N	94	0	43	18	0
6	Q	94	0	41	19	0
6	T	94	0	43	13	0
6	W	94	0	44	21	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	H	1	0	0	0	0
7	K	1	0	0	0	0
7	N	1	0	0	0	0
7	Q	1	0	0	0	0
7	T	1	0	0	0	0
7	W	1	0	0	0	0
8	C	43	0	30	8	0
8	F	43	0	30	25	0
8	I	43	0	30	29	0
8	L	43	0	30	6	0
8	O	43	0	30	11	0
8	R	43	0	30	5	0
8	U	43	0	30	4	0
8	X	43	0	30	15	0
9	C	2	0	0	0	0
9	F	2	0	0	0	0
9	I	2	0	0	0	0
9	L	2	0	0	0	0
9	O	2	0	0	0	0
9	R	2	0	0	0	0
9	U	2	0	0	0	0
9	X	2	0	0	1	0
10	A	37	0	0	0	0
10	B	72	0	0	7	0
10	C	35	0	0	1	0
10	D	6	0	0	0	0
10	E	13	0	0	1	0
10	F	8	0	0	0	0
10	G	25	0	0	1	0
10	H	83	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	20	0	0	1	0
10	J	28	0	0	2	0
10	K	74	0	0	3	0
10	L	30	0	0	0	0
10	M	10	0	0	0	0
10	N	76	0	0	5	0
10	O	17	0	0	3	0
10	P	16	0	0	4	0
10	Q	43	0	0	3	0
10	R	22	0	0	1	0
10	S	20	0	0	1	0
10	T	62	0	0	4	0
10	U	25	0	0	3	0
10	V	12	0	0	1	0
10	W	41	0	0	3	0
10	X	24	0	0	3	0
All	All	115931	0	105822	4154	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 19.

All (4154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:939:PHE:CE2	2:W:1004:ARG:CD	1.78	1.66
1:V:16:PRO:CG	1:V:128:TRP:CE2	1.81	1.62
2:W:939:PHE:CE2	2:W:1004:ARG:HD2	1.10	1.59
1:V:16:PRO:HG3	1:V:128:TRP:CZ2	0.98	1.50
1:V:241:ARG:HH12	1:V:257:ARG:CG	1.20	1.50
1:V:16:PRO:HG3	1:V:128:TRP:CE2	1.38	1.47
2:W:939:PHE:CD2	2:W:1004:ARG:HD2	1.50	1.45
2:E:663:VAL:C	2:E:664:TYR:N	1.68	1.45
1:V:16:PRO:CG	1:V:128:TRP:CZ2	1.85	1.44
1:V:241:ARG:NH1	1:V:257:ARG:CG	1.77	1.41
1:V:16:PRO:CG	1:V:128:TRP:NE1	1.80	1.39
1:V:126:ASN:ND2	3:X:88:PHE:HE1	1.22	1.35
2:E:193:SER:CB	2:E:217:ALA:O	1.78	1.31
2:Q:446:ARG:NH2	2:Q:821:PHE:O	1.59	1.30
1:V:16:PRO:CD	1:V:128:TRP:HE1	1.44	1.29
3:I:302:ASN:OD1	8:I:401:HEM:HAA2	1.29	1.28
1:V:241:ARG:HH12	1:V:257:ARG:CD	1.46	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:551:ASN:O	2:Q:557:SER:CB	1.81	1.27
2:Q:311:GLU:OE2	2:Q:1019:LYS:NZ	1.64	1.27
1:V:241:ARG:NH2	2:W:90:GLU:OE2	1.67	1.26
1:V:16:PRO:HG2	1:V:128:TRP:NE1	1.39	1.26
1:V:241:ARG:NH1	1:V:257:ARG:HG2	0.91	1.23
2:E:356:THR:OG1	2:E:847:HIS:CB	1.86	1.23
2:E:193:SER:CA	2:E:217:ALA:O	1.89	1.21
2:B:433:VAL:CG1	2:B:444:ILE:HD13	1.71	1.19
1:V:126:ASN:ND2	3:X:88:PHE:CE1	1.99	1.19
1:V:16:PRO:HG2	1:V:128:TRP:CE2	1.56	1.18
1:V:189:ARG:HG3	1:V:211:TYR:HE2	1.02	1.17
2:W:923:HIS:O	2:W:1021:SER:HB3	1.44	1.17
3:C:305:LYS:HE3	8:C:401:HEM:NB	1.58	1.17
1:M:336:ARG:NH2	1:M:359:GLU:HG2	1.60	1.16
3:X:81:LEU:HD21	3:X:308:SER:CA	1.73	1.16
2:E:192:TYR:O	2:E:197:GLY:HA3	1.46	1.15
3:I:155:MET:CE	3:I:241:PHE:HA	1.76	1.15
3:I:154:ARG:HG2	8:I:401:HEM:HBB1	1.23	1.14
1:V:252:ARG:NH2	1:V:386:ASP:OD2	1.78	1.14
2:W:939:PHE:CE2	2:W:1004:ARG:HD3	1.77	1.14
3:I:154:ARG:CB	8:I:401:HEM:HBB2	1.76	1.14
1:V:189:ARG:HG3	1:V:211:TYR:CE2	1.83	1.13
2:W:937:ASN:ND2	2:W:954:GLU:O	1.80	1.13
3:F:120:ASP:HB3	3:F:258:PHE:CE1	1.84	1.12
1:V:189:ARG:HG2	8:X:401:HEM:HBA2	1.26	1.12
1:V:189:ARG:NH2	1:V:207:ARG:O	1.82	1.12
2:N:1135:MET:CE	2:N:1138:PHE:HD2	1.62	1.12
3:I:154:ARG:HG2	8:I:401:HEM:CBB	1.78	1.12
3:I:305:LYS:NZ	8:I:401:HEM:NB	1.97	1.12
2:W:974:TYR:HE1	2:W:1052:ARG:HD3	1.03	1.12
2:W:924:SER:OG	6:W:5801:MD1:O2A	1.67	1.12
3:I:154:ARG:HB3	8:I:401:HEM:HBB2	1.32	1.11
2:Q:91:GLN:NE2	2:Q:113:ARG:O	1.81	1.11
1:A:126:ASN:ND2	3:C:90:ASN:OD1	1.83	1.11
1:P:257:ARG:NH1	2:Q:89:VAL:O	1.85	1.10
2:N:1135:MET:HE2	2:N:1139:LEU:HD21	1.31	1.10
3:I:154:ARG:CG	8:I:401:HEM:CBB	2.29	1.10
1:M:257:ARG:HH22	2:N:90:GLU:HG3	1.17	1.09
1:M:209:ARG:NH1	3:O:234:GLU:OE1	1.82	1.09
1:V:189:ARG:NH1	1:V:209:ARG:HB2	1.67	1.09
1:M:21:ARG:NH2	1:M:180:TYR:OH	1.86	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:435:ASP:HB2	2:W:442:LYS:HD2	1.29	1.08
3:I:48:VAL:HG22	3:I:313:PRO:HB2	1.36	1.07
3:I:155:MET:HE2	3:I:241:PHE:HB3	1.32	1.06
1:M:189:ARG:NH2	3:O:244:LEU:O	1.87	1.06
2:B:433:VAL:HG11	2:B:444:ILE:HD13	1.31	1.06
2:W:1124:THR:HG23	2:W:1126:TYR:CD2	1.91	1.06
2:N:1135:MET:HE1	2:N:1138:PHE:CD2	1.90	1.05
2:Q:394:ARG:HH22	2:Q:829:GLN:NE2	1.54	1.05
3:F:171:TRP:CE2	3:F:229:ARG:NE	2.24	1.05
2:N:1119:TRP:O	2:N:1122:VAL:HG23	1.56	1.05
1:V:252:ARG:HH22	1:V:386:ASP:CG	1.60	1.04
1:V:212:ARG:NH2	3:X:129:GLU:O	1.90	1.04
2:W:939:PHE:CD2	2:W:1004:ARG:CD	2.22	1.04
2:T:661:LYS:O	2:T:1060:THR:OG1	1.76	1.03
2:T:823:THR:HB	2:T:829:GLN:HE21	1.16	1.03
1:M:257:ARG:NH2	2:N:90:GLU:HG3	1.73	1.03
2:Q:857:LEU:HB2	2:Q:900:THR:HG21	1.36	1.03
3:X:81:LEU:HD21	3:X:308:SER:N	1.73	1.03
2:Q:499:SER:OG	2:Q:894:TRP:NE1	1.89	1.02
2:W:381:THR:HG22	2:W:383:PHE:H	1.21	1.02
2:Q:394:ARG:NH2	2:Q:829:GLN:HE22	1.57	1.02
3:C:305:LYS:HE3	8:C:401:HEM:C1B	1.95	1.01
2:K:937:ASN:ND2	2:K:954:GLU:H	1.56	1.01
1:M:243:GLU:OE1	2:N:54:ARG:NH1	1.93	1.01
2:Q:258:PRO:O	2:Q:608:ARG:NH2	1.93	1.01
2:W:974:TYR:HE1	2:W:1052:ARG:CD	1.72	1.01
2:E:123:ARG:HH11	3:F:194:ASP:HB2	1.23	1.01
3:I:302:ASN:HD22	3:I:303:GLY:N	1.58	1.01
1:D:149:ALA:O	2:E:1009:PRO:HG2	1.58	1.01
2:W:974:TYR:CE1	2:W:1052:ARG:HD3	1.95	1.01
3:I:302:ASN:CG	8:I:401:HEM:HAA2	1.81	1.01
2:Q:937:ASN:ND2	2:Q:954:GLU:O	1.93	1.01
2:W:38:ASP:O	10:W:5901:HOH:O	1.77	1.00
2:E:848:ARG:CB	2:E:860:ALA:O	2.09	1.00
2:W:857:LEU:HB2	2:W:900:THR:HG21	1.44	1.00
2:Q:937:ASN:HD21	2:Q:954:GLU:N	1.60	1.00
2:W:1124:THR:HG23	2:W:1126:TYR:HD2	1.23	1.00
2:Q:549:THR:OG1	2:Q:551:ASN:OD1	1.80	0.99
2:N:115:CYS:HB3	4:N:5804:SF4:S2	2.02	0.99
1:V:189:ARG:HH12	1:V:209:ARG:HB2	1.18	0.99
3:I:155:MET:HE3	3:I:241:PHE:HA	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:305:LYS:NZ	8:I:401:HEM:NA	2.09	0.99
1:M:336:ARG:HH22	1:M:359:GLU:HG2	1.24	0.98
1:M:239:TYR:OH	2:N:50:GLU:O	1.81	0.98
3:I:155:MET:HE2	3:I:241:PHE:CB	1.93	0.98
2:Q:433:VAL:HG21	2:Q:460:PRO:HB3	1.43	0.98
3:O:155:MET:SD	8:O:401:HEM:ND	2.38	0.97
2:K:917:LYS:O	2:K:1019:LYS:HE2	1.64	0.97
2:T:193:SER:O	2:T:216:GLY:O	1.81	0.97
1:V:16:PRO:HD3	1:V:128:TRP:HE1	1.30	0.96
3:F:171:TRP:CD2	3:F:229:ARG:HD2	2.01	0.96
3:X:81:LEU:CD2	3:X:307:ILE:C	2.34	0.96
2:H:658:ASN:OD1	2:H:1024:ILE:HG12	1.65	0.96
2:E:193:SER:CB	2:E:217:ALA:C	2.34	0.96
3:F:120:ASP:HB3	3:F:258:PHE:CD1	2.00	0.95
3:I:53:TYR:CE1	3:I:319:ILE:HA	2.01	0.95
3:O:303:GLY:O	3:O:305:LYS:HD3	1.67	0.95
1:V:33:ASN:ND2	1:V:331:PHE:CZ	2.34	0.95
3:X:81:LEU:HD21	3:X:308:SER:HA	1.48	0.95
2:N:923:HIS:O	2:N:1021:SER:HB3	1.66	0.95
3:O:130:PHE:CE2	3:O:301:ARG:HD3	2.00	0.95
3:I:302:ASN:ND2	3:I:303:GLY:H	1.64	0.94
2:N:1135:MET:CE	2:N:1138:PHE:CD2	2.47	0.94
1:V:241:ARG:NH2	2:W:90:GLU:CD	2.19	0.94
2:W:939:PHE:HE2	2:W:1004:ARG:CB	1.80	0.94
1:V:149:ALA:HB2	1:V:168:PHE:HD2	1.31	0.94
2:B:1135:MET:CE	2:B:1138:PHE:CD2	2.50	0.93
2:N:1135:MET:CE	2:N:1139:LEU:HD21	1.98	0.93
3:O:294:TRP:NE1	3:O:305:LYS:HB3	1.83	0.93
1:V:207:ARG:HG2	1:V:207:ARG:HH11	1.31	0.93
1:V:241:ARG:HH22	2:W:90:GLU:CD	1.71	0.93
3:I:155:MET:CE	3:I:241:PHE:CA	2.47	0.93
2:W:654:VAL:HG12	6:W:5801:MD1:O2B	1.69	0.92
2:Q:640:THR:OG1	2:Q:1071:ASP:OD1	1.87	0.92
3:X:81:LEU:HD22	3:X:307:ILE:C	1.89	0.92
2:W:438:SER:OG	10:W:5902:HOH:O	1.86	0.91
2:Q:445:THR:HG22	2:Q:448:ASP:OD2	1.70	0.91
2:B:1135:MET:HE1	2:B:1138:PHE:CD2	2.05	0.91
1:V:15:TYR:CE2	1:V:185:ALA:HB2	2.03	0.91
3:I:302:ASN:OD1	8:I:401:HEM:CAA	2.16	0.91
2:K:917:LYS:HZ1	6:K:5801:MD1:H15	0.93	0.91
2:B:433:VAL:HG13	2:B:444:ILE:HD13	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:16:PRO:CD	1:V:128:TRP:NE1	2.21	0.91
3:F:229:ARG:HG2	3:F:229:ARG:HH11	1.35	0.91
2:Q:70:ASN:H	2:Q:231:LEU:HD11	1.36	0.91
2:E:663:VAL:C	2:E:664:TYR:CA	2.39	0.91
2:W:435:ASP:CB	2:W:442:LYS:HD2	2.00	0.91
1:P:255:GLU:OE1	1:P:346:ARG:NH2	2.03	0.90
1:V:259:MET:CE	1:V:269:GLN:HG3	2.01	0.90
3:X:275:ASP:HB3	3:X:278:ASP:HB2	1.53	0.90
2:N:1135:MET:HE1	2:N:1138:PHE:HD2	1.24	0.90
2:B:1135:MET:CE	2:B:1138:PHE:HD2	1.83	0.90
2:W:977:VAL:HG22	2:W:1001:LEU:HD23	1.51	0.90
2:Q:69:PRO:O	2:Q:922:VAL:HG11	1.71	0.90
3:F:155:MET:SD	8:F:401:HEM:NC	2.45	0.89
1:P:276:PRO:HB3	1:P:286:HIS:NE2	1.88	0.89
2:W:939:PHE:HE2	2:W:1004:ARG:HB3	1.36	0.89
3:I:305:LYS:HD3	3:I:307:ILE:CG2	2.03	0.89
2:W:976:TYR:CD1	2:W:1000:ARG:NH2	2.41	0.89
2:B:101:LEU:HD12	2:B:802:LEU:HD11	1.54	0.89
2:N:1034:GLU:OE2	2:N:1053:TYR:OH	1.88	0.89
2:Q:433:VAL:CG2	2:Q:460:PRO:HB3	2.02	0.89
2:W:893:SER:O	2:W:897:THR:HG23	1.71	0.89
2:Q:394:ARG:NH2	2:Q:829:GLN:NE2	2.17	0.89
2:W:977:VAL:CG2	2:W:1001:LEU:HD23	2.03	0.89
2:K:31:LEU:HD11	3:R:107:ILE:HD11	1.55	0.89
2:Q:759:LYS:O	2:Q:763:GLU:HG3	1.72	0.89
3:L:302:ASN:O	3:L:305:LYS:HE2	1.71	0.88
3:I:154:ARG:CB	8:I:401:HEM:CBB	2.51	0.88
1:M:336:ARG:NH2	1:M:359:GLU:CG	2.35	0.88
3:O:155:MET:SD	8:O:401:HEM:NC	2.46	0.88
3:L:84:GLN:NE2	3:L:303:GLY:O	2.06	0.88
2:T:653:ASN:O	2:T:653:ASN:ND2	2.07	0.88
2:W:655:ASN:ND2	2:W:685:THR:HB	1.89	0.88
2:E:218:GLY:O	2:E:219:THR:HG22	1.72	0.88
3:I:302:ASN:HD22	3:I:303:GLY:H	0.92	0.88
1:V:68:TYR:OH	2:W:1131:GLU:OE2	1.91	0.88
3:X:41:GLU:HB3	3:X:309:ILE:HB	1.55	0.88
3:I:155:MET:CE	3:I:241:PHE:CB	2.51	0.87
3:I:302:ASN:ND2	3:I:303:GLY:N	2.20	0.87
2:W:857:LEU:HB2	2:W:900:THR:CG2	2.04	0.87
3:I:303:GLY:HA2	3:I:305:LYS:HE3	1.57	0.87
2:B:58:GLN:OE1	10:B:5901:HOH:O	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:153:PRO:O	2:W:157:THR:HG23	1.73	0.87
3:I:48:VAL:CG2	3:I:313:PRO:HB2	2.05	0.87
2:Q:917:LYS:HD2	6:Q:5802:MD1:H15	1.40	0.87
3:F:171:TRP:CE2	3:F:229:ARG:CD	2.58	0.86
2:Q:96:GLN:HG2	2:Q:108:ARG:HG2	1.56	0.86
3:I:154:ARG:CG	8:I:401:HEM:HBB2	2.01	0.86
3:O:303:GLY:HA2	3:O:305:LYS:CD	2.05	0.86
2:E:193:SER:HA	2:E:217:ALA:O	1.75	0.86
1:P:108:TYR:OH	10:P:601:HOH:O	1.93	0.86
3:X:81:LEU:CD2	3:X:308:SER:N	2.38	0.86
2:Q:1138:PHE:HA	2:Q:1143:LEU:HD23	1.55	0.86
2:W:934:ILE:HD11	2:W:952:VAL:HG13	1.55	0.86
2:B:433:VAL:CG1	2:B:444:ILE:CD1	2.54	0.86
3:F:164:LEU:N	3:F:236:LEU:O	2.08	0.85
2:Q:394:ARG:HH12	2:Q:829:GLN:NE2	1.74	0.85
2:Q:821:PHE:HE2	2:Q:828:LEU:HD21	1.41	0.85
3:C:301:ARG:HH21	3:C:301:ARG:HG2	1.41	0.85
3:I:242:GLY:HA2	8:I:401:HEM:O1A	1.76	0.85
2:W:977:VAL:HG22	2:W:1001:LEU:CD2	2.06	0.85
2:N:1135:MET:HE3	2:N:1138:PHE:HD2	1.41	0.85
2:Q:115:CYS:HB2	2:Q:314:MET:HE1	1.58	0.85
2:E:77:ILE:HD13	2:E:114:MET:CE	2.05	0.85
2:K:917:LYS:NZ	6:K:5801:MD1:H15	1.73	0.85
2:W:974:TYR:CE1	2:W:1052:ARG:CD	2.59	0.85
3:F:171:TRP:CZ2	3:F:229:ARG:NE	2.45	0.84
2:Q:394:ARG:HH22	2:Q:829:GLN:CD	1.81	0.84
2:T:983:ASP:OD2	2:T:1061:ARG:NH1	2.10	0.84
1:V:33:ASN:ND2	1:V:331:PHE:CE2	2.46	0.84
2:K:425:ARG:HG2	2:K:425:ARG:HH11	1.42	0.84
2:Q:937:ASN:ND2	2:Q:954:GLU:H	1.75	0.83
2:H:36:VAL:HG12	3:I:243:THR:HG21	1.58	0.83
2:E:1003:LEU:O	2:E:1003:LEU:HD23	1.77	0.83
2:K:937:ASN:ND2	2:K:954:GLU:N	2.26	0.83
2:B:225:ARG:HH11	2:B:656:LEU:HD12	1.44	0.83
2:Q:625:ILE:CD1	2:Q:633:ARG:HE	1.92	0.83
2:B:276:GLN:HE22	2:B:1092:HIS:H	1.27	0.82
2:W:892:LYS:HB3	2:W:897:THR:HG22	1.61	0.82
2:B:641:HIS:CE1	2:B:1087:PHE:HB2	2.14	0.82
2:B:950:PRO:HD2	2:B:954:GLU:HB3	1.62	0.82
2:N:1020:HIS:HE1	6:N:5801:MD1:O11	1.63	0.82
1:V:189:ARG:CG	1:V:211:TYR:HE2	1.88	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:81:LEU:CD2	3:X:308:SER:HA	2.10	0.82
3:F:171:TRP:CZ2	3:F:229:ARG:CD	2.62	0.82
2:E:1063:TRP:H	2:E:1096:THR:HG23	1.43	0.81
2:H:709:THR:HG22	2:H:718:GLN:HB2	1.61	0.81
2:K:379:LYS:HB3	2:K:450:GLY:HA2	1.62	0.81
2:Q:383:PHE:HE2	2:Q:548:LEU:HD21	1.44	0.81
2:T:316:GLU:OE1	10:T:5901:HOH:O	1.97	0.81
1:V:189:ARG:HG2	8:X:401:HEM:CBA	2.07	0.81
3:X:81:LEU:CD2	3:X:308:SER:CA	2.58	0.81
2:Q:115:CYS:HB2	2:Q:314:MET:CE	2.10	0.81
2:B:433:VAL:HG11	2:B:444:ILE:CD1	2.10	0.81
3:I:305:LYS:CD	3:I:307:ILE:HG23	2.11	0.81
1:M:15:TYR:HE1	2:N:41:LEU:HD11	1.45	0.81
2:B:46:ASP:OD1	2:B:48:ARG:HG3	1.81	0.81
2:Q:640:THR:HB	2:Q:1087:PHE:HB3	1.62	0.81
3:F:157:ASP:C	3:F:239:GLU:O	2.20	0.80
3:I:154:ARG:CG	8:I:401:HEM:HBB1	1.99	0.80
2:T:115:CYS:HB3	4:T:5804:SF4:S2	2.20	0.80
1:V:25:GLN:HG2	1:V:302:ASN:HD22	1.46	0.80
2:B:923:HIS:O	2:B:1021:SER:HB3	1.80	0.80
3:I:53:TYR:CE1	3:I:319:ILE:HG23	2.17	0.80
2:T:113:ARG:HG3	2:T:315:PRO:HB2	1.63	0.80
3:F:171:TRP:CE2	3:F:229:ARG:HD2	2.17	0.80
2:W:974:TYR:O	2:W:1108:ALA:HB3	1.82	0.80
2:N:1124:THR:CG2	2:N:1126:TYR:CD2	2.64	0.80
2:W:153:PRO:O	2:W:157:THR:CG2	2.30	0.80
3:X:139:PRO:HB3	3:X:151:PHE:CE1	2.16	0.80
3:C:305:LYS:HE3	8:C:401:HEM:C4B	2.16	0.80
3:F:305:LYS:HE3	8:F:401:HEM:C4D	1.83	0.80
1:V:101:GLN:O	1:V:104:THR:HG22	1.81	0.80
2:N:305:THR:HG23	2:N:525:TYR:HB3	1.61	0.79
2:Q:307:LYS:HD3	2:Q:562:TRP:HB2	1.63	0.79
2:Q:937:ASN:HD21	2:Q:954:GLU:H	1.24	0.79
2:W:398:LYS:O	2:W:471:ILE:HD11	1.83	0.79
2:B:1135:MET:HE3	2:B:1138:PHE:HD2	1.47	0.79
1:V:262:CYS:SG	1:V:266:ILE:HG12	2.21	0.79
2:H:275:ASP:HB3	2:H:563:ALA:HB1	1.65	0.79
1:P:107:PRO:HG3	1:P:285:ARG:HH11	1.46	0.79
2:Q:351:ARG:HG3	2:Q:354:THR:HG21	1.64	0.79
3:X:109:ILE:O	3:X:110:TYR:HD1	1.66	0.79
2:B:217:ALA:HB2	2:B:262:LEU:CD1	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:501:THR:HG23	2:E:503:SER:H	1.46	0.79
2:K:91:GLN:HE21	2:K:114:MET:HB2	1.47	0.79
1:D:263:VAL:HA	2:E:112:PRO:CB	2.13	0.79
2:B:71:ASP:O	2:B:72:THR:HG22	1.82	0.79
2:Q:937:ASN:ND2	2:Q:954:GLU:N	2.30	0.78
2:B:655:ASN:ND2	2:B:924:SER:OG	2.16	0.78
2:T:823:THR:HB	2:T:829:GLN:NE2	1.96	0.78
2:W:939:PHE:CE2	2:W:1004:ARG:HB3	2.18	0.78
2:Q:336:GLU:OE2	6:Q:5802:MD1:O3'	2.02	0.78
2:Q:603:LEU:HD11	2:Q:772:ARG:HD3	1.65	0.78
2:K:433:VAL:HG21	2:K:460:PRO:HB3	1.66	0.78
2:N:51:SER:O	2:N:52:VAL:C	2.22	0.78
1:M:4:VAL:HG23	1:M:19:GLU:HB2	1.64	0.78
1:D:149:ALA:O	2:E:1009:PRO:CG	2.31	0.78
3:I:53:TYR:CD1	3:I:319:ILE:HA	2.18	0.78
1:M:194:LYS:HG3	1:M:201:VAL:HG22	1.66	0.78
2:E:1063:TRP:H	2:E:1096:THR:CG2	1.97	0.78
1:V:16:PRO:CB	1:V:128:TRP:CZ2	2.65	0.78
2:W:222:PHE:HD1	2:W:648:VAL:HG13	1.49	0.78
2:W:974:TYR:CE1	2:W:1052:ARG:NH1	2.50	0.78
3:O:110:TYR:CD1	3:O:268:CYS:HB2	2.19	0.77
2:Q:394:ARG:NH1	2:Q:829:GLN:NE2	2.31	0.77
2:B:977:VAL:HG12	2:B:1103:VAL:HG11	1.66	0.77
1:M:190:LYS:HD2	2:N:37:VAL:HG13	1.66	0.77
2:B:1022:ALA:HB1	2:B:1050:SER:HB2	1.66	0.77
1:P:267:ARG:NH1	4:P:503:SF4:S1	2.58	0.77
1:G:25:GLN:HG2	1:G:302:ASN:ND2	1.98	0.77
3:L:302:ASN:CG	3:L:303:GLY:H	1.87	0.77
1:P:231:VAL:CG2	10:P:604:HOH:O	2.31	0.77
1:V:40:THR:HG22	1:V:261:ALA:HB1	1.66	0.77
1:P:262:CYS:HB2	1:P:267:ARG:HD3	1.66	0.77
2:B:225:ARG:NH1	2:B:656:LEU:HD12	2.00	0.77
1:V:9:LEU:HD23	1:V:111:TYR:HD2	1.49	0.77
2:W:853:ALA:HA	2:W:1102:LEU:HD21	1.67	0.77
2:W:91:GLN:NE2	2:W:114:MET:HB2	1.99	0.77
2:W:551:ASN:O	2:W:557:SER:HB2	1.84	0.77
3:X:138:PHE:HB2	3:X:279:VAL:HG21	1.66	0.77
2:K:957:ILE:HB	2:K:1003:LEU:HD11	1.67	0.77
2:T:381:THR:HG22	2:T:383:PHE:H	1.51	0.77
3:U:51:VAL:HG22	3:U:316:LEU:HA	1.67	0.77
3:X:81:LEU:CD2	3:X:307:ILE:O	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:109:ILE:HB	3:X:271:LEU:CD2	2.15	0.77
2:E:617:TRP:HA	2:E:621:GLU:HG3	1.67	0.76
3:F:171:TRP:CE3	3:F:229:ARG:HD2	2.19	0.76
1:M:259:MET:HG2	1:M:269:GLN:HB2	1.65	0.76
1:P:107:PRO:HG3	1:P:285:ARG:NH1	2.00	0.76
2:Q:357:ALA:HB2	2:Q:847:HIS:CD2	2.20	0.76
1:M:23:LYS:HD2	1:M:23:LYS:O	1.84	0.76
1:S:262:CYS:SG	1:S:266:ILE:HG12	2.25	0.76
3:F:140:LEU:HD21	3:F:163:ASN:HB2	1.68	0.76
3:U:43:THR:HG22	3:U:147:PRO:HG3	1.66	0.76
1:J:62:ASN:HD22	1:J:71:PHE:HB3	1.50	0.76
1:V:149:ALA:HB2	1:V:168:PHE:CD2	2.18	0.76
1:M:126:ASN:HA	3:O:88:PHE:CE1	2.21	0.76
2:N:923:HIS:O	2:N:1021:SER:CB	2.33	0.76
2:W:321:THR:HG22	2:W:343:LYS:HD2	1.68	0.76
8:X:401:HEM:HBC2	8:X:401:HEM:HHD	1.68	0.76
3:I:51:VAL:HG13	3:I:104:HIS:HD2	1.50	0.76
2:E:926:TRP:HD1	2:E:932:ASN:OD1	1.68	0.75
3:F:155:MET:SD	8:F:401:HEM:ND	2.60	0.75
3:F:305:LYS:HE3	8:F:401:HEM:CHA	2.03	0.75
2:K:31:LEU:N	2:K:31:LEU:HD13	2.02	0.75
1:V:116:ILE:HG13	1:V:129:ALA:HB1	1.67	0.75
2:W:857:LEU:CB	2:W:900:THR:HG21	2.16	0.75
2:W:923:HIS:O	2:W:1021:SER:CB	2.32	0.75
2:E:192:TYR:C	2:E:197:GLY:HA3	2.06	0.75
1:J:262:CYS:HB2	1:J:267:ARG:HD3	1.67	0.75
2:Q:575:LYS:HD3	2:Q:575:LYS:H	1.50	0.75
1:V:241:ARG:NH1	1:V:257:ARG:CD	2.31	0.75
2:N:1124:THR:HG22	2:N:1126:TYR:CD2	2.20	0.75
3:C:309:ILE:HG13	3:C:310:GLN:HG3	1.69	0.75
2:K:918:SER:HB2	2:K:1019:LYS:HD3	1.67	0.75
2:N:213:ARG:HD2	2:N:642:MET:HB3	1.66	0.75
2:B:537:LEU:HD21	2:B:842:GLU:HG2	1.66	0.75
2:H:36:VAL:HG12	3:I:243:THR:CG2	2.15	0.75
2:K:917:LYS:O	2:K:1019:LYS:CE	2.34	0.75
1:V:213:LYS:HD2	3:X:301:ARG:HH21	1.52	0.75
2:W:937:ASN:CG	2:W:954:GLU:O	2.24	0.75
2:E:414:SER:O	2:E:420:LEU:HB2	1.87	0.75
1:M:125:ILE:O	1:M:125:ILE:HG12	1.85	0.75
3:O:140:LEU:CG	3:O:161:PRO:O	2.34	0.75
3:U:305:LYS:HE2	8:U:401:HEM:C4C	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:178:CYS:O	1:V:181:PRO:HD3	1.86	0.75
2:W:1124:THR:O	2:W:1126:TYR:CD2	2.39	0.75
3:X:278:ASP:OD2	9:X:402:CA:CA	1.64	0.75
2:B:1088:GLU:HG2	2:B:1091:ASN:HB3	1.69	0.75
2:H:49:TRP:O	2:H:52:VAL:HG23	1.87	0.75
1:M:15:TYR:HE2	1:M:185:ALA:HB2	1.50	0.75
3:O:137:MET:SD	3:O:155:MET:HA	2.27	0.75
3:R:236:LEU:HB2	3:R:245:THR:O	1.86	0.75
2:B:236:LYS:NZ	2:B:734:ASP:OD1	2.20	0.75
3:I:155:MET:CE	3:I:241:PHE:HB3	2.13	0.75
3:O:303:GLY:HA2	3:O:305:LYS:HD2	1.67	0.75
1:V:36:ILE:HG13	2:W:310:ILE:HG23	1.68	0.74
2:B:879:ALA:HB3	2:B:888:ARG:HH21	1.51	0.74
1:V:257:ARG:HD2	2:W:90:GLU:OE1	1.86	0.74
2:K:445:THR:HG22	2:K:448:ASP:OD2	1.86	0.74
1:M:23:LYS:HD2	1:M:23:LYS:C	2.07	0.74
1:S:34:ARG:HA	2:T:321:THR:HG21	1.69	0.74
2:E:193:SER:C	2:E:217:ALA:O	2.25	0.74
2:N:78:ARG:NH1	2:N:92:ASN:OD1	2.20	0.74
1:D:149:ALA:HB2	1:D:168:PHE:HD2	1.53	0.74
2:Q:950:PRO:HD2	2:Q:954:GLU:HB3	1.68	0.74
1:V:241:ARG:HH11	1:V:257:ARG:HG2	0.91	0.74
2:Q:394:ARG:NH1	2:Q:831:TYR:O	2.21	0.74
3:L:51:VAL:HG22	3:L:316:LEU:HA	1.70	0.74
2:Q:356:THR:HG22	2:Q:538:MET:HA	1.69	0.74
2:Q:1022:ALA:HB1	2:Q:1050:SER:HB2	1.69	0.74
2:E:628:THR:HG22	2:E:630:LYS:H	1.53	0.74
1:M:190:LYS:NZ	2:N:37:VAL:O	2.20	0.74
2:Q:531:HIS:O	2:Q:1099:LYS:HB2	1.86	0.74
2:W:545:PRO:O	2:W:549:THR:HG23	1.87	0.74
2:Q:93:TYR:O	2:Q:96:GLN:NE2	2.21	0.74
3:X:229:ARG:NH1	10:X:502:HOH:O	2.18	0.74
1:G:126:ASN:O	1:G:127:GLN:HG2	1.87	0.74
2:N:1078:LYS:HG3	2:N:1079:ILE:HG12	1.70	0.74
2:E:664:TYR:HB3	2:E:995:PHE:HE2	1.50	0.73
2:B:217:ALA:HB2	2:B:262:LEU:HD12	1.69	0.73
1:D:6:ASN:ND2	1:D:13:MET:SD	2.57	0.73
1:D:190:LYS:HB2	2:E:37:VAL:HG21	1.69	0.73
1:M:149:ALA:HB2	1:M:168:PHE:HD2	1.53	0.73
3:O:301:ARG:HG2	3:O:301:ARG:HH11	1.53	0.73
2:T:546:VAL:HG12	2:T:552:VAL:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:LEU:HB2	1:G:305:TYR:HE1	1.51	0.73
1:P:76:ASP:OD2	2:Q:1138:PHE:CZ	2.41	0.73
2:B:135:LEU:HB2	2:B:694:ALA:HB3	1.69	0.73
2:H:267:TRP:NE1	2:H:612:GLU:OE1	2.20	0.73
2:N:1022:ALA:HB1	2:N:1050:SER:CB	2.18	0.73
1:S:257:ARG:NH1	2:T:89:VAL:O	2.20	0.73
3:X:81:LEU:O	3:X:96:ASN:HA	1.89	0.73
3:X:302:ASN:HB2	8:X:401:HEM:HAA1	1.70	0.73
2:H:1024:ILE:HG22	2:H:1055:SER:CB	2.19	0.73
2:N:73:HIS:O	2:N:113:ARG:NH1	2.21	0.73
2:N:880:GLU:O	2:N:885:ARG:NH1	2.21	0.73
1:S:292:PRO:HG2	1:S:295:PRO:HG3	1.69	0.73
2:W:91:GLN:HE21	2:W:114:MET:HB2	1.52	0.73
2:B:302:LEU:HD11	2:B:524:HIS:CD2	2.23	0.73
2:E:385:LEU:HA	2:E:433:VAL:HG11	1.70	0.73
2:Q:332:VAL:HG23	2:Q:344:ALA:HB2	1.70	0.73
2:E:998:VAL:O	2:E:1054:GLY:HA2	1.88	0.73
8:I:401:HEM:HBA2	8:I:401:HEM:CHA	2.18	0.73
2:K:115:CYS:HB3	4:K:5804:SF4:S2	2.28	0.73
2:N:519:LYS:NZ	2:N:549:THR:O	2.21	0.73
2:K:265:ARG:HE	2:K:612:GLU:HB2	1.53	0.72
3:X:109:ILE:HB	3:X:271:LEU:HD23	1.71	0.72
3:L:271:LEU:HD12	3:L:281:PHE:HB2	1.71	0.72
3:O:155:MET:SD	8:O:401:HEM:FE	1.82	0.72
3:R:148:GLU:OE2	3:R:148:GLU:N	2.20	0.72
2:T:1022:ALA:HB1	2:T:1050:SER:HB2	1.71	0.72
2:W:655:ASN:HD21	2:W:685:THR:HB	1.54	0.72
2:K:138:LYS:HG3	2:K:170:LEU:HD11	1.70	0.72
2:K:937:ASN:HD21	2:K:954:GLU:H	1.36	0.72
2:Q:275:ASP:HB3	2:Q:563:ALA:HB1	1.70	0.72
2:Q:394:ARG:CZ	2:Q:829:GLN:HE22	2.02	0.72
3:R:91:GLY:HA3	3:R:304:GLN:HG3	1.71	0.72
2:B:652:THR:HG22	2:B:680:THR:HB	1.71	0.72
2:K:1061:ARG:NH1	2:K:1062:ASP:O	2.22	0.72
1:M:189:ARG:HG2	1:M:189:ARG:NH1	2.03	0.72
2:T:394:ARG:NH2	2:T:829:GLN:OE1	2.23	0.72
2:W:776:GLY:H	2:W:781:LYS:HZ3	1.35	0.72
1:D:362:LYS:HA	1:D:376:TYR:HA	1.71	0.72
2:E:194:GLY:O	2:E:197:GLY:N	2.22	0.72
2:Q:383:PHE:CE2	2:Q:548:LEU:HD21	2.24	0.72
1:V:9:LEU:HD23	1:V:111:TYR:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HD3	2:B:1010:ALA:HA	1.70	0.72
2:B:123:ARG:NH2	2:B:930:ASP:OD2	2.22	0.72
3:F:112:GLN:HG3	3:F:266:VAL:HG22	1.72	0.72
2:K:418:GLN:OE1	2:K:446:ARG:NH2	2.23	0.72
2:N:96:GLN:HB3	2:N:108:ARG:HG2	1.71	0.72
2:Q:622:ARG:NH1	10:Q:5901:HOH:O	2.23	0.72
3:X:277:LEU:N	3:X:277:LEU:HD23	2.05	0.72
2:H:124:ARG:NH1	2:H:925:GLN:OE1	2.23	0.72
2:H:527:GLU:HG2	6:H:5802:MD1:H101	1.71	0.72
3:I:157:ASP:OD1	3:I:158:ARG:N	2.22	0.72
2:K:241:ARG:HG3	2:K:584:TRP:O	1.89	0.72
2:E:113:ARG:O	2:E:315:PRO:CB	2.38	0.71
2:H:1024:ILE:HG22	2:H:1055:SER:HB2	1.72	0.71
2:T:824:PRO:HD2	2:T:829:GLN:HE22	1.55	0.71
1:G:309:ARG:HG2	1:G:310:TRP:HE3	1.54	0.71
1:V:259:MET:HE3	1:V:269:GLN:HG3	1.70	0.71
3:C:301:ARG:HH21	3:C:301:ARG:CG	2.01	0.71
2:K:135:LEU:HB2	2:K:694:ALA:HB3	1.72	0.71
2:K:275:ASP:HB3	2:K:563:ALA:HB1	1.71	0.71
3:R:236:LEU:HA	3:R:247:GLN:HG3	1.73	0.71
1:D:257:ARG:NH1	2:E:90:GLU:OE2	2.24	0.71
2:E:1062:ASP:HA	2:E:1096:THR:CG2	2.20	0.71
2:K:225:ARG:HH21	2:K:269:ASN:HA	1.56	0.71
3:L:142:LYS:NZ	3:L:286:SER:O	2.22	0.71
2:Q:265:ARG:NH2	2:Q:644:SER:OG	2.23	0.71
2:W:648:VAL:HG23	2:W:676:GLN:HB3	1.70	0.71
1:M:15:TYR:CE2	1:M:185:ALA:HB2	2.26	0.71
2:Q:661:LYS:NZ	2:Q:1096:THR:OG1	2.22	0.71
1:D:271:PHE:O	1:D:278:ASN:ND2	2.23	0.71
3:F:241:PHE:HB2	8:F:401:HEM:CHB	2.20	0.71
1:M:16:PRO:HG3	1:M:128:TRP:CE3	2.25	0.71
1:M:207:ARG:NH2	2:N:44:TYR:OH	2.24	0.71
1:V:211:TYR:CE1	3:X:302:ASN:HB3	2.25	0.71
3:F:211:SER:O	3:F:215:LEU:HB2	1.91	0.71
2:Q:356:THR:HG23	2:Q:538:MET:HG2	1.71	0.71
2:Q:917:LYS:NZ	6:Q:5801:MD1:H15	1.88	0.71
2:W:1124:THR:O	2:W:1126:TYR:HD2	1.74	0.71
1:G:62:ASN:HD22	1:G:71:PHE:HB3	1.56	0.71
2:K:110:TRP:HZ3	2:K:316:GLU:OE1	1.73	0.71
1:M:256:THR:HG22	1:M:259:MET:HB2	1.73	0.71
2:Q:72:THR:HG21	2:Q:713:SER:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:453:LEU:HD11	2:W:827:ARG:HH12	1.55	0.71
2:W:939:PHE:HE2	2:W:1004:ARG:CG	2.04	0.71
2:T:376:TYR:CD2	2:T:550:GLY:HA2	2.26	0.70
2:W:96:GLN:HB3	2:W:108:ARG:HG2	1.71	0.70
2:B:499:SER:OG	2:B:894:TRP:NE1	2.24	0.70
2:K:917:LYS:NZ	6:K:5801:MD1:S13	2.64	0.70
2:T:135:LEU:HB2	2:T:694:ALA:HB3	1.73	0.70
3:L:301:ARG:HH21	3:L:301:ARG:CG	2.03	0.70
2:T:467:LYS:HD3	2:T:477:GLU:OE1	1.91	0.70
2:B:96:GLN:HB3	2:B:108:ARG:HG2	1.71	0.70
2:W:658:ASN:ND2	2:W:1024:ILE:HG23	2.05	0.70
3:O:269:ARG:NH2	3:O:279:VAL:O	2.24	0.70
1:P:149:ALA:HB2	1:P:168:PHE:HD2	1.57	0.70
2:T:407:GLN:O	2:T:425:ARG:NH2	2.21	0.70
1:V:126:ASN:ND2	3:X:88:PHE:CZ	2.49	0.70
2:W:950:PRO:HD2	2:W:954:GLU:HG3	1.73	0.70
3:X:309:ILE:HD13	3:X:309:ILE:N	2.06	0.70
2:B:225:ARG:HH11	2:B:656:LEU:CD1	2.05	0.70
1:D:219:PRO:HB2	1:D:297:PHE:CD1	2.27	0.70
1:S:395:VAL:O	2:T:326:ARG:NH1	2.24	0.70
1:V:386:ASP:N	1:V:386:ASP:OD1	2.23	0.70
1:G:408:ASN:ND2	2:H:805:THR:OG1	2.23	0.70
2:W:222:PHE:CD1	2:W:648:VAL:HG13	2.27	0.70
1:J:2:THR:HG22	1:J:15:TYR:O	1.91	0.70
2:W:934:ILE:HD11	2:W:952:VAL:CG1	2.21	0.70
3:I:305:LYS:NZ	8:I:401:HEM:FE	1.58	0.70
3:O:42:LEU:O	3:O:44:PRO:HD3	1.91	0.70
3:O:235:ASP:N	3:O:250:GLN:OE1	2.25	0.70
2:W:434:TRP:HB3	2:W:461:VAL:HG22	1.74	0.70
1:D:65:THR:HG21	1:D:147:ASP:H	1.57	0.70
3:I:305:LYS:HD3	3:I:307:ILE:HG23	1.72	0.70
2:K:1078:LYS:HG3	2:K:1079:ILE:HG12	1.73	0.70
1:P:230:ARG:NH2	3:R:182:GLU:O	2.25	0.70
2:Q:179:THR:OG1	2:Q:744:LYS:NZ	2.24	0.70
3:C:305:LYS:CE	8:C:401:HEM:C1B	2.72	0.69
2:N:71:ASP:OD2	2:N:73:HIS:HD2	1.75	0.69
2:B:983:ASP:OD1	2:B:1061:ARG:NH1	2.26	0.69
1:D:53:LYS:O	1:D:226:ARG:NH1	2.25	0.69
2:E:57:TYR:O	2:E:88:ARG:NH1	2.24	0.69
2:E:1012:PRO:HG2	2:E:1015:CYS:HB3	1.74	0.69
1:V:62:ASN:HD22	1:V:71:PHE:HB3	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:857:LEU:N	2:W:900:THR:HG23	2.08	0.69
1:G:127:GLN:HE22	3:I:89:PRO:HB3	1.55	0.69
3:I:51:VAL:CG1	3:I:104:HIS:HD2	2.06	0.69
1:J:209:ARG:NH2	8:L:401:HEM:O2D	2.25	0.69
1:M:188:PRO:HB2	3:O:302:ASN:OD1	1.92	0.69
8:R:401:HEM:HHD	8:R:401:HEM:HBC2	1.75	0.69
2:W:435:ASP:HB2	2:W:442:LYS:CD	2.15	0.69
2:W:939:PHE:CZ	2:W:1004:ARG:HD3	2.25	0.69
3:C:305:LYS:HE2	8:C:401:HEM:NA	2.07	0.69
2:W:1001:LEU:HA	2:W:1054:GLY:HA3	1.72	0.69
2:B:293:MET:O	2:B:296:VAL:HG12	1.92	0.69
2:B:983:ASP:HB3	2:B:984:ARG:HD3	1.73	0.69
2:B:1022:ALA:HB1	2:B:1050:SER:CB	2.22	0.69
1:D:34:ARG:HA	2:E:321:THR:HG21	1.74	0.69
1:D:346:ARG:O	2:E:111:ASN:HB3	1.93	0.69
2:H:917:LYS:HE3	6:H:5801:MD1:H15	1.57	0.69
1:M:166:ARG:NH1	2:N:1009:PRO:O	2.25	0.69
1:P:108:TYR:HE2	1:P:291:LEU:HD22	1.58	0.69
3:I:155:MET:HE2	3:I:241:PHE:CA	2.18	0.69
1:V:225:TYR:HB3	3:X:127:THR:HG22	1.73	0.69
2:W:857:LEU:H	2:W:900:THR:HG23	1.55	0.69
2:B:628:THR:HG21	2:B:873:TYR:HB3	1.73	0.69
1:G:4:VAL:HG23	1:G:19:GLU:HB2	1.74	0.69
3:I:307:ILE:HD13	8:I:401:HEM:HAB	1.74	0.69
2:Q:394:ARG:CZ	2:Q:829:GLN:NE2	2.56	0.69
1:V:267:ARG:NH1	4:V:503:SF4:S1	2.64	0.69
3:X:139:PRO:HB3	3:X:151:PHE:HE1	1.55	0.69
1:A:21:ARG:NH2	1:A:103:GLY:O	2.26	0.69
3:F:89:PRO:HD2	3:F:302:ASN:HD21	1.58	0.69
2:K:73:HIS:O	2:K:113:ARG:NH1	2.26	0.69
2:Q:336:GLU:OE1	6:Q:5802:MD1:O2'	2.10	0.69
2:Q:821:PHE:CE2	2:Q:828:LEU:HD21	2.26	0.69
2:B:57:TYR:O	2:B:88:ARG:NH1	2.26	0.69
1:V:66:LYS:N	1:V:169:PHE:O	2.25	0.69
2:B:407:GLN:O	2:B:425:ARG:NH2	2.26	0.68
1:G:262:CYS:SG	1:G:266:ILE:HG12	2.34	0.68
3:I:241:PHE:HD1	3:I:241:PHE:H	1.40	0.68
1:A:313:ARG:O	1:A:317:ARG:HG3	1.94	0.68
2:B:314:MET:HG3	2:B:315:PRO:HD3	1.74	0.68
3:I:51:VAL:HG13	3:I:104:HIS:CD2	2.28	0.68
2:Q:1052:ARG:NH1	2:Q:1109:GLU:OE2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:528:GLY:HA2	2:T:1099:LYS:HZ2	1.56	0.68
1:V:16:PRO:HG3	1:V:128:TRP:HZ2	0.86	0.68
2:B:463:GLU:HG2	2:B:486:LYS:NZ	2.09	0.68
2:K:658:ASN:HD21	2:K:1023:TRP:HA	1.58	0.68
1:V:211:TYR:O	3:X:301:ARG:NE	2.26	0.68
2:W:939:PHE:CD2	2:W:1004:ARG:NE	2.61	0.68
3:X:129:GLU:OE1	3:X:187:ARG:NH1	2.26	0.68
2:H:858:PRO:O	2:H:888:ARG:NH1	2.25	0.68
1:J:34:ARG:HB3	1:J:266:ILE:HG22	1.75	0.68
2:W:852:GLU:OE2	2:W:984:ARG:NH1	2.23	0.68
3:F:204:TYR:O	3:F:208:VAL:HG23	1.94	0.68
2:K:313:LYS:NZ	2:K:563:ALA:O	2.27	0.68
2:K:880:GLU:O	2:K:885:ARG:NH1	2.27	0.68
1:M:190:LYS:HB3	2:N:37:VAL:HG11	1.74	0.68
1:S:209:ARG:NH2	8:U:401:HEM:O2D	2.26	0.68
2:W:950:PRO:CD	2:W:954:GLU:HG3	2.24	0.68
8:X:401:HEM:HBB2	8:X:401:HEM:HHC	1.74	0.68
2:H:152:THR:HG22	2:H:155:ASN:H	1.58	0.68
3:I:51:VAL:CG1	3:I:104:HIS:CD2	2.75	0.68
2:N:868:ILE:HB	2:N:891:LYS:HE2	1.76	0.68
2:B:665:GLN:OE1	2:B:987:GLU:N	2.21	0.68
1:D:136:ASP:OD1	1:D:137:LYS:N	2.26	0.68
2:E:986:TYR:OH	2:E:993:ASP:CB	2.42	0.68
2:H:823:THR:HG21	2:H:829:GLN:HG3	1.76	0.68
1:M:15:TYR:CE1	2:N:41:LEU:HD11	2.28	0.68
2:B:275:ASP:HB3	2:B:563:ALA:HB1	1.74	0.68
1:D:408:ASN:HD21	2:E:805:THR:H	1.40	0.68
2:E:135:LEU:HB2	2:E:694:ALA:HB3	1.76	0.68
2:T:546:VAL:HG13	2:T:551:ASN:HB2	1.76	0.68
2:E:680:THR:HG22	6:E:5801:MD1:N2	2.08	0.68
2:H:227:GLY:O	2:H:228:MET:O	2.12	0.68
2:N:811:PHE:HA	2:N:814:GLN:HG3	1.75	0.68
1:V:15:TYR:HE2	1:V:185:ALA:HB2	1.56	0.68
2:W:275:ASP:HB3	2:W:563:ALA:HB1	1.76	0.68
3:X:84:GLN:HB2	3:X:307:ILE:HG12	1.75	0.68
2:N:942:PRO:HA	2:N:952:VAL:HG13	1.75	0.68
2:Q:547:MET:HE1	2:Q:830:ALA:HB2	1.74	0.68
1:V:211:TYR:O	3:X:301:ARG:CD	2.41	0.68
3:X:309:ILE:HD13	3:X:309:ILE:H	1.59	0.68
2:B:153:PRO:O	2:B:157:THR:HG23	1.94	0.67
2:T:917:LYS:NZ	6:T:5801:MD1:H15	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:852:GLU:HG2	2:W:1101:THR:HA	1.76	0.67
2:E:52:VAL:HG11	3:F:221:ALA:HB2	1.76	0.67
2:H:166:ASN:HB3	2:Q:1035:THR:HG23	1.76	0.67
2:Q:917:LYS:O	2:Q:1019:LYS:NZ	2.26	0.67
1:S:36:ILE:O	2:T:919:ARG:NH2	2.27	0.67
1:A:356:LYS:HG2	1:A:383:PHE:HE2	1.59	0.67
1:D:212:ARG:N	5:D:504:F3S:S4	2.65	0.67
2:Q:494:ILE:O	2:Q:497:VAL:HG22	1.94	0.67
2:Q:942:PRO:HA	2:Q:952:VAL:HG13	1.75	0.67
2:Q:1138:PHE:HA	2:Q:1143:LEU:CD2	2.24	0.67
2:T:824:PRO:HD2	2:T:829:GLN:NE2	2.09	0.67
1:V:166:ARG:HD3	2:W:1010:ALA:HA	1.75	0.67
2:W:355:ASP:OD2	6:W:5802:MD1:N1	2.26	0.67
3:X:273:THR:HG22	3:X:275:ASP:H	1.60	0.67
3:L:123:GLN:NE2	3:L:125:ILE:HD12	2.08	0.67
2:N:1135:MET:HE1	2:N:1138:PHE:CE2	2.28	0.67
2:H:57:TYR:O	2:H:88:ARG:NH1	2.24	0.67
2:K:425:ARG:HG2	2:K:425:ARG:NH1	2.02	0.67
3:F:120:ASP:HB3	3:F:258:PHE:HE1	1.52	0.67
3:I:154:ARG:CD	8:I:401:HEM:CBB	2.73	0.67
3:L:51:VAL:HG12	3:L:102:ALA:HB3	1.77	0.67
3:X:302:ASN:O	3:X:305:LYS:HE3	1.93	0.67
1:A:104:THR:O	1:A:285:ARG:NH1	2.28	0.67
1:D:390:VAL:HG23	1:D:391:VAL:HG23	1.77	0.67
2:E:658:ASN:HD21	2:E:1023:TRP:HA	1.60	0.67
6:E:5802:MD1:O11	6:E:5802:MD1:N15	2.28	0.67
3:F:171:TRP:NE1	3:F:229:ARG:NE	2.43	0.67
3:O:301:ARG:HH11	3:O:301:ARG:CG	2.06	0.67
1:P:333:VAL:HG13	1:P:373:PHE:HB2	1.77	0.67
2:Q:1078:LYS:HG3	2:Q:1079:ILE:HG12	1.77	0.67
3:R:237:ASN:OD1	3:R:247:GLN:NE2	2.28	0.67
2:B:442:LYS:HG2	2:B:458:ILE:HD12	1.76	0.67
2:E:160:MET:SD	2:E:167:ASP:HB2	2.35	0.67
2:H:528:GLY:HA2	2:H:1099:LYS:HZ2	1.58	0.67
2:N:117:LYS:NZ	2:N:919:ARG:O	2.27	0.67
3:R:143:ILE:HD12	3:R:143:ILE:O	1.95	0.67
1:V:336:ARG:HD2	1:V:376:TYR:CE1	2.30	0.67
2:W:381:THR:CG2	2:W:383:PHE:H	2.02	0.67
2:B:395:VAL:HG13	2:B:432:VAL:HB	1.77	0.67
2:H:294:ASN:OD1	2:H:295:ASP:N	2.28	0.67
1:M:80:LEU:HD23	1:M:83:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:139:PRO:HB3	3:R:151:PHE:HE2	1.59	0.67
1:V:100:SER:OG	1:V:104:THR:HG23	1.94	0.67
2:W:123:ARG:NH2	2:W:930:ASP:OD2	2.26	0.67
2:W:584:TRP:HB2	2:W:773:LEU:HD11	1.77	0.67
2:B:305:THR:HG22	2:B:525:TYR:HB3	1.76	0.67
3:L:123:GLN:HE21	3:L:125:ILE:HD12	1.60	0.67
2:T:445:THR:OG1	2:T:448:ASP:OD2	2.13	0.67
1:V:29:VAL:HG21	1:V:283:LEU:HD23	1.77	0.67
1:G:402:ARG:NH2	10:G:601:HOH:O	2.26	0.66
2:H:681:ASP:OD1	2:H:682:ILE:N	2.28	0.66
3:I:53:TYR:HE1	3:I:319:ILE:HG23	1.59	0.66
2:W:974:TYR:HD1	2:W:1002:MET:SD	2.17	0.66
3:X:130:PHE:CE1	3:X:301:ARG:HD3	2.30	0.66
3:C:294:TRP:NE1	3:C:305:LYS:HB3	2.11	0.66
2:E:414:SER:C	2:E:420:LEU:HB2	2.15	0.66
2:T:1078:LYS:HG3	2:T:1079:ILE:HG12	1.78	0.66
1:V:34:ARG:CB	1:V:266:ILE:HG22	2.25	0.66
1:V:128:TRP:CD1	1:V:185:ALA:HB1	2.30	0.66
2:H:156:LYS:NZ	2:H:673:ASN:OD1	2.28	0.66
2:H:763:GLU:OE1	2:H:765:ARG:NH1	2.28	0.66
3:I:110:TYR:CE1	3:I:268:CYS:HB2	2.31	0.66
1:M:318:GLN:HE22	2:N:1138:PHE:HD1	1.43	0.66
1:V:13:MET:HG3	1:V:118:GLU:OE1	1.95	0.66
2:E:77:ILE:HD13	2:E:114:MET:HE2	1.76	0.66
2:E:1062:ASP:OD1	2:E:1096:THR:HG21	1.94	0.66
2:H:1078:LYS:HG3	2:H:1079:ILE:HG12	1.75	0.66
3:O:237:ASN:ND2	3:O:277:LEU:O	2.27	0.66
2:Q:547:MET:CE	2:Q:830:ALA:HB2	2.25	0.66
2:Q:977:VAL:HG12	2:Q:1059:ILE:HG21	1.77	0.66
1:M:258:CYS:HB2	1:M:267:ARG:HH12	1.59	0.66
1:P:195:ARG:HH12	1:P:239:TYR:HB2	1.60	0.66
2:T:275:ASP:HB3	2:T:563:ALA:HB1	1.77	0.66
2:W:795:GLU:HB3	2:W:798:VAL:HG12	1.76	0.66
2:W:865:ASN:OD1	2:W:866:PRO:HD2	1.95	0.66
1:D:21:ARG:CZ	1:D:179:THR:HG21	2.25	0.66
1:D:187:CYS:HB2	1:D:192:ILE:HD13	1.76	0.66
2:H:922:VAL:HG23	2:H:926:TRP:CE3	2.30	0.66
2:H:922:VAL:HG23	2:H:926:TRP:CZ3	2.31	0.66
1:M:15:TYR:CD2	1:M:16:PRO:HD2	2.29	0.66
1:M:262:CYS:SG	1:M:266:ILE:HG12	2.36	0.66
2:Q:937:ASN:ND2	2:Q:954:GLU:C	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1099:LYS:NZ	10:Q:5905:HOH:O	2.28	0.66
1:V:207:ARG:HH11	1:V:207:ARG:CG	2.07	0.66
2:E:192:TYR:O	2:E:197:GLY:CA	2.35	0.66
2:H:236:LYS:HG2	2:H:653:ASN:HB3	1.78	0.66
2:Q:491:ASP:OD2	2:Q:864:THR:N	2.24	0.66
1:M:45:CYS:HB2	4:M:501:SF4:S2	2.35	0.66
1:S:166:ARG:HD3	2:T:1010:ALA:HA	1.78	0.66
1:J:262:CYS:SG	1:J:266:ILE:HG12	2.36	0.66
2:K:175:ASP:O	2:K:179:THR:HG23	1.96	0.66
2:Q:278:PRO:HB2	2:Q:536:THR:HB	1.76	0.66
2:Q:859:ASN:ND2	2:Q:885:ARG:O	2.27	0.66
2:W:124:ARG:NH2	2:W:925:GLN:OE1	2.29	0.66
2:W:681:ASP:OD1	2:W:682:ILE:N	2.27	0.66
1:J:16:PRO:HG2	1:J:185:ALA:HB1	1.77	0.66
2:T:678:MET:HG2	2:T:693:PHE:HB2	1.77	0.66
2:W:647:LYS:O	2:W:675:GLU:N	2.29	0.66
2:B:790:ASN:OD1	10:B:5902:HOH:O	2.14	0.65
2:B:1088:GLU:HB3	2:B:1091:ASN:O	1.95	0.65
2:N:425:ARG:NH2	2:N:430:ASP:OD1	2.27	0.65
2:Q:462:LEU:HB3	2:Q:482:LEU:HD12	1.78	0.65
2:W:868:ILE:HG22	2:W:870:PRO:HD3	1.78	0.65
3:I:305:LYS:HD3	3:I:307:ILE:HG21	1.77	0.65
1:M:209:ARG:NH1	3:O:234:GLU:CD	2.49	0.65
2:N:1061:ARG:NH1	2:N:1062:ASP:O	2.28	0.65
2:Q:57:TYR:O	2:Q:88:ARG:NH1	2.29	0.65
1:V:262:CYS:HA	4:V:503:SF4:S3	2.37	0.65
2:B:1132:ASN:O	2:B:1136:LYS:HG3	1.95	0.65
2:K:241:ARG:NH1	2:K:757:ASN:O	2.29	0.65
2:Q:91:GLN:HG3	2:Q:114:MET:SD	2.36	0.65
2:Q:220:ARG:HD3	2:Q:265:ARG:HD3	1.78	0.65
1:V:64:GLU:OE2	1:V:70:GLY:HA2	1.96	0.65
2:N:388:ARG:HG3	2:N:395:VAL:HG22	1.77	0.65
2:N:1135:MET:CE	2:N:1139:LEU:CD2	2.74	0.65
2:T:113:ARG:CG	2:T:315:PRO:HB2	2.26	0.65
2:W:57:TYR:O	2:W:88:ARG:NH1	2.25	0.65
1:D:407:TYR:HE2	2:E:576:TRP:HZ2	1.45	0.65
2:H:1024:ILE:HG22	2:H:1055:SER:OG	1.96	0.65
2:K:476:ILE:HD12	2:K:476:ILE:O	1.97	0.65
1:P:262:CYS:SG	1:P:266:ILE:HG12	2.36	0.65
2:Q:124:ARG:NH2	2:Q:925:GLN:OE1	2.30	0.65
2:T:718:GLN:NE2	10:T:5906:HOH:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:ASP:OD1	2:B:376:TYR:N	2.20	0.65
3:O:192:HIS:NE2	3:O:194:ASP:OD1	2.28	0.65
1:P:115:THR:O	1:P:119:VAL:HG23	1.97	0.65
1:P:157:GLU:OE1	1:P:166:ARG:NH1	2.20	0.65
1:S:79:THR:HA	1:S:82:LEU:HD12	1.78	0.65
1:V:15:TYR:CD2	1:V:16:PRO:HD2	2.32	0.65
1:V:259:MET:HE2	1:V:269:GLN:HG3	1.79	0.65
2:W:382:ASP:HA	2:W:385:LEU:HD13	1.78	0.65
2:E:94:ASP:OD2	2:E:98:TYR:CZ	2.50	0.65
2:H:923:HIS:O	2:H:1021:SER:HB2	1.97	0.65
1:J:207:ARG:NH2	2:K:44:TYR:OH	2.29	0.65
2:K:276:GLN:HB3	2:K:1095:ASN:ND2	2.11	0.65
2:K:861:ILE:HB	2:K:891:LYS:HA	1.78	0.65
2:E:963:ALA:O	2:E:967:LEU:HD12	1.96	0.65
3:F:158:ARG:N	3:F:239:GLU:O	2.30	0.65
2:Q:658:ASN:OD1	2:Q:1024:ILE:HG23	1.97	0.65
1:V:309:ARG:NH1	2:W:345:ASP:OD1	2.30	0.65
2:W:381:THR:HG22	2:W:383:PHE:N	2.05	0.65
2:W:976:TYR:CD1	2:W:1000:ARG:CZ	2.79	0.65
3:X:117:ASP:HB3	3:X:263:TRP:HD1	1.60	0.65
2:B:641:HIS:CE1	2:B:1069:GLN:HA	2.32	0.65
2:B:686:GLY:HA2	2:B:689:GLU:HB2	1.78	0.65
3:I:305:LYS:HZ3	8:I:401:HEM:FE	1.09	0.65
2:K:250:ASP:OD2	2:K:254:ARG:NH1	2.29	0.65
1:M:91:TYR:HA	2:N:1147:ASP:OD2	1.97	0.65
2:N:51:SER:O	2:N:54:ARG:N	2.30	0.65
1:D:35:CYS:HA	1:D:266:ILE:HD11	1.77	0.65
2:W:857:LEU:H	2:W:900:THR:CG2	2.10	0.65
2:B:446:ARG:NH1	2:B:823:THR:O	2.30	0.64
2:B:527:GLU:HA	2:B:530:ASN:HB2	1.78	0.64
2:E:1029:THR:HG21	2:E:1049:SER:HB2	1.78	0.64
2:N:970:GLU:OE2	2:N:1130:ASN:ND2	2.29	0.64
3:R:131:ARG:NH1	10:R:501:HOH:O	2.29	0.64
2:T:480:THR:HG23	2:T:483:GLU:H	1.61	0.64
2:T:937:ASN:OD1	2:T:940:GLY:N	2.30	0.64
2:W:35:VAL:H	3:X:245:THR:HG21	1.62	0.64
2:W:977:VAL:CG2	2:W:1001:LEU:CD2	2.68	0.64
3:X:287:THR:HG22	3:X:314:LEU:HD11	1.79	0.64
2:B:386:LEU:O	2:B:395:VAL:HG12	1.97	0.64
2:B:913:CYS:HB2	2:B:1103:VAL:HG21	1.80	0.64
2:H:61:ARG:HG2	2:H:81:VAL:HB	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:227:GLY:O	2:H:228:MET:C	2.33	0.64
2:N:1099:LYS:NZ	10:N:5901:HOH:O	2.20	0.64
2:Q:821:PHE:HE2	2:Q:828:LEU:CD2	2.10	0.64
3:R:168:LYS:HD2	3:R:171:TRP:CE2	2.32	0.64
1:V:201:VAL:O	1:V:234:LYS:NZ	2.30	0.64
2:W:123:ARG:HD2	3:X:194:ASP:HB2	1.78	0.64
2:B:852:GLU:OE2	2:B:984:ARG:NH2	2.30	0.64
1:D:292:PRO:HG3	1:D:304:TYR:HE2	1.62	0.64
3:I:112:GLN:HG3	3:I:266:VAL:HG12	1.79	0.64
2:N:1135:MET:HE3	2:N:1138:PHE:CD2	2.26	0.64
2:Q:625:ILE:HD12	2:Q:633:ARG:HG2	1.77	0.64
2:T:342:GLN:HG3	2:T:343:LYS:HD2	1.79	0.64
2:W:333:ILE:O	6:W:5802:MD1:N2	2.29	0.64
3:C:112:GLN:HG3	3:C:266:VAL:HG12	1.80	0.64
2:E:313:LYS:O	2:E:317:ALA:N	2.30	0.64
3:F:111:PHE:CE1	3:F:165:TRP:HZ3	2.16	0.64
3:F:137:MET:HE1	3:F:155:MET:HA	1.79	0.64
2:Q:357:ALA:HB2	2:Q:847:HIS:HD2	1.59	0.64
1:S:4:VAL:HG23	1:S:19:GLU:HB2	1.79	0.64
2:B:305:THR:CG2	2:B:525:TYR:HB3	2.28	0.64
2:B:661:LYS:HD3	2:B:1098:PRO:HG3	1.79	0.64
2:E:33:PRO:HG3	3:O:321:TRP:CZ3	2.33	0.64
2:E:926:TRP:CD1	2:E:932:ASN:OD1	2.50	0.64
1:G:166:ARG:HD3	2:H:1010:ALA:HA	1.78	0.64
2:H:164:ARG:NH2	2:H:674:ILE:O	2.30	0.64
2:Q:821:PHE:CE2	2:Q:828:LEU:CD2	2.80	0.64
1:V:2:THR:N	1:V:14:GLU:OE1	2.31	0.64
2:E:1014:ASN:ND2	2:E:1014:ASN:H	1.94	0.64
1:J:190:LYS:HD2	2:K:37:VAL:HB	1.78	0.64
2:T:915:THR:HA	2:T:1018:MET:O	1.98	0.64
2:W:969:ILE:HG12	2:W:1107:LYS:HB2	1.80	0.64
2:H:917:LYS:HG2	6:H:5802:MD1:H15	1.62	0.64
1:J:190:LYS:HB3	2:K:40:PRO:HG3	1.80	0.64
1:M:64:GLU:HG3	1:M:66:LYS:HD3	1.80	0.64
2:Q:115:CYS:HB3	4:Q:5804:SF4:S2	2.37	0.64
1:V:4:VAL:N	1:V:13:MET:O	2.27	0.64
2:W:192:TYR:CZ	2:W:647:LYS:HE2	2.33	0.64
2:W:877:GLU:OE2	2:W:892:LYS:NZ	2.30	0.64
3:X:95:VAL:O	3:X:306:ASN:ND2	2.31	0.64
3:X:137:MET:SD	3:X:290:ASN:HB3	2.37	0.64
1:M:188:PRO:HG2	3:O:302:ASN:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:811:PHE:HA	2:Q:814:GLN:HG2	1.79	0.64
1:S:36:ILE:HD11	2:T:317:ALA:HB3	1.79	0.64
1:D:263:VAL:HG11	2:E:114:MET:O	1.97	0.64
2:H:381:THR:HG22	2:H:383:PHE:H	1.63	0.64
2:H:446:ARG:NH2	2:H:823:THR:O	2.31	0.64
2:K:661:LYS:HA	2:K:1057:GLN:NE2	2.12	0.64
2:Q:1064:SER:OG	2:Q:1069:GLN:NE2	2.25	0.64
1:S:172:GLN:HB3	1:S:267:ARG:HH21	1.62	0.64
3:F:37:VAL:HA	3:F:154:ARG:NH2	2.13	0.64
2:K:388:ARG:HG3	2:K:395:VAL:HG22	1.78	0.64
3:L:51:VAL:HG21	3:L:316:LEU:HG	1.80	0.64
3:L:151:PHE:CE1	3:L:160:LYS:HB3	2.33	0.64
2:N:353:ASN:ND2	2:N:1100:GLU:OE2	2.31	0.64
2:Q:385:LEU:HD23	2:Q:431:PHE:HB2	1.79	0.64
2:Q:497:VAL:HA	2:Q:500:MET:HG3	1.79	0.64
1:V:296:GLN:NE2	1:V:318:GLN:O	2.30	0.64
2:W:386:LEU:HD12	2:W:432:VAL:HG23	1.79	0.64
2:B:312:ASN:O	6:B:5802:MD1:N8	2.31	0.63
3:C:247:GLN:O	3:C:250:GLN:NE2	2.31	0.63
2:E:915:THR:OG1	6:E:5801:MD1:N17	2.30	0.63
1:M:21:ARG:NH1	1:M:103:GLY:O	2.31	0.63
2:N:505:LYS:NZ	2:N:509:GLU:OE2	2.24	0.63
2:N:653:ASN:ND2	2:N:653:ASN:O	2.30	0.63
2:N:861:ILE:HB	2:N:891:LYS:HA	1.80	0.63
2:E:970:GLU:HG2	2:E:1118:VAL:HG21	1.79	0.63
2:E:1012:PRO:CG	2:E:1015:CYS:HB3	2.28	0.63
3:I:163:ASN:HD22	3:I:164:LEU:N	1.97	0.63
2:T:438:SER:O	2:T:440:GLY:N	2.32	0.63
1:V:211:TYR:HB2	5:V:504:F3S:S1	2.38	0.63
2:E:1003:LEU:HD23	2:E:1003:LEU:C	2.19	0.63
3:R:51:VAL:HG23	3:R:104:HIS:HD2	1.63	0.63
3:R:143:ILE:HD13	3:R:145:ILE:HG13	1.81	0.63
2:B:528:GLY:HA2	2:B:1099:LYS:HZ2	1.64	0.63
2:B:790:ASN:O	2:B:790:ASN:ND2	2.31	0.63
1:D:219:PRO:HB2	1:D:297:PHE:CE1	2.34	0.63
2:E:1033:HIS:NE2	2:E:1052:ARG:HG3	2.14	0.63
2:K:925:GLN:HE21	6:K:5801:MD1:H5'1	1.62	0.63
2:N:120:THR:HG22	2:N:931:TRP:HE3	1.63	0.63
2:Q:705:GLU:HG3	2:Q:706:PHE:N	2.13	0.63
2:B:913:CYS:HB2	2:B:1103:VAL:CG2	2.29	0.63
1:D:150:LYS:O	1:D:166:ARG:HA	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:959:ILE:HD13	2:E:1016:THR:HG23	1.80	0.63
2:K:31:LEU:H	2:K:31:LEU:HD22	1.64	0.63
2:Q:382:ASP:HA	2:Q:385:LEU:HD13	1.78	0.63
1:D:66:LYS:N	1:D:169:PHE:O	2.30	0.63
2:E:77:ILE:HD13	2:E:114:MET:HE3	1.81	0.63
2:E:1002:MET:O	2:E:1002:MET:HG3	1.97	0.63
1:G:95:LYS:CB	1:G:109:GLY:HA2	2.28	0.63
2:K:117:LYS:HD2	2:K:922:VAL:HG23	1.81	0.63
1:M:102:TYR:N	1:M:274:ASP:OD1	2.21	0.63
3:U:191:MET:HG2	3:U:192:HIS:N	2.13	0.63
2:W:265:ARG:HE	2:W:612:GLU:HB2	1.62	0.63
2:B:213:ARG:HD3	2:B:642:MET:HB3	1.80	0.63
1:D:6:ASN:ND2	1:D:298:GLY:O	2.31	0.63
1:D:149:ALA:HB2	1:D:168:PHE:CD2	2.33	0.63
1:G:15:TYR:HE1	2:H:41:LEU:HD11	1.64	0.63
2:N:179:THR:OG1	2:N:744:LYS:NZ	2.28	0.63
2:H:389:THR:HG23	2:H:867:TYR:HE1	1.64	0.63
1:J:195:ARG:HD3	1:J:200:ILE:HB	1.80	0.63
2:Q:909:TYR:CD1	2:Q:1104:LYS:HB2	2.34	0.63
1:S:252:ARG:NH1	1:S:386:ASP:OD1	2.32	0.63
2:T:640:THR:HB	2:T:1087:PHE:HB3	1.80	0.63
2:K:334:THR:HG22	2:K:336:GLU:H	1.63	0.63
3:L:301:ARG:HH21	3:L:301:ARG:HG2	1.63	0.63
2:N:453:LEU:HD11	2:N:827:ARG:HH12	1.62	0.63
2:Q:135:LEU:HB2	2:Q:694:ALA:HB3	1.81	0.63
2:W:684:ILE:O	2:W:684:ILE:HD12	1.99	0.63
2:E:415:TYR:HA	2:E:420:LEU:H	1.64	0.62
2:K:69:PRO:HG2	2:K:71:ASP:HB2	1.81	0.62
2:K:312:ASN:O	6:K:5802:MD1:N8	2.31	0.62
2:W:882:TRP:CD1	2:W:883:GLU:HG2	2.34	0.62
2:W:1001:LEU:HD11	2:W:1003:LEU:HD22	1.81	0.62
2:B:652:THR:O	2:B:654:VAL:HG22	1.99	0.62
1:D:8:HIS:HD2	1:D:292:PRO:HG2	1.63	0.62
3:F:81:LEU:CD2	3:F:293:VAL:HG23	2.30	0.62
2:T:115:CYS:CB	4:T:5804:SF4:S2	2.85	0.62
2:W:844:PHE:HB2	2:W:868:ILE:HD11	1.81	0.62
3:O:121:ASN:N	3:O:132:ASP:OD2	2.28	0.62
2:B:28:PHE:HA	3:U:107:ILE:HD12	1.80	0.62
2:B:491:ASP:OD2	2:B:864:THR:N	2.30	0.62
2:E:680:THR:HG22	6:E:5801:MD1:HN21	1.64	0.62
3:F:81:LEU:HD21	3:F:293:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:TYR:CD1	2:H:507:LEU:HD11	2.34	0.62
3:I:294:TRP:CE2	3:I:305:LYS:HB2	2.33	0.62
2:N:1016:THR:HG21	2:N:1105:ILE:HD11	1.80	0.62
1:V:212:ARG:HH11	1:V:212:ARG:CG	2.11	0.62
1:A:159:SER:HB2	2:B:347:TRP:HB3	1.81	0.62
2:E:333:ILE:O	6:E:5802:MD1:N2	2.32	0.62
2:E:930:ASP:O	2:E:934:ILE:HG13	1.99	0.62
2:H:1001:LEU:HA	2:H:1054:GLY:HA3	1.81	0.62
1:M:240:PRO:HG3	2:N:54:ARG:HG2	1.81	0.62
3:I:306:ASN:N	3:I:306:ASN:HD22	1.96	0.62
1:M:243:GLU:CD	2:N:54:ARG:NH1	2.52	0.62
2:T:763:GLU:OE1	2:T:765:ARG:NH1	2.33	0.62
3:X:81:LEU:N	3:X:96:ASN:O	2.25	0.62
2:E:1036:ARG:NH1	2:E:1038:ASP:OD1	2.33	0.62
3:F:219:TYR:HE2	3:F:227:LEU:HD23	1.65	0.62
2:N:653:ASN:C	2:N:653:ASN:HD22	2.01	0.62
2:Q:68:SER:O	2:Q:231:LEU:HD12	1.98	0.62
2:Q:425:ARG:HH11	2:Q:425:ARG:CG	2.12	0.62
2:T:151:LEU:HD12	2:T:675:GLU:HG2	1.80	0.62
2:W:527:GLU:HA	2:W:530:ASN:HB2	1.82	0.62
3:F:171:TRP:NE1	3:F:229:ARG:CZ	2.63	0.62
3:F:241:PHE:HB2	8:F:401:HEM:HBB	1.82	0.62
3:I:321:TRP:CE2	3:X:161:PRO:HG3	2.34	0.62
3:O:294:TRP:CE2	3:O:305:LYS:HB3	2.35	0.62
8:R:401:HEM:HBB2	8:R:401:HEM:HMB1	1.82	0.62
3:U:118:ALA:HA	3:U:261:LYS:HG2	1.79	0.62
1:V:64:GLU:HB3	1:V:70:GLY:HA2	1.82	0.62
2:W:939:PHE:CE2	2:W:1004:ARG:CG	2.75	0.62
2:B:271:THR:HG23	2:B:1090:ASP:HA	1.81	0.62
8:C:401:HEM:HBB2	8:C:401:HEM:HMB1	1.81	0.62
3:I:305:LYS:CG	3:I:307:ILE:HG23	2.28	0.62
1:M:125:ILE:HD13	1:M:127:GLN:HB2	1.82	0.62
2:N:275:ASP:HB3	2:N:563:ALA:HB1	1.80	0.62
1:A:365:GLU:OE2	1:A:372:LYS:NZ	2.32	0.62
2:B:435:ASP:OD1	2:B:437:LYS:N	2.29	0.62
2:B:446:ARG:HH11	2:B:446:ARG:CG	2.12	0.62
1:D:137:LYS:HA	1:D:140:ARG:HD2	1.80	0.62
2:E:1033:HIS:CE1	2:E:1052:ARG:HD3	2.35	0.62
3:I:305:LYS:HG2	3:I:307:ILE:HG23	1.81	0.62
8:O:401:HEM:HMB1	8:O:401:HEM:HBB2	1.81	0.62
1:V:211:TYR:HD2	5:V:504:F3S:S1	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ARG:NH1	10:B:5906:HOH:O	2.32	0.61
1:G:160:THR:HG23	2:H:346:TYR:HB3	1.81	0.61
2:K:421:LYS:HB2	2:K:424:GLN:HG3	1.81	0.61
2:N:100:ASP:OD1	2:N:102:TYR:N	2.31	0.61
2:N:312:ASN:O	6:N:5802:MD1:N8	2.33	0.61
2:T:823:THR:CB	2:T:829:GLN:HE21	2.02	0.61
1:V:36:ILE:O	2:W:919:ARG:NH2	2.33	0.61
2:W:123:ARG:NH2	3:X:193:ASP:OD1	2.33	0.61
2:B:678:MET:HG2	2:B:693:PHE:HB2	1.83	0.61
3:I:231:ARG:NH1	3:I:250:GLN:O	2.33	0.61
3:L:107:ILE:HD11	2:Q:31:LEU:HD11	1.82	0.61
1:M:205:GLN:NE2	1:M:232:SER:O	2.33	0.61
2:Q:865:ASN:O	2:Q:891:LYS:NZ	2.29	0.61
2:T:752:LYS:O	2:T:753:ARG:HG2	2.00	0.61
2:W:759:LYS:O	2:W:763:GLU:HG3	2.01	0.61
3:X:109:ILE:O	3:X:110:TYR:CD1	2.52	0.61
2:B:681:ASP:OD1	2:B:682:ILE:N	2.31	0.61
8:L:401:HEM:HBB2	8:L:401:HEM:HMB1	1.81	0.61
2:Q:760:PHE:HB2	2:Q:769:TYR:CE2	2.36	0.61
1:A:402:ARG:O	2:B:804:ARG:NH2	2.34	0.61
3:C:105:ASP:OD2	2:T:29:ARG:NH2	2.32	0.61
2:E:235:GLY:N	2:E:707:GLU:OE2	2.34	0.61
1:G:15:TYR:CD2	1:G:16:PRO:HD2	2.36	0.61
1:J:133:ILE:HG13	1:J:216:GLU:HG3	1.81	0.61
1:J:365:GLU:HG2	1:J:372:LYS:HZ1	1.66	0.61
2:K:123:ARG:HD2	3:L:194:ASP:HB2	1.81	0.61
2:N:1124:THR:HG21	2:N:1126:TYR:CD2	2.35	0.61
2:Q:267:TRP:CD2	2:Q:614:VAL:HG22	2.35	0.61
2:W:311:GLU:OE2	2:W:1019:LYS:NZ	2.33	0.61
2:B:628:THR:CG2	2:B:873:TYR:HB3	2.30	0.61
1:D:292:PRO:HG3	1:D:304:TYR:CE2	2.34	0.61
3:F:155:MET:SD	8:F:401:HEM:FE	1.88	0.61
3:I:98:ALA:HB3	3:I:291:MET:HE2	1.81	0.61
1:P:302:ASN:HA	1:P:304:TYR:CE2	2.35	0.61
1:V:64:GLU:OE2	1:V:70:GLY:CA	2.49	0.61
1:V:212:ARG:HG3	1:V:212:ARG:NH1	2.14	0.61
3:C:235:ASP:HB2	3:C:252:VAL:HG12	1.82	0.61
2:E:275:ASP:HB3	2:E:563:ALA:HB1	1.81	0.61
2:E:1062:ASP:CG	2:E:1096:THR:CG2	2.69	0.61
2:H:974:TYR:CZ	2:H:1004:ARG:HD3	2.36	0.61
1:M:88:ASN:ND2	1:M:111:TYR:OH	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:16:PRO:CG	1:V:128:TRP:HE1	1.62	0.61
1:V:212:ARG:HH11	1:V:212:ARG:HG3	1.66	0.61
1:V:227:GLY:HA3	3:X:125:ILE:HG22	1.82	0.61
2:W:922:VAL:O	2:W:922:VAL:HG12	2.01	0.61
2:E:349:PRO:O	2:E:503:SER:HB3	2.01	0.61
1:G:293:LEU:HB2	1:G:305:TYR:CE1	2.35	0.61
2:H:625:ILE:HG12	2:H:635:VAL:HG22	1.83	0.61
2:K:681:ASP:OD1	2:K:682:ILE:N	2.30	0.61
2:K:915:THR:HA	2:K:1018:MET:O	1.99	0.61
2:K:1076:LYS:NZ	2:K:1080:GLY:O	2.33	0.61
1:M:256:THR:CG2	1:M:259:MET:HB2	2.31	0.61
1:M:256:THR:HG23	1:M:259:MET:H	1.66	0.61
2:N:91:GLN:HE21	2:N:114:MET:HB2	1.65	0.61
2:N:954:GLU:OE1	2:N:1004:ARG:HG3	2.01	0.61
3:O:303:GLY:C	3:O:305:LYS:HD3	2.21	0.61
2:Q:641:HIS:CE1	2:Q:1087:PHE:HB2	2.36	0.61
2:Q:678:MET:HG2	2:Q:693:PHE:HB2	1.82	0.61
2:Q:928:VAL:HA	2:Q:933:PHE:CD1	2.35	0.61
1:V:150:LYS:HG2	1:V:167:TRP:NE1	2.16	0.61
2:W:795:GLU:HB3	2:W:798:VAL:CG1	2.31	0.61
2:E:272:TRP:CH2	2:E:618:ASN:HB2	2.36	0.61
2:E:618:ASN:HD21	2:E:661:LYS:CB	2.13	0.61
1:M:34:ARG:HB2	1:M:266:ILE:HG22	1.81	0.61
2:N:446:ARG:NH2	2:N:821:PHE:O	2.34	0.61
3:O:303:GLY:CA	3:O:305:LYS:CD	2.79	0.61
1:V:37:ALA:HA	1:V:63:VAL:HG11	1.82	0.61
2:W:113:ARG:HG3	2:W:113:ARG:HH11	1.66	0.61
2:W:853:ALA:N	2:W:1100:GLU:OE2	2.22	0.61
2:E:959:ILE:CD1	2:E:1016:THR:HG23	2.30	0.61
3:F:111:PHE:HE1	3:F:165:TRP:HZ3	1.49	0.61
2:H:658:ASN:OD1	2:H:1024:ILE:CG1	2.45	0.61
2:K:116:LEU:HD21	2:K:919:ARG:O	2.01	0.61
2:K:918:SER:HA	2:K:1019:LYS:HE2	1.83	0.61
2:N:916:PRO:HA	6:N:5802:MD1:O1A	2.01	0.61
2:Q:307:LYS:NZ	2:Q:313:LYS:NZ	2.48	0.61
2:T:823:THR:HG21	2:T:829:GLN:HG3	1.82	0.61
8:U:401:HEM:HBB2	8:U:401:HEM:HMB1	1.81	0.61
2:E:262:LEU:CG	2:E:608:ARG:CB	2.79	0.61
3:I:143:ILE:HG22	3:I:145:ILE:HG22	1.83	0.61
2:K:865:ASN:O	2:K:891:LYS:NZ	2.33	0.61
1:M:189:ARG:HE	1:M:209:ARG:HG3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:GLN:HG2	2:B:112:PRO:HB2	1.83	0.60
2:B:353:ASN:ND2	2:B:1100:GLU:OE1	2.34	0.60
3:C:236:LEU:HA	3:C:247:GLN:HG3	1.83	0.60
2:E:51:SER:O	2:E:54:ARG:N	2.34	0.60
3:F:115:TRP:NE1	3:F:293:VAL:HG11	2.15	0.60
2:Q:848:ARG:NH1	2:Q:889:ASN:OD1	2.33	0.60
2:Q:1057:GLN:HE22	6:Q:5801:MD1:H162	1.47	0.60
1:V:333:VAL:HG13	1:V:373:PHE:HB2	1.83	0.60
2:W:274:GLY:HA2	2:W:1095:ASN:OD1	2.01	0.60
2:B:113:ARG:NH2	2:B:316:GLU:OE2	2.33	0.60
2:B:469:LYS:HA	2:B:475:GLU:HA	1.82	0.60
2:B:950:PRO:CD	2:B:954:GLU:HB3	2.31	0.60
1:J:149:ALA:HB2	1:J:168:PHE:HD2	1.65	0.60
2:Q:625:ILE:HD13	2:Q:633:ARG:HE	1.65	0.60
2:Q:852:GLU:HG3	2:Q:1063:TRP:HZ2	1.65	0.60
1:V:25:GLN:HG2	1:V:302:ASN:ND2	2.14	0.60
2:E:700:TRP:NE1	6:E:5801:MD1:N7	2.47	0.60
3:F:171:TRP:CH2	3:F:229:ARG:HD3	2.35	0.60
1:G:149:ALA:HB2	1:G:168:PHE:HD2	1.66	0.60
2:K:848:ARG:NH2	2:K:859:ASN:OD1	2.35	0.60
2:W:293:MET:CE	2:W:313:LYS:HD2	2.30	0.60
2:B:355:ASP:H	2:B:538:MET:HE3	1.67	0.60
1:D:8:HIS:CD2	1:D:292:PRO:HG2	2.36	0.60
2:N:917:LYS:O	2:N:1019:LYS:NZ	2.31	0.60
2:Q:531:HIS:C	2:Q:1097:VAL:HG23	2.21	0.60
2:E:1020:HIS:CD2	6:E:5801:MD1:C20	2.84	0.60
1:P:4:VAL:O	1:P:13:MET:N	2.29	0.60
2:T:373:ASP:O	2:T:377:VAL:HG23	2.01	0.60
1:V:34:ARG:NH2	2:W:322:GLU:OE2	2.35	0.60
1:V:187:CYS:SG	1:V:191:ALA:HB3	2.42	0.60
1:V:408:ASN:ND2	2:W:805:THR:OG1	2.32	0.60
2:W:113:ARG:HH11	2:W:113:ARG:CG	2.14	0.60
2:H:947:LYS:NZ	10:H:5907:HOH:O	2.34	0.60
1:P:34:ARG:HB2	1:P:266:ILE:HG22	1.84	0.60
1:P:161:LEU:HD21	1:P:309:ARG:HD3	1.84	0.60
2:E:920:HIS:CD2	2:E:935:TRP:O	2.55	0.60
3:F:117:ASP:N	3:F:261:LYS:O	2.35	0.60
1:J:349:GLN:NE2	2:K:90:GLU:OE1	2.35	0.60
1:S:397:GLU:HG3	1:S:398:PRO:HD2	1.83	0.60
2:T:152:THR:HG22	2:T:154:GLU:HG2	1.81	0.60
1:V:64:GLU:OE1	1:V:173:ARG:HD3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:458:ILE:H	2:W:458:ILE:HD12	1.67	0.60
3:I:154:ARG:HA	8:I:401:HEM:CBB	2.31	0.60
2:K:918:SER:CB	2:K:1019:LYS:HD3	2.31	0.60
1:M:188:PRO:CB	3:O:302:ASN:OD1	2.49	0.60
3:O:165:TRP:CZ2	3:O:269:ARG:HD3	2.37	0.60
3:O:282:VAL:HG23	3:O:285:GLU:CB	2.31	0.60
2:W:438:SER:O	2:W:440:GLY:N	2.35	0.60
2:B:302:LEU:HD23	2:B:320:VAL:HG23	1.84	0.60
2:Q:72:THR:CG2	2:Q:713:SER:OG	2.49	0.60
1:A:64:GLU:HG3	1:A:66:LYS:HE3	1.82	0.60
1:G:160:THR:HG21	2:H:510:ARG:HH22	1.67	0.60
2:H:294:ASN:OD1	2:H:807:PRO:HB3	2.01	0.60
2:K:115:CYS:SG	2:K:117:LYS:HE3	2.42	0.60
2:K:1004:ARG:NH2	2:K:1111:GLY:O	2.34	0.60
1:M:166:ARG:HD3	2:N:1010:ALA:HA	1.83	0.60
1:S:83:ILE:HG22	1:S:119:VAL:HG21	1.82	0.60
2:W:315:PRO:HG3	4:W:5804:SF4:S2	2.42	0.60
3:X:48:VAL:HG12	3:X:313:PRO:HB2	1.84	0.60
3:F:111:PHE:HE1	3:F:165:TRP:CZ3	2.20	0.59
2:K:98:TYR:CE1	2:K:798:VAL:HG21	2.37	0.59
3:L:303:GLY:HA2	3:L:305:LYS:CE	2.32	0.59
2:N:80:PHE:HE1	2:N:90:GLU:HB2	1.67	0.59
2:Q:852:GLU:HG3	2:Q:1063:TRP:CZ2	2.37	0.59
2:W:919:ARG:HG3	2:W:920:HIS:ND1	2.16	0.59
1:A:90:TRP:HB2	2:B:1146:VAL:HG12	1.85	0.59
2:E:582:TYR:O	2:E:586:ALA:N	2.29	0.59
2:E:971:ASP:HB2	2:E:1007:TYR:CD2	2.38	0.59
3:F:219:TYR:CE2	3:F:227:LEU:HD23	2.36	0.59
3:L:305:LYS:HE3	8:L:401:HEM:C4A	2.30	0.59
2:B:1088:GLU:HB3	2:B:1091:ASN:HB3	1.84	0.59
2:E:77:ILE:CD1	2:E:114:MET:CE	2.79	0.59
2:K:546:VAL:HG13	2:K:551:ASN:HB2	1.83	0.59
2:N:915:THR:HA	2:N:1018:MET:O	2.02	0.59
2:Q:82:ARG:NH1	10:Q:5904:HOH:O	2.27	0.59
2:Q:383:PHE:N	2:Q:384:PRO:HD2	2.17	0.59
3:R:112:GLN:HG3	3:R:266:VAL:HG12	1.84	0.59
3:R:305:LYS:HE2	8:R:401:HEM:ND	2.16	0.59
1:A:404:ASP:HA	2:B:804:ARG:NH2	2.17	0.59
2:B:117:LYS:NZ	2:B:919:ARG:O	2.35	0.59
1:D:6:ASN:HB2	1:D:13:MET:HG2	1.83	0.59
1:D:262:CYS:SG	1:D:266:ILE:HD12	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:VAL:HG11	3:F:291:MET:SD	2.42	0.59
1:G:121:LYS:NZ	3:I:32:GLU:OE2	2.32	0.59
2:H:312:ASN:O	6:H:5802:MD1:N8	2.35	0.59
2:H:759:LYS:O	2:H:763:GLU:HG3	2.03	0.59
3:I:282:VAL:O	3:I:316:LEU:HD12	2.02	0.59
1:M:190:LYS:CB	2:N:37:VAL:HG11	2.32	0.59
2:N:434:TRP:O	2:N:461:VAL:HG22	2.03	0.59
1:P:296:GLN:NE2	1:P:318:GLN:O	2.34	0.59
2:Q:404:TYR:HE2	2:Q:406:LEU:HD23	1.67	0.59
1:V:353:TYR:CE2	1:V:385:GLU:HG3	2.37	0.59
2:W:406:LEU:CD2	2:W:429:GLY:HA2	2.33	0.59
2:Q:306:GLY:HA3	2:Q:529:VAL:HG22	1.84	0.59
2:Q:445:THR:CG2	2:Q:448:ASP:OD2	2.46	0.59
2:T:822:TYR:CE1	2:T:1076:LYS:HD2	2.38	0.59
2:W:388:ARG:HG3	2:W:395:VAL:HB	1.82	0.59
2:W:410:SER:HA	2:W:415:TYR:CD2	2.37	0.59
2:W:834:GLU:OE1	2:W:837:ILE:HD12	2.03	0.59
3:X:140:LEU:HD22	3:X:161:PRO:HB2	1.84	0.59
3:C:302:ASN:O	3:C:305:LYS:CG	2.50	0.59
2:E:110:TRP:N	2:E:110:TRP:CD1	2.71	0.59
1:G:192:ILE:HG12	1:G:203:ILE:HG12	1.84	0.59
8:L:401:HEM:HHD	8:L:401:HEM:HBC2	1.83	0.59
2:N:1124:THR:HG22	2:N:1126:TYR:CG	2.38	0.59
2:Q:70:ASN:H	2:Q:231:LEU:CD1	2.14	0.59
2:B:217:ALA:HB2	2:B:262:LEU:HD13	1.85	0.59
1:M:184:LEU:HD21	2:N:40:PRO:HB2	1.85	0.59
1:P:266:ILE:HG13	1:P:267:ARG:HG3	1.84	0.59
1:P:276:PRO:CB	1:P:286:HIS:NE2	2.62	0.59
2:T:922:VAL:O	2:T:922:VAL:HG12	2.02	0.59
2:W:332:VAL:HG23	2:W:344:ALA:HB2	1.84	0.59
1:D:212:ARG:NH2	3:F:129:GLU:O	2.36	0.59
2:E:913:CYS:HA	2:E:1016:THR:O	2.03	0.59
1:G:178:CYS:HB3	1:G:299:THR:O	2.02	0.59
2:K:353:ASN:ND2	2:K:1100:GLU:OE2	2.36	0.59
2:N:1022:ALA:HB1	2:N:1050:SER:HB2	1.83	0.59
2:T:375:ASP:OD2	2:T:379:LYS:NZ	2.34	0.59
1:V:149:ALA:O	2:W:1009:PRO:HG2	2.02	0.59
2:W:382:ASP:OD2	2:W:394:ARG:NH2	2.36	0.59
3:C:302:ASN:O	3:C:305:LYS:HG2	2.03	0.59
2:E:746:GLY:O	2:E:750:ARG:N	2.35	0.59
8:F:401:HEM:HBA1	8:F:401:HEM:HMA1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:GLU:OE1	2:H:47:ARG:NH2	2.33	0.59
2:H:803:PHE:CG	2:H:808:ARG:HG3	2.37	0.59
2:N:1124:THR:HB	2:N:1126:TYR:H	1.68	0.59
3:O:231:ARG:HD3	3:O:233:VAL:O	2.02	0.59
3:O:241:PHE:HD2	3:O:241:PHE:N	2.01	0.59
1:S:192:ILE:HG12	1:S:203:ILE:HG12	1.85	0.59
2:W:96:GLN:O	2:W:105:LYS:NZ	2.36	0.59
2:W:621:GLU:O	2:W:622:ARG:HD3	2.03	0.59
2:W:996:TYR:CE2	2:W:1000:ARG:HD2	2.38	0.59
2:B:922:VAL:HG12	2:B:922:VAL:O	2.02	0.59
3:C:294:TRP:CE2	3:C:305:LYS:HB3	2.37	0.59
1:G:16:PRO:HG3	1:G:128:TRP:CE3	2.38	0.59
2:H:678:MET:HG2	2:H:693:PHE:HB2	1.84	0.59
3:L:318[B]:ARG:HE	3:R:143:ILE:HG22	1.68	0.59
1:M:188:PRO:CG	3:O:302:ASN:OD1	2.51	0.59
2:Q:394:ARG:HH12	2:Q:829:GLN:HE21	1.50	0.59
2:B:882:TRP:CD1	2:B:883:GLU:HG2	2.38	0.58
2:E:916:PRO:O	2:E:1020:HIS:N	2.33	0.58
2:N:135:LEU:HB2	2:N:694:ALA:HB3	1.83	0.58
2:Q:865:ASN:HB3	2:Q:868:ILE:HD12	1.85	0.58
2:T:640:THR:OG1	2:T:1071:ASP:OD1	2.20	0.58
2:W:130:ARG:NH1	2:W:702:GLU:OE2	2.36	0.58
2:W:684:ILE:HA	2:W:688:ILE:HD12	1.85	0.58
2:W:858:PRO:O	2:W:888:ARG:NH2	2.27	0.58
2:B:114:MET:HE2	2:B:119:TYR:CD1	2.38	0.58
3:C:87:ALA:O	3:C:90:ASN:ND2	2.36	0.58
2:E:916:PRO:HA	6:E:5802:MD1:O1A	2.02	0.58
3:F:171:TRP:CH2	3:F:229:ARG:CD	2.86	0.58
2:K:152:THR:HG22	2:K:155:ASN:HB2	1.85	0.58
2:K:1087:PHE:HD1	2:K:1093:CYS:HB3	1.68	0.58
2:N:856:TYR:O	2:N:902:ASN:HB2	2.03	0.58
2:T:1027:ASP:O	2:T:1031:GLN:HG3	2.03	0.58
1:V:209:ARG:NH1	3:X:234:GLU:OE1	2.36	0.58
2:B:113:ARG:HG3	2:B:315:PRO:HB2	1.86	0.58
2:B:375:ASP:OD1	2:B:379:LYS:HE3	2.02	0.58
1:D:52:ASN:ND2	3:F:215:LEU:HA	2.18	0.58
2:E:1129:GLY:N	2:E:1131:GLU:OE2	2.31	0.58
3:F:300:ASP:HA	3:F:304:GLN:CB	2.34	0.58
1:G:51:PHE:HZ	3:I:214:GLU:HG3	1.68	0.58
2:H:250:ASP:OD2	2:H:254:ARG:NH1	2.35	0.58
1:M:90:TRP:HB2	2:N:1146:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:433:VAL:N	2:W:442:LYS:O	2.36	0.58
3:X:35:LYS:HG3	3:X:86:LYS:HA	1.85	0.58
1:D:294:TYR:HB3	1:D:297:PHE:CE2	2.39	0.58
8:F:401:HEM:HBC2	8:F:401:HEM:HHD	1.85	0.58
2:H:138:LYS:HB2	2:H:170:LEU:HD21	1.84	0.58
2:E:527:GLU:HA	2:E:530:ASN:HB2	1.86	0.58
2:H:100:ASP:OD2	2:H:103:GLY:N	2.36	0.58
2:H:922:VAL:CG2	2:H:926:TRP:CZ3	2.86	0.58
2:K:937:ASN:ND2	2:K:954:GLU:O	2.35	0.58
3:L:302:ASN:CG	3:L:303:GLY:N	2.55	0.58
2:Q:101:LEU:HD12	2:Q:802:LEU:HD11	1.86	0.58
2:Q:335:PRO:HG3	2:Q:352:ASN:OD1	2.03	0.58
2:Q:485:TYR:O	2:Q:489:LEU:HG	2.03	0.58
2:T:77:ILE:HG23	2:T:114:MET:SD	2.44	0.58
2:T:814:GLN:OE1	2:T:814:GLN:N	2.36	0.58
1:V:15:TYR:OH	1:V:181:PRO:O	2.17	0.58
2:W:498:VAL:HG12	2:W:503:SER:O	2.03	0.58
3:C:132:ASP:OD2	3:C:295:ASN:HA	2.04	0.58
6:E:5801:MD1:N8	10:E:5902:HOH:O	2.32	0.58
2:H:123:ARG:NH2	2:H:930:ASP:OD2	2.37	0.58
2:H:236:LYS:HG2	2:H:653:ASN:CB	2.34	0.58
2:K:434:TRP:HB3	2:K:461:VAL:HG22	1.86	0.58
1:M:193:TYR:CE2	2:N:47:ARG:HD3	2.38	0.58
2:N:61:ARG:HH11	2:N:61:ARG:HG3	1.67	0.58
2:Q:373:ASP:O	2:Q:377:VAL:HG23	2.03	0.58
3:L:303:GLY:HA2	3:L:305:LYS:CD	2.34	0.58
1:M:163:GLU:HG2	1:M:312:PRO:HA	1.86	0.58
2:Q:95:HIS:ND1	2:Q:111:ASN:OD1	2.34	0.58
2:Q:100:ASP:HB2	2:Q:802:LEU:HD21	1.85	0.58
2:T:353:ASN:ND2	2:T:1100:GLU:OE2	2.37	0.58
1:V:34:ARG:HB2	1:V:266:ILE:HG22	1.86	0.58
2:W:758:TRP:O	2:W:762:ILE:HG13	2.03	0.58
2:E:651:PHE:N	2:E:651:PHE:CD1	2.71	0.58
2:E:700:TRP:N	2:E:700:TRP:CD1	2.72	0.58
1:G:15:TYR:CE1	2:H:41:LEU:HD11	2.38	0.58
1:M:309:ARG:HG2	1:M:310:TRP:HE3	1.67	0.58
2:Q:47:ARG:HG2	2:Q:47:ARG:O	2.03	0.58
2:Q:388:ARG:HG2	2:Q:476:ILE:HD12	1.84	0.58
2:T:611:ASP:HB3	2:T:1089:ALA:HB2	1.85	0.58
2:W:293:MET:HE1	2:W:313:LYS:HD2	1.85	0.58
3:X:89:PRO:HG3	3:X:302:ASN:HD21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1078:LYS:HG3	2:B:1079:ILE:HG12	1.85	0.58
1:D:65:THR:HG21	1:D:147:ASP:N	2.17	0.58
2:E:498:VAL:HA	2:E:501:THR:HG22	1.86	0.58
3:F:130:PHE:CE1	3:F:301:ARG:HD3	2.38	0.58
8:F:401:HEM:HBB2	8:F:401:HEM:HMB1	1.84	0.58
1:J:132:TYR:O	1:J:221:LYS:NZ	2.37	0.58
2:Q:1078:LYS:HB3	2:Q:1091:ASN:ND2	2.18	0.58
3:X:81:LEU:HD21	3:X:308:SER:CB	2.33	0.58
2:E:760:PHE:HB3	2:E:765:ARG:O	2.03	0.58
2:H:69:PRO:HD2	2:H:71:ASP:OD1	2.03	0.58
2:Q:67:CYS:HB2	2:Q:77:ILE:HD11	1.84	0.58
2:Q:73:HIS:CD2	2:Q:73:HIS:N	2.68	0.58
2:T:376:TYR:CE2	2:T:550:GLY:HA2	2.39	0.58
3:U:305:LYS:HD2	3:U:307:ILE:HG22	1.85	0.58
2:W:861:ILE:HB	2:W:891:LYS:HA	1.85	0.58
2:B:566:TYR:OH	2:B:567:LYS:NZ	2.36	0.57
2:E:69:PRO:HB3	2:E:700:TRP:HH2	1.68	0.57
3:I:32:GLU:HG3	3:I:32:GLU:O	2.01	0.57
2:K:209:GLU:OE1	2:K:209:GLU:N	2.34	0.57
2:N:1135:MET:HE2	2:N:1139:LEU:CD2	2.21	0.57
1:P:279:PRO:O	1:P:283:LEU:HB2	2.04	0.57
3:U:145:ILE:HG12	3:U:288:TYR:CE2	2.39	0.57
1:V:336:ARG:NH1	1:V:376:TYR:CD1	2.72	0.57
2:W:501:THR:O	2:W:501:THR:OG1	2.12	0.57
2:W:1078:LYS:HG3	2:W:1079:ILE:N	2.19	0.57
2:B:629:PRO:HG2	2:B:874:GLY:O	2.04	0.57
3:F:110:TYR:HA	3:F:267:PHE:O	2.04	0.57
2:K:390:ASP:OD1	2:K:391:THR:N	2.32	0.57
1:M:189:ARG:HG2	1:M:189:ARG:HH11	1.67	0.57
1:M:373:PHE:CE2	1:M:375:MET:HB2	2.39	0.57
2:N:917:LYS:HD2	6:N:5802:MD1:H15	1.69	0.57
3:R:137:MET:SD	3:R:155:MET:HA	2.44	0.57
2:W:72:THR:HG21	2:W:313:LYS:HE3	1.86	0.57
2:W:388:ARG:NH2	2:W:390:ASP:OD2	2.34	0.57
2:W:504:PRO:HG3	2:W:507:LEU:HD12	1.86	0.57
3:C:269:ARG:NH2	10:C:501:HOH:O	2.36	0.57
1:D:173:ARG:NH2	1:D:220:TYR:O	2.37	0.57
1:D:211:TYR:N	5:D:504:F3S:S4	2.77	0.57
2:E:192:TYR:CA	2:E:197:GLY:HA3	2.34	0.57
2:E:915:THR:HA	2:E:1018:MET:O	2.04	0.57
2:E:1062:ASP:CG	2:E:1096:THR:HG21	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:332:VAL:HG23	2:H:344:ALA:HB2	1.87	0.57
2:H:983:ASP:OD2	2:H:1061:ARG:HD2	2.04	0.57
3:I:42:LEU:HD21	3:I:150:PRO:HA	1.86	0.57
2:K:678:MET:HG2	2:K:693:PHE:HB2	1.86	0.57
3:O:235:ASP:CB	3:O:250:GLN:OE1	2.52	0.57
1:P:267:ARG:HD2	4:P:503:SF4:S1	2.44	0.57
2:Q:1022:ALA:HB1	2:Q:1050:SER:CB	2.34	0.57
2:W:377:VAL:CG2	2:W:548:LEU:HA	2.34	0.57
2:B:463:GLU:OE2	2:B:486:LYS:NZ	2.37	0.57
2:E:110:TRP:HD1	2:E:110:TRP:H	1.52	0.57
2:N:117:LYS:HB3	2:N:926:TRP:CD2	2.39	0.57
2:N:311:GLU:OE2	2:N:1019:LYS:NZ	2.35	0.57
2:N:678:MET:HG2	2:N:693:PHE:HB2	1.85	0.57
1:P:262:CYS:O	2:Q:112:PRO:HG3	2.04	0.57
2:Q:425:ARG:HG3	2:Q:425:ARG:NH1	2.19	0.57
2:W:52:VAL:HG11	3:X:221:ALA:HB2	1.86	0.57
2:W:897:THR:O	2:W:900:THR:HG22	2.04	0.57
2:B:376:TYR:CD2	2:B:550:GLY:HA2	2.39	0.57
1:J:30:PHE:CE1	1:J:267:ARG:HG2	2.39	0.57
1:J:55:GLN:HG3	1:J:226:ARG:HD2	1.87	0.57
3:O:241:PHE:N	3:O:241:PHE:CD2	2.71	0.57
2:Q:1119:TRP:CD2	2:Q:1121:PRO:HD2	2.40	0.57
2:Q:1131:GLU:OE1	2:Q:1131:GLU:N	2.33	0.57
3:R:151:PHE:CE1	3:R:160:LYS:HB3	2.39	0.57
2:W:930:ASP:OD1	2:W:931:TRP:N	2.38	0.57
1:D:249:THR:HG21	1:D:254:MET:HB3	1.87	0.57
1:D:331:PHE:CE1	2:E:325:GLU:HG2	2.40	0.57
3:F:252:VAL:HG12	3:F:269:ARG:HB2	1.85	0.57
2:K:190:LYS:HA	2:K:193:SER:HB2	1.85	0.57
2:N:984:ARG:NH1	10:N:5912:HOH:O	2.38	0.57
2:Q:225:ARG:HB2	2:Q:267:TRP:HB2	1.86	0.57
2:Q:534:HIS:O	2:Q:538:MET:HG3	2.05	0.57
2:Q:681:ASP:OD2	2:Q:682:ILE:N	2.37	0.57
2:Q:882:TRP:CD1	2:Q:883:GLU:HG2	2.40	0.57
2:T:528:GLY:HA2	2:T:1099:LYS:NZ	2.18	0.57
3:U:58:VAL:HG22	3:U:59:PRO:HD2	1.86	0.57
2:B:400:ILE:HG21	2:B:468:LEU:HD23	1.87	0.57
2:E:337:TYR:HB3	2:E:1010:ALA:HB1	1.86	0.57
3:I:247:GLN:O	3:I:250:GLN:NE2	2.38	0.57
3:O:303:GLY:HA2	3:O:305:LYS:CE	2.35	0.57
1:A:178:CYS:HB3	1:A:299:THR:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ALA:HA	1:D:168:PHE:HB3	1.86	0.57
2:H:139:GLY:O	2:H:159:TYR:HB3	2.05	0.57
3:L:51:VAL:CG2	3:L:316:LEU:HG	2.34	0.57
1:M:219:PRO:HB2	1:M:297:PHE:CD1	2.40	0.57
2:Q:503:SER:HB2	2:Q:508:ILE:HD11	1.86	0.57
1:V:149:ALA:HA	1:V:168:PHE:HB3	1.86	0.57
1:V:189:ARG:HD2	8:X:401:HEM:CGA	2.34	0.57
2:W:456:LYS:HB2	2:W:458:ILE:HD12	1.86	0.57
2:W:666:MET:HE3	2:W:670:VAL:HG21	1.86	0.57
2:E:1063:TRP:N	2:E:1096:THR:HG23	2.17	0.57
3:I:321:TRP:O	3:I:322:GLN:OXT	2.21	0.57
2:N:82:ARG:NH1	3:O:214:GLU:OE2	2.38	0.57
2:T:917:LYS:HZ1	6:T:5801:MD1:H15	1.49	0.57
2:W:976:TYR:CD2	2:W:1108:ALA:HB2	2.38	0.57
1:A:259:MET:HA	1:A:267:ARG:HD3	1.87	0.57
2:E:386:LEU:H	2:E:433:VAL:HG12	1.70	0.57
2:E:920:HIS:HD2	2:E:935:TRP:O	1.87	0.57
3:F:273:THR:HG22	3:F:275:ASP:H	1.68	0.57
2:N:961:PRO:O	2:N:965:ARG:HG3	2.04	0.57
2:Q:544:LEU:HB2	2:Q:545:PRO:HD3	1.86	0.57
2:Q:648:VAL:HG13	2:Q:676:GLN:HB3	1.85	0.57
1:V:252:ARG:HD2	1:V:350:THR:HG21	1.87	0.57
2:W:924:SER:OG	6:W:5801:MD1:PA	2.63	0.57
2:B:302:LEU:HD11	2:B:524:HIS:HD2	1.65	0.56
2:E:1062:ASP:OD1	2:E:1096:THR:CG2	2.53	0.56
3:F:121:ASN:HB3	3:F:130:PHE:O	2.05	0.56
1:G:399:ILE:HD11	2:H:298:PHE:CE2	2.40	0.56
2:K:930:ASP:OD1	2:K:931:TRP:N	2.38	0.56
3:O:235:ASP:HB3	3:O:250:GLN:OE1	2.05	0.56
2:Q:514:ASP:O	2:Q:518:ILE:HG22	2.05	0.56
3:U:236:LEU:N	3:U:236:LEU:HD23	2.19	0.56
1:V:150:LYS:HG2	1:V:167:TRP:CE2	2.40	0.56
2:W:916:PRO:HA	6:W:5802:MD1:O1A	2.04	0.56
1:A:402:ARG:NH1	2:B:803:PHE:O	2.31	0.56
2:B:433:VAL:HG13	2:B:444:ILE:CD1	2.28	0.56
1:D:41:CYS:N	4:D:503:SF4:S3	2.76	0.56
2:E:663:VAL:C	2:E:664:TYR:HA	2.26	0.56
3:F:301:ARG:H	3:F:304:GLN:CB	2.18	0.56
3:I:155:MET:HE1	3:I:241:PHE:CB	2.35	0.56
3:I:321:TRP:CE3	3:I:321:TRP:HA	2.39	0.56
1:V:252:ARG:NH2	1:V:386:ASP:CG	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:467:LYS:O	2:W:468:LEU:HD13	2.04	0.56
2:B:392:LEU:HD11	2:B:869:ARG:HG3	1.88	0.56
3:C:285:GLU:OE1	3:U:142:LYS:HD3	2.06	0.56
1:D:407:TYR:CE2	2:E:576:TRP:HZ2	2.23	0.56
2:E:851:PRO:O	2:E:858:PRO:HB3	2.05	0.56
2:H:418:GLN:OE1	2:H:446:ARG:NH1	2.38	0.56
3:L:236:LEU:HA	3:L:247:GLN:HG3	1.86	0.56
1:M:78:LYS:O	1:M:82:LEU:HD13	2.05	0.56
1:P:34:ARG:CB	1:P:266:ILE:HG22	2.36	0.56
2:Q:311:GLU:HG3	2:Q:919:ARG:HB3	1.86	0.56
2:Q:312:ASN:O	6:Q:5802:MD1:N8	2.38	0.56
1:S:164:HIS:HD1	2:T:337:TYR:HH	1.51	0.56
2:T:91:GLN:HE21	2:T:114:MET:HB2	1.69	0.56
2:T:115:CYS:SG	2:T:117:LYS:NZ	2.76	0.56
1:V:213:LYS:HB2	5:V:504:F3S:S2	2.45	0.56
2:W:438:SER:OG	2:W:438:SER:O	2.24	0.56
1:A:98:GLU:O	1:A:98:GLU:HG3	2.05	0.56
2:B:114:MET:HE2	2:B:119:TYR:HD1	1.70	0.56
2:B:528:GLY:HA2	2:B:1099:LYS:NZ	2.20	0.56
2:E:586:ALA:O	2:E:606:LYS:O	2.23	0.56
2:E:617:TRP:HA	2:E:621:GLU:CG	2.35	0.56
2:K:709:THR:HG22	2:K:718:GLN:HB2	1.87	0.56
3:R:51:VAL:CG2	3:R:104:HIS:HD2	2.18	0.56
2:T:921:THR:O	6:T:5802:MD1:N17	2.39	0.56
2:W:79:ALA:HA	2:W:89:VAL:HG23	1.86	0.56
2:W:709:THR:HG22	2:W:718:GLN:HB2	1.87	0.56
2:W:976:TYR:HD2	2:W:1108:ALA:HB2	1.70	0.56
2:B:923:HIS:CG	6:B:5801:MD1:H102	2.40	0.56
2:E:527:GLU:OE2	6:E:5802:MD1:H101	2.04	0.56
2:H:916:PRO:HA	6:H:5802:MD1:O1A	2.06	0.56
1:J:178:CYS:HB3	1:J:299:THR:O	2.06	0.56
2:N:51:SER:O	2:N:53:TYR:N	2.39	0.56
3:O:103:ILE:CG2	3:O:110:TYR:HB2	2.36	0.56
2:Q:142[A]:ARG:NH1	2:Q:146:ASP:OD1	2.39	0.56
1:V:16:PRO:CG	1:V:128:TRP:HZ2	1.65	0.56
2:W:865:ASN:O	2:W:891:LYS:NZ	2.23	0.56
2:B:117:LYS:HE3	2:B:922:VAL:HG23	1.88	0.56
2:H:917:LYS:O	2:H:1019:LYS:NZ	2.33	0.56
1:J:192:ILE:HG12	1:J:203:ILE:HG12	1.88	0.56
2:K:164:ARG:NH2	2:K:674:ILE:O	2.35	0.56
2:K:227:GLY:HA3	2:K:654:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:388:ARG:NH2	2:K:390:ASP:OD2	2.39	0.56
2:K:938:ASN:ND2	10:K:5904:HOH:O	2.33	0.56
3:L:136:LEU:HD23	3:L:291:MET:HB3	1.86	0.56
3:L:303:GLY:HA2	3:L:305:LYS:HE3	1.87	0.56
2:N:996:TYR:CE2	2:N:1000:ARG:HB2	2.41	0.56
2:N:1132:ASN:O	2:N:1136:LYS:HG3	2.05	0.56
2:Q:123:ARG:HH21	3:R:194:ASP:HB2	1.69	0.56
3:U:236:LEU:HB2	3:U:245:THR:O	2.04	0.56
1:V:126:ASN:HA	3:X:88:PHE:CZ	2.41	0.56
2:W:98:TYR:CE1	2:W:798:VAL:HG11	2.40	0.56
2:W:222:PHE:HD1	2:W:648:VAL:CG1	2.18	0.56
2:E:139:GLY:HA3	2:E:160:MET:HB2	1.88	0.56
3:F:258:PHE:HB2	3:F:263:TRP:CZ3	2.39	0.56
1:G:242:ILE:HD11	1:G:256:THR:HG22	1.87	0.56
1:M:81:LYS:HB2	2:N:1134:PHE:CE1	2.41	0.56
2:N:71:ASP:O	2:N:72:THR:HG22	2.06	0.56
3:O:285:GLU:OE1	3:O:285:GLU:HA	2.04	0.56
1:P:195:ARG:NH2	1:P:243:GLU:OE2	2.36	0.56
2:Q:900:THR:O	2:Q:901:LYS:HD2	2.05	0.56
1:S:34:ARG:CB	1:S:266:ILE:HG22	2.36	0.56
2:T:225:ARG:HH11	2:T:656:LEU:HD12	1.69	0.56
2:W:970:GLU:OE2	2:W:1130:ASN:ND2	2.38	0.56
2:B:499:SER:HG	2:B:894:TRP:HE1	1.52	0.56
2:B:941:ASP:OD2	2:B:944:ARG:N	2.39	0.56
1:G:2:THR:HG21	1:G:18:PHE:HD2	1.70	0.56
1:G:25:GLN:CG	1:G:302:ASN:ND2	2.69	0.56
2:Q:94:ASP:OD1	2:Q:94:ASP:N	2.39	0.56
2:Q:307:LYS:HZ1	2:Q:313:LYS:HZ3	1.54	0.56
2:Q:386:LEU:HD23	2:Q:480:THR:HG22	1.88	0.56
2:Q:641:HIS:ND1	2:Q:1087:PHE:HB2	2.20	0.56
2:T:431:PHE:CE1	2:T:825:THR:HA	2.41	0.56
2:T:1132:ASN:HB3	2:T:1135:MET:H	1.70	0.56
2:B:32:LYS:HE3	2:B:35:VAL:HA	1.87	0.56
1:D:15:TYR:HE1	1:D:180:TYR:HA	1.71	0.56
1:M:16:PRO:HG3	1:M:128:TRP:CZ3	2.40	0.56
2:N:305:THR:CG2	2:N:525:TYR:HB3	2.34	0.56
2:Q:616:TYR:CE2	2:Q:623:PRO:HA	2.41	0.56
3:R:86:LYS:HE2	3:R:309:ILE:CD1	2.36	0.56
2:T:1064:SER:OG	2:T:1069:GLN:NE2	2.32	0.56
1:V:15:TYR:HE1	2:W:41:LEU:HD11	1.70	0.56
2:W:33:PRO:HA	3:X:277:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:915:THR:HA	2:W:1018:MET:O	2.05	0.56
2:W:976:TYR:HD1	2:W:1000:ARG:NE	2.03	0.56
2:B:671:ASN:HA	2:B:674:ILE:HG13	1.86	0.56
2:B:841:GLY:HA3	2:B:870:PRO:HB3	1.88	0.56
1:D:143:ASN:ND2	2:E:920:HIS:NE2	2.54	0.56
1:D:192:ILE:HD11	5:D:504:F3S:S3	2.46	0.56
2:H:90:GLU:HG2	2:H:91:GLN:H	1.71	0.56
2:H:135:LEU:HB2	2:H:694:ALA:HB3	1.87	0.56
1:M:34:ARG:CB	1:M:266:ILE:HG22	2.36	0.56
2:Q:588:ASP:OD2	2:Q:590:PHE:N	2.39	0.56
2:W:44:TYR:CG	2:W:45:PRO:HD2	2.40	0.56
2:W:631:TYR:OH	2:W:871:ASP:OD1	2.20	0.56
3:X:55:GLN:HG3	3:X:55:GLN:O	2.06	0.56
3:X:242:GLY:H	8:X:401:HEM:HBA1	1.70	0.56
2:B:913:CYS:CB	2:B:1103:VAL:HG21	2.35	0.55
2:B:1135:MET:HE3	2:B:1138:PHE:CD2	2.27	0.55
3:F:171:TRP:CZ2	3:F:229:ARG:HD3	2.41	0.55
2:H:977:VAL:HB	2:H:1001:LEU:HD23	1.87	0.55
2:K:937:ASN:HD21	2:K:954:GLU:N	1.99	0.55
2:Q:900:THR:HG22	2:Q:901:LYS:H	1.70	0.55
2:Q:969:ILE:HG12	2:Q:1107:LYS:HB2	1.87	0.55
1:D:209:ARG:HH12	3:F:244:LEU:HD23	1.71	0.55
1:D:314:ALA:HB1	2:E:1141:GLY:HA3	1.88	0.55
2:H:336:GLU:OE2	6:H:5802:MD1:O3'	2.22	0.55
2:H:1057:GLN:HA	2:H:1060:THR:HG22	1.88	0.55
2:K:342:GLN:HG3	2:K:343:LYS:HD2	1.88	0.55
1:M:115:THR:HG23	1:M:298:GLY:HA3	1.87	0.55
2:T:551:ASN:O	2:T:557:SER:HB2	2.06	0.55
1:V:42:THR:HG23	1:V:61:ASN:O	2.06	0.55
1:V:184:LEU:HD21	2:W:40:PRO:HB2	1.88	0.55
2:B:928:VAL:CG2	2:B:1048:GLN:HG2	2.36	0.55
2:T:268:SER:HB2	2:T:1090:ASP:OD2	2.05	0.55
3:U:43:THR:HG22	3:U:147:PRO:CG	2.36	0.55
1:V:211:TYR:CD2	5:V:504:F3S:S1	2.99	0.55
2:W:917:LYS:HZ3	6:W:5801:MD1:H15	1.54	0.55
1:A:259:MET:HG3	1:A:269:GLN:HB2	1.88	0.55
2:B:916:PRO:HA	6:B:5802:MD1:O1A	2.06	0.55
3:F:210:GLN:HB2	2:Q:208:LYS:HE2	1.86	0.55
3:I:145:ILE:HG23	3:I:288:TYR:CE2	2.42	0.55
2:K:462:LEU:HB3	2:K:482:LEU:HD23	1.88	0.55
3:O:258:PHE:HB2	3:O:263:TRP:CE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:30:PHE:CD1	1:P:267:ARG:HG2	2.41	0.55
1:P:76:ASP:OD2	2:Q:1138:PHE:HZ	1.90	0.55
1:P:96:ASP:OD2	1:P:106:ALA:N	2.29	0.55
2:W:178:PHE:HB3	2:W:744:LYS:HG3	1.87	0.55
2:B:468:LEU:O	2:B:475:GLU:HG3	2.05	0.55
3:F:166:HIS:CE1	3:F:168:LYS:HE3	2.42	0.55
2:N:250:ASP:OD2	2:N:254:ARG:NH1	2.39	0.55
2:Q:1018:MET:HE3	2:Q:1056:GLN:HA	1.89	0.55
2:T:296:VAL:HG11	2:T:320:VAL:HG22	1.89	0.55
2:T:312:ASN:O	6:T:5802:MD1:N8	2.40	0.55
2:T:804:ARG:NH2	2:T:817:GLU:OE2	2.40	0.55
3:U:129:GLU:CD	3:U:187:ARG:HH12	2.08	0.55
1:V:72:PRO:HG3	1:V:139:TRP:CZ3	2.42	0.55
2:W:428:ILE:HD11	2:W:1074:PHE:CG	2.41	0.55
3:X:84:GLN:O	3:X:90:ASN:HB2	2.06	0.55
3:C:227:LEU:O	3:C:229:ARG:NH2	2.39	0.55
2:E:77:ILE:HA	2:E:114:MET:HE3	1.89	0.55
2:E:618:ASN:HD21	2:E:661:LYS:H	1.52	0.55
2:E:917:LYS:HE2	6:E:5801:MD1:S13	2.46	0.55
1:M:400:HIS:CD2	2:N:104:ASN:HB3	2.41	0.55
2:N:47:ARG:HH21	2:N:47:ARG:HG3	1.70	0.55
3:O:131:ARG:HE	3:O:170:ASP:CG	2.10	0.55
2:Q:321:THR:O	2:Q:324:MET:HG2	2.06	0.55
2:Q:372:TYR:HD2	2:Q:377:VAL:HG21	1.71	0.55
2:W:139:GLY:O	2:W:159:TYR:HB3	2.06	0.55
2:W:1023:TRP:CD1	2:W:1023:TRP:N	2.72	0.55
3:X:50:ASN:ND2	3:X:317:GLU:OE1	2.38	0.55
2:E:664:TYR:CD1	2:E:999:SER:HA	2.42	0.55
3:I:107:ILE:HG13	3:I:108:THR:HG23	1.87	0.55
3:I:132:ASP:OD1	3:I:295:ASN:HA	2.06	0.55
1:J:329:GLU:OE1	1:J:371:LYS:NZ	2.37	0.55
2:K:124:ARG:NH1	2:K:925:GLN:OE1	2.40	0.55
2:K:270:TYR:CE2	2:K:276:GLN:HG3	2.42	0.55
3:O:122:LYS:HB3	3:O:169:ALA:HB1	1.89	0.55
2:Q:424:GLN:NE2	2:Q:1083:PHE:O	2.39	0.55
3:U:302:ASN:CG	3:U:303:GLY:H	2.09	0.55
2:B:868:ILE:HG22	2:B:870:PRO:HD3	1.88	0.55
2:B:915:THR:HA	2:B:1018:MET:O	2.06	0.55
1:D:178:CYS:HB3	1:D:299:THR:O	2.07	0.55
1:D:313:ARG:NH1	1:D:325:ASP:HA	2.22	0.55
2:E:709:THR:N	2:E:718:GLN:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:229:ARG:HG2	3:F:229:ARG:NH1	2.08	0.55
3:F:305:LYS:CE	8:F:401:HEM:C4D	2.64	0.55
1:G:66:LYS:NZ	1:G:76:ASP:OD2	2.38	0.55
3:I:83:LYS:HE2	3:I:92:GLY:O	2.06	0.55
3:I:231:ARG:NH1	3:I:250:GLN:HB2	2.21	0.55
2:K:124:ARG:NH2	2:K:683:GLU:OE2	2.39	0.55
2:K:276:GLN:HB3	2:K:1095:ASN:HD21	1.71	0.55
2:K:382:ASP:HA	2:K:385:LEU:HD13	1.88	0.55
2:K:834:GLU:HB2	2:K:837:ILE:HD12	1.89	0.55
1:V:28:ALA:HB2	1:V:259:MET:HE3	1.88	0.55
2:W:976:TYR:HD1	2:W:1000:ARG:HE	1.55	0.55
1:A:317:ARG:NH1	1:A:325:ASP:OD2	2.40	0.55
2:B:415:TYR:CD1	2:B:420:LEU:HB3	2.42	0.55
2:E:964:ALA:HB3	2:E:1007:TYR:HE1	1.70	0.55
3:F:172:GLU:OE1	3:F:255:CYS:HA	2.07	0.55
2:K:1011:TYR:CE2	2:K:1017:MET:HB2	2.42	0.55
1:M:262:CYS:HA	4:M:503:SF4:S3	2.47	0.55
2:N:77:ILE:HD11	4:N:5804:SF4:S1	2.47	0.55
2:N:485:TYR:HA	2:N:488:HIS:HB3	1.88	0.55
1:P:346:ARG:HA	1:P:346:ARG:NE	2.22	0.55
2:Q:307:LYS:HZ1	2:Q:313:LYS:NZ	2.04	0.55
2:Q:381:THR:O	2:Q:827:ARG:NH1	2.39	0.55
2:Q:434:TRP:HB3	2:Q:461:VAL:HG12	1.88	0.55
3:R:269:ARG:NH1	3:R:279:VAL:O	2.40	0.55
1:A:259:MET:SD	1:A:267:ARG:HD3	2.47	0.55
2:E:917:LYS:HZ1	6:E:5801:MD1:C16	2.19	0.55
2:E:1062:ASP:HA	2:E:1096:THR:HG21	1.88	0.55
3:F:302:ASN:O	3:F:305:LYS:HD2	2.06	0.55
3:I:298:ARG:O	3:I:299:GLU:HB2	2.07	0.55
2:K:916:PRO:HA	6:K:5802:MD1:O1A	2.07	0.55
1:M:115:THR:HG22	1:M:117:PHE:H	1.72	0.55
2:N:977:VAL:HG11	2:N:1001:LEU:HD23	1.89	0.55
2:Q:310:ILE:CG1	2:Q:340:SER:HA	2.37	0.55
2:Q:654:VAL:HG12	6:Q:5801:MD1:O2B	2.06	0.55
3:R:305:LYS:HE2	8:R:401:HEM:C1D	2.41	0.55
1:V:241:ARG:NH2	2:W:90:GLU:OE1	2.25	0.55
2:B:971:ASP:HB2	2:B:1007:TYR:CG	2.42	0.54
2:B:972:GLY:O	2:B:1004:ARG:NH1	2.40	0.54
2:K:925:GLN:NE2	6:K:5801:MD1:H5'1	2.22	0.54
1:S:34:ARG:HA	2:T:321:THR:CG2	2.37	0.54
2:W:236:LYS:HG2	2:W:653:ASN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:235:ASP:O	3:X:250:GLN:NE2	2.40	0.54
2:B:515:ILE:HG22	2:B:549:THR:HG21	1.89	0.54
1:D:257:ARG:HB3	4:D:501:SF4:S2	2.46	0.54
2:E:305:THR:O	6:E:5802:MD1:N2	2.39	0.54
3:F:155:MET:CG	8:F:401:HEM:NC	2.69	0.54
2:H:100:ASP:OD2	2:H:104:ASN:N	2.40	0.54
2:H:236:LYS:HE3	2:H:734:ASP:OD2	2.06	0.54
2:H:1061:ARG:HG2	2:H:1062:ASP:N	2.22	0.54
2:K:394:ARG:NH1	2:K:831:TYR:O	2.40	0.54
2:K:984:ARG:NH2	10:K:5907:HOH:O	2.39	0.54
2:N:1001:LEU:HD22	2:N:1055:SER:O	2.07	0.54
2:N:1020:HIS:CE1	6:N:5801:MD1:O11	2.52	0.54
2:W:250:ASP:OD2	2:W:254:ARG:NH1	2.39	0.54
1:D:168:PHE:HE1	2:E:342:GLN:HE21	1.56	0.54
1:G:271:PHE:O	1:G:278:ASN:ND2	2.39	0.54
1:J:189:ARG:HH12	3:L:244:LEU:HB3	1.73	0.54
2:K:900:THR:O	2:K:901:LYS:HG3	2.07	0.54
2:K:1001:LEU:HA	2:K:1054:GLY:HA3	1.89	0.54
2:N:882:TRP:CZ3	2:N:983:ASP:OD1	2.60	0.54
1:P:284:ILE:CD1	1:P:304:TYR:CD2	2.91	0.54
2:Q:213:ARG:NE	2:Q:642:MET:HB3	2.22	0.54
1:S:177:HIS:NE2	1:S:237:ALA:HB2	2.22	0.54
1:V:16:PRO:HD3	1:V:128:TRP:NE1	2.08	0.54
2:W:300:LYS:H	2:W:520:PRO:HD2	1.72	0.54
2:W:974:TYR:O	2:W:1108:ALA:CB	2.54	0.54
3:X:302:ASN:HB2	8:X:401:HEM:CAA	2.38	0.54
2:B:706:PHE:CD1	2:B:789:LEU:HD11	2.42	0.54
2:B:1027:ASP:O	2:B:1031:GLN:HG3	2.07	0.54
2:E:73:HIS:HD2	2:E:315:PRO:CB	2.21	0.54
3:I:53:TYR:CZ	3:I:319:ILE:HG23	2.42	0.54
2:K:977:VAL:HB	2:K:1001:LEU:HD23	1.90	0.54
3:L:303:GLY:C	3:L:305:LYS:HD2	2.28	0.54
2:N:533:PHE:HB2	2:N:1100:GLU:HG3	1.89	0.54
1:P:231:VAL:HG22	10:P:604:HOH:O	2.03	0.54
2:Q:527:GLU:O	2:Q:531:HIS:HB2	2.07	0.54
2:T:983:ASP:HB3	2:T:984:ARG:HD3	1.89	0.54
2:T:1032:ALA:HB1	2:T:1036:ARG:HD2	1.87	0.54
2:B:213:ARG:NH2	2:B:642:MET:O	2.40	0.54
2:E:956:GLN:C	2:E:1003:LEU:HD11	2.27	0.54
2:H:434:TRP:CZ3	2:H:441:PRO:HD3	2.42	0.54
2:H:571:PHE:HB2	2:H:581:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:222:PHE:CD1	2:K:648:VAL:HG22	2.42	0.54
2:K:497:VAL:O	2:K:501:THR:OG1	2.23	0.54
3:O:103:ILE:HG22	3:O:110:TYR:HB2	1.90	0.54
2:Q:229:GLY:HA3	2:Q:237:TYR:CD1	2.42	0.54
2:Q:974:TYR:CZ	2:Q:1004:ARG:HD3	2.43	0.54
2:W:135:LEU:HB2	2:W:694:ALA:HB3	1.89	0.54
3:C:54:MET:O	3:C:56:ILE:HG13	2.07	0.54
1:D:117:PHE:CE1	1:D:129:ALA:HB2	2.43	0.54
2:E:445:THR:HG22	2:E:446:ARG:H	1.73	0.54
2:H:923:HIS:O	2:H:1021:SER:CB	2.55	0.54
1:M:225:TYR:HD1	3:O:127:THR:HA	1.73	0.54
2:N:394:ARG:NH1	2:N:831:TYR:O	2.40	0.54
2:N:641:HIS:CE1	2:N:1087:PHE:HB2	2.43	0.54
1:P:282:TRP:CE3	1:P:283:LEU:HD12	2.43	0.54
1:S:104:THR:O	1:S:285:ARG:NH1	2.41	0.54
3:X:81:LEU:O	3:X:96:ASN:O	2.24	0.54
2:E:657:ILE:HD12	2:E:657:ILE:H	1.70	0.54
2:E:924:SER:HB3	6:E:5801:MD1:O2A	2.08	0.54
2:K:71:ASP:O	2:K:72:THR:HG22	2.07	0.54
2:K:376:TYR:CD2	2:K:550:GLY:HA2	2.43	0.54
3:O:137:MET:HE3	3:O:290:ASN:HB3	1.89	0.54
2:W:124:ARG:NH1	2:W:683:GLU:OE1	2.40	0.54
2:W:130:ARG:HH12	2:W:702:GLU:CD	2.11	0.54
2:W:228:MET:O	2:W:231:LEU:HG	2.08	0.54
2:W:1040:ARG:HH12	3:X:192:HIS:CE1	2.26	0.54
1:A:16:PRO:HG3	1:A:128:TRP:CE3	2.43	0.54
2:B:227:GLY:HA3	2:B:654:VAL:HG22	1.90	0.54
2:E:651:PHE:HD2	2:E:654:VAL:HA	1.73	0.54
3:I:154:ARG:CA	8:I:401:HEM:CBB	2.86	0.54
2:N:321:THR:HG22	2:N:343:LYS:HG2	1.90	0.54
2:Q:917:LYS:HZ3	6:Q:5801:MD1:H15	1.53	0.54
2:Q:1030:VAL:HG13	2:Q:1053:TYR:HE2	1.72	0.54
1:S:45:CYS:HB2	4:S:501:SF4:S2	2.47	0.54
1:S:289:ILE:HD11	1:S:331:PHE:HB2	1.90	0.54
3:U:138:PHE:HB3	3:U:279:VAL:HG21	1.88	0.54
1:V:396:GLU:HA	1:V:396:GLU:OE2	2.07	0.54
2:W:661:LYS:O	2:W:1060:THR:OG1	2.25	0.54
2:W:909:TYR:CD2	2:W:1104:LYS:HB2	2.43	0.54
2:W:974:TYR:CE1	2:W:1052:ARG:HD2	2.42	0.54
2:B:64:THR:CG2	2:B:76:ARG:HD2	2.38	0.54
2:B:276:GLN:HB3	2:B:1095:ASN:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:VAL:O	2:B:501:THR:OG1	2.22	0.54
2:B:776:GLY:H	2:B:781:LYS:HZ2	1.55	0.54
2:E:656:LEU:O	2:E:660:ALA:N	2.41	0.54
1:M:356:LYS:HB3	1:M:383:PHE:HE2	1.71	0.54
2:N:648:VAL:HG13	2:N:676:GLN:HB3	1.90	0.54
3:O:87:ALA:CB	3:O:241:PHE:HE1	2.20	0.54
2:Q:115:CYS:CB	4:Q:5804:SF4:S2	2.96	0.54
2:Q:532:TYR:C	2:Q:1097:VAL:HG21	2.28	0.54
2:T:753:ARG:HA	2:T:756:ASP:HB2	1.90	0.54
2:T:909:TYR:CD1	2:T:1104:LYS:HB2	2.42	0.54
2:W:115:CYS:HB2	2:W:314:MET:HE2	1.89	0.54
2:W:354:THR:HA	2:W:847:HIS:HE1	1.73	0.54
3:X:81:LEU:HD23	3:X:307:ILE:O	2.07	0.54
2:B:984:ARG:HH11	2:B:1061:ARG:HB2	1.73	0.54
2:E:33:PRO:HG2	3:F:161:PRO:HB3	1.90	0.54
3:F:114:ILE:HA	3:F:263:TRP:O	2.07	0.54
2:K:321:THR:O	2:K:324:MET:HG2	2.08	0.54
2:N:814:GLN:HA	2:N:819:LEU:HB2	1.91	0.54
2:N:917:LYS:NZ	6:N:5801:MD1:H15	2.06	0.54
1:P:178:CYS:HB3	1:P:299:THR:O	2.08	0.54
3:U:137:MET:HB2	8:U:401:HEM:CBC	2.38	0.54
1:V:318:GLN:OE1	2:W:1143:LEU:HB2	2.07	0.54
2:W:976:TYR:HD1	2:W:1000:ARG:NH2	2.03	0.54
2:B:970:GLU:HG2	2:B:1118:VAL:HG21	1.90	0.53
3:F:299:GLU:O	3:F:301:ARG:NH1	2.41	0.53
3:I:53:TYR:OH	3:I:319:ILE:HG23	2.07	0.53
3:I:95:VAL:HG22	3:I:306:ASN:OD1	2.08	0.53
2:K:453:LEU:HD11	2:K:827:ARG:HH12	1.72	0.53
2:K:531:HIS:CG	2:K:1098:PRO:HD2	2.43	0.53
2:N:308:ASN:HD21	2:N:339:PRO:HD2	1.73	0.53
2:Q:533:PHE:CE2	2:Q:1065:MET:HG3	2.43	0.53
2:T:409:ILE:HG21	2:T:445:THR:HG21	1.90	0.53
2:T:434:TRP:HB3	2:T:461:VAL:HG22	1.91	0.53
2:W:308:ASN:ND2	2:W:311:GLU:OE1	2.40	0.53
2:B:311:GLU:OE2	2:B:339:PRO:HG2	2.08	0.53
1:D:225:TYR:HB3	3:F:127:THR:HG23	1.89	0.53
2:E:1051:PHE:CD2	2:E:1055:SER:HA	2.43	0.53
2:H:140:TRP:HZ2	2:H:676:GLN:HE21	1.54	0.53
3:I:154:ARG:CA	8:I:401:HEM:HBB2	2.38	0.53
3:I:236:LEU:HD23	3:I:246:SER:HA	1.90	0.53
2:K:30:LEU:HD12	2:K:31:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:212:ARG:N	5:M:504:F3S:S4	2.72	0.53
2:N:114:MET:HG2	4:N:5804:SF4:S1	2.47	0.53
2:Q:842:GLU:OE2	2:Q:848:ARG:NH2	2.41	0.53
3:F:41:GLU:OE1	3:F:154:ARG:NH2	2.42	0.53
2:H:663:VAL:HG21	2:H:1024:ILE:HD13	1.89	0.53
2:K:415:TYR:HE1	2:K:420:LEU:HD23	1.73	0.53
2:W:390:ASP:N	2:W:390:ASP:OD1	2.37	0.53
3:X:137:MET:HG2	8:X:401:HEM:CBC	2.38	0.53
2:B:225:ARG:NE	2:B:269:ASN:OD1	2.31	0.53
2:B:588:ASP:OD1	2:B:608:ARG:NH2	2.41	0.53
2:K:116:LEU:H	2:K:116:LEU:HD23	1.74	0.53
2:K:286:LEU:HD12	2:K:287:GLN:H	1.73	0.53
2:K:1064:SER:OG	2:K:1069:GLN:NE2	2.42	0.53
1:V:34:ARG:HB3	1:V:266:ILE:HG22	1.89	0.53
2:W:381:THR:O	2:W:827:ARG:HD3	2.09	0.53
3:X:224:LEU:O	10:X:501:HOH:O	2.18	0.53
2:E:128:PRO:HD3	3:F:194:ASP:HB3	1.91	0.53
2:E:506:ASP:O	2:E:510:ARG:N	2.40	0.53
2:E:572:GLN:HA	2:E:1079:ILE:O	2.09	0.53
2:H:76:ARG:HD3	2:H:718:GLN:OE1	2.08	0.53
2:H:1016:THR:HG21	2:H:1105:ILE:HD11	1.89	0.53
2:K:485:TYR:OH	2:K:830:ALA:O	2.22	0.53
2:N:265:ARG:NH1	2:N:643:PRO:HA	2.23	0.53
2:N:1069:GLN:HE21	2:N:1094:ILE:HD11	1.74	0.53
2:Q:659:ASN:OD1	2:Q:1021:SER:OG	2.26	0.53
2:Q:768:VAL:O	2:Q:772:ARG:HG3	2.08	0.53
2:T:114:MET:HG2	4:T:5804:SF4:S1	2.48	0.53
2:B:1088:GLU:CG	2:B:1091:ASN:HB3	2.38	0.53
2:B:1119:TRP:CD2	2:B:1121:PRO:HD2	2.44	0.53
2:E:85:VAL:HG12	2:E:87:MET:HG2	1.90	0.53
2:E:957:ILE:CB	2:E:1018:MET:HG2	2.39	0.53
3:R:238:ALA:HB2	3:R:244:LEU:HD12	1.90	0.53
2:W:551:ASN:O	2:W:558:GLY:N	2.42	0.53
2:B:373:ASP:O	2:B:377:VAL:HG23	2.08	0.53
2:H:528:GLY:HA2	2:H:1099:LYS:NZ	2.23	0.53
1:M:175:CYS:SG	1:M:234:LYS:NZ	2.68	0.53
2:Q:433:VAL:HG21	2:Q:460:PRO:CB	2.29	0.53
2:Q:1024:ILE:HG22	2:Q:1055:SER:HB2	1.90	0.53
2:T:164:ARG:NH1	2:T:677:ILE:HD12	2.24	0.53
2:W:34:ALA:HA	3:X:245:THR:HG21	1.90	0.53
1:A:6:ASN:OD1	1:A:8:HIS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:TRP:HB3	2:B:461:VAL:HG22	1.90	0.53
3:C:237:ASN:OD1	3:C:247:GLN:NE2	2.41	0.53
2:E:1051:PHE:CE2	2:E:1055:SER:HA	2.43	0.53
2:H:462:LEU:O	2:H:480:THR:HG21	2.09	0.53
3:I:142:LYS:HG2	3:X:285:GLU:OE1	2.08	0.53
1:J:207:ARG:HD3	2:K:44:TYR:OH	2.09	0.53
2:N:641:HIS:CE1	2:N:1069:GLN:HA	2.44	0.53
2:N:823:THR:HG21	2:N:829:GLN:HG3	1.91	0.53
2:N:991:PRO:HA	2:N:996:TYR:CD1	2.44	0.53
1:P:284:ILE:HD11	1:P:304:TYR:CD2	2.44	0.53
2:Q:69:PRO:HB3	2:Q:700:TRP:CH2	2.43	0.53
2:Q:660:ALA:O	2:Q:1057:GLN:OE1	2.27	0.53
2:Q:915:THR:HA	2:Q:1018:MET:O	2.09	0.53
2:T:1001:LEU:HA	2:T:1054:GLY:HA3	1.91	0.53
1:V:291:LEU:HB2	1:V:320:PHE:HB3	1.91	0.53
2:W:883:GLU:O	2:W:886:THR:OG1	2.26	0.53
6:W:5801:MD1:H11	6:W:5801:MD1:H7	1.90	0.53
2:B:662:HIS:H	2:B:1060:THR:HG23	1.74	0.53
3:O:247:GLN:CB	10:O:502:HOH:O	2.56	0.53
2:Q:915:THR:OG1	6:Q:5801:MD1:N16	2.40	0.53
1:S:20:SER:HG	1:S:196:LYS:HZ1	1.52	0.53
2:T:1057:GLN:OE1	6:T:5801:MD1:N16	2.37	0.53
1:V:116:ILE:HA	1:V:119:VAL:HG12	1.90	0.53
2:W:513:LYS:O	2:W:517:THR:OG1	2.23	0.53
2:B:166:ASN:ND2	2:B:1031:GLN:OE1	2.42	0.53
2:B:485:TYR:OH	2:B:830:ALA:O	2.21	0.53
2:E:793:TYR:HB2	2:E:798:VAL:O	2.08	0.53
2:H:868:ILE:HG22	2:H:870:PRO:HD3	1.90	0.53
2:K:227:GLY:O	2:K:653:ASN:HB3	2.09	0.53
2:N:61:ARG:HG2	2:N:81:VAL:HB	1.91	0.53
2:Q:611:ASP:HB3	2:Q:1089:ALA:HB2	1.91	0.53
2:Q:903:PHE:CE2	2:Q:904:LEU:HG	2.44	0.53
2:Q:957:ILE:HB	2:Q:1003:LEU:HD21	1.90	0.53
2:T:711:SER:HB3	2:T:714:ASN:OD1	2.09	0.53
3:U:51:VAL:HG23	3:U:104:HIS:HD2	1.74	0.53
1:V:126:ASN:HA	3:X:88:PHE:CE1	2.44	0.53
3:C:163:ASN:HD22	3:C:164:LEU:H	1.57	0.52
1:D:331:PHE:HZ	2:E:324:MET:HG3	1.73	0.52
1:J:36:ILE:HD12	2:K:314:MET:HB2	1.91	0.52
2:N:117:LYS:HB3	2:N:926:TRP:CE2	2.44	0.52
2:N:916:PRO:O	2:N:1020:HIS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:228:MET:HB3	2:Q:231:LEU:HD23	1.90	0.52
2:Q:902:ASN:O	2:Q:906:GLU:HG2	2.08	0.52
2:Q:973:ASP:OD1	2:Q:1111:GLY:N	2.37	0.52
1:S:149:ALA:HB2	1:S:168:PHE:HD2	1.73	0.52
2:T:128:PRO:HG2	2:T:129:TYR:CE2	2.44	0.52
2:T:546:VAL:CG1	2:T:552:VAL:HG23	2.39	0.52
1:V:285:ARG:NH2	10:V:603:HOH:O	2.41	0.52
1:V:311:ALA:HB3	1:V:316:LEU:HD11	1.91	0.52
1:V:336:ARG:HD2	1:V:376:TYR:CD1	2.43	0.52
2:W:892:LYS:HB3	2:W:897:THR:CG2	2.37	0.52
1:A:296:GLN:NE2	1:A:318:GLN:O	2.43	0.52
1:D:229:THR:OG1	1:D:231:VAL:HG12	2.09	0.52
2:E:651:PHE:CD2	2:E:654:VAL:HA	2.44	0.52
2:H:113:ARG:HD2	2:H:316:GLU:OE2	2.09	0.52
1:J:11:ARG:NH1	1:J:113:GLY:O	2.42	0.52
2:K:985:PRO:HB2	2:K:999:SER:HB3	1.92	0.52
1:M:178:CYS:O	1:M:194:LYS:NZ	2.43	0.52
2:N:872:ASP:OD1	2:N:890:ILE:HG12	2.10	0.52
3:O:234:GLU:OE2	3:O:246:SER:OG	2.20	0.52
2:Q:625:ILE:CD1	2:Q:633:ARG:CG	2.88	0.52
1:S:4:VAL:N	1:S:13:MET:O	2.34	0.52
2:T:117:LYS:HB3	2:T:926:TRP:CD2	2.43	0.52
3:X:138:PHE:CB	3:X:279:VAL:HG21	2.39	0.52
3:X:229:ARG:CD	3:X:229:ARG:H	2.21	0.52
2:H:661:LYS:O	2:H:1057:GLN:HB3	2.08	0.52
2:N:977:VAL:HG12	2:N:1001:LEU:HB3	1.91	0.52
3:O:58:VAL:HG22	3:O:59:PRO:HD2	1.91	0.52
1:P:108:TYR:CE2	1:P:291:LEU:HD22	2.40	0.52
1:P:282:TRP:CH2	1:P:287:GLN:HG3	2.45	0.52
2:Q:916:PRO:HA	6:Q:5802:MD1:O1A	2.10	0.52
1:V:259:MET:CE	1:V:269:GLN:CG	2.83	0.52
2:B:1001:LEU:HD22	2:B:1055:SER:O	2.08	0.52
2:E:957:ILE:HA	2:E:1017:MET:O	2.09	0.52
2:E:998:VAL:O	2:E:1054:GLY:CA	2.57	0.52
2:N:228:MET:SD	2:N:269:ASN:HB3	2.50	0.52
3:O:236:LEU:HD23	3:O:246:SER:HA	1.91	0.52
1:P:64:GLU:HG3	1:P:66:LYS:HD3	1.91	0.52
2:T:641:HIS:CG	2:T:1087:PHE:HB2	2.44	0.52
1:V:126:ASN:O	1:V:127:GLN:HG2	2.08	0.52
1:V:189:ARG:HD2	8:X:401:HEM:O2A	2.09	0.52
2:W:409:ILE:HD11	2:W:445:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LYS:HG2	1:A:383:PHE:CE2	2.41	0.52
2:B:483:GLU:O	2:B:487:ILE:HG13	2.08	0.52
2:B:665:GLN:NE2	2:B:669:ASN:OD1	2.42	0.52
2:E:1012:PRO:HG2	2:E:1012:PRO:O	2.09	0.52
3:F:215:LEU:HD13	3:F:219:TYR:CE1	2.45	0.52
1:J:16:PRO:HG3	1:J:128:TRP:CE3	2.44	0.52
3:L:290:ASN:OD1	3:L:308:SER:OG	2.26	0.52
1:M:38:CYS:O	2:N:116:LEU:HD22	2.10	0.52
1:M:243:GLU:CD	2:N:54:ARG:HH12	2.11	0.52
1:P:395:VAL:O	2:Q:326:ARG:NH1	2.30	0.52
2:Q:114:MET:HG2	4:Q:5804:SF4:S1	2.50	0.52
2:Q:124:ARG:NH1	2:Q:683:GLU:OE2	2.42	0.52
2:T:433:VAL:HG21	2:T:460:PRO:HB3	1.91	0.52
2:T:834:GLU:HB2	2:T:837:ILE:HD12	1.90	0.52
1:V:7:TRP:HB2	1:V:105:GLY:O	2.09	0.52
2:B:317:ALA:O	2:B:320:VAL:HG12	2.09	0.52
2:B:924:SER:OG	2:B:924:SER:O	2.28	0.52
1:D:296:GLN:NE2	1:D:318:GLN:O	2.42	0.52
2:K:872:ASP:OD1	2:K:890:ILE:HG12	2.09	0.52
3:L:51:VAL:HG12	3:L:102:ALA:CB	2.38	0.52
6:N:5802:MD1:N15	6:N:5802:MD1:O11	2.43	0.52
1:P:184:LEU:HA	1:P:192:ILE:HB	1.90	0.52
2:T:661:LYS:HE3	2:T:1096:THR:HG21	1.92	0.52
2:B:943:TYR:HB3	3:C:188:TYR:HB3	1.91	0.52
2:B:1074:PHE:HB2	2:B:1085:PHE:CE1	2.45	0.52
1:D:363:VAL:HG13	1:D:377:ASN:HB2	1.92	0.52
2:E:617:TRP:O	2:E:666:MET:HE2	2.10	0.52
2:E:1062:ASP:CG	2:E:1096:THR:HG23	2.30	0.52
3:F:111:PHE:CE1	3:F:165:TRP:CZ3	2.96	0.52
3:F:115:TRP:CE2	3:F:293:VAL:HG11	2.45	0.52
1:G:34:ARG:HB2	1:G:266:ILE:HG22	1.90	0.52
1:G:241:ARG:NH2	1:G:255:GLU:O	2.31	0.52
2:H:882:TRP:CD1	2:H:883:GLU:HG2	2.44	0.52
8:I:401:HEM:CHA	8:I:401:HEM:CBA	2.85	0.52
1:J:365:GLU:HG2	1:J:372:LYS:NZ	2.24	0.52
2:N:611:ASP:HB3	2:N:1089:ALA:HB2	1.92	0.52
2:Q:496:SER:O	2:Q:500:MET:HG3	2.08	0.52
3:U:137:MET:SD	3:U:155:MET:HA	2.50	0.52
2:W:389:THR:HG23	2:W:867:TYR:HE1	1.75	0.52
2:B:271:THR:HB	2:B:1094:ILE:O	2.10	0.52
2:B:641:HIS:ND1	2:B:1087:PHE:HB2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:GLN:HE21	2:B:669:ASN:HB2	1.75	0.52
2:E:156:LYS:O	2:E:161:PHE:HB2	2.10	0.52
2:E:218:GLY:O	2:E:219:THR:CG2	2.53	0.52
3:F:155:MET:HG3	8:F:401:HEM:CHC	2.40	0.52
3:I:321:TRP:HA	3:I:321:TRP:HE3	1.73	0.52
2:K:174:TRP:HE1	2:K:730:GLU:HG2	1.75	0.52
2:K:311:GLU:HG3	2:K:919:ARG:HB3	1.91	0.52
1:P:60:TRP:HZ2	1:P:233:GLU:HB3	1.74	0.52
2:Q:1020:HIS:CE1	6:Q:5801:MD1:N8	2.78	0.52
3:U:151:PHE:CE1	3:U:160:LYS:HB3	2.45	0.52
2:W:376:TYR:O	2:W:379:LYS:O	2.27	0.52
2:B:381:THR:O	2:B:827:ARG:NH2	2.39	0.52
3:C:285:GLU:CD	3:U:142:LYS:HD3	2.31	0.52
2:E:920:HIS:N	2:E:920:HIS:HD1	2.07	0.52
2:H:219:THR:HG21	2:H:250:ASP:HB2	1.92	0.52
2:H:435:ASP:HB3	2:H:438:SER:HB3	1.92	0.52
3:I:272:ASN:ND2	3:X:272:ASN:OD1	2.43	0.52
2:K:116:LEU:HD11	2:K:920:HIS:HA	1.92	0.52
2:N:527:GLU:HA	2:N:530:ASN:HB2	1.90	0.52
2:N:882:TRP:CD1	2:N:883:GLU:HG2	2.44	0.52
3:O:91:GLY:HA3	3:O:304:GLN:HB3	1.91	0.52
3:O:294:TRP:CE2	3:O:305:LYS:CB	2.93	0.52
2:Q:625:ILE:CD1	2:Q:633:ARG:NE	2.69	0.52
2:T:706:PHE:CZ	2:T:722:LYS:HD2	2.45	0.52
1:V:252:ARG:CZ	1:V:386:ASP:OD2	2.54	0.52
1:D:177:HIS:NE2	1:D:237:ALA:HB2	2.24	0.52
2:E:356:THR:HG1	2:E:847:HIS:CB	2.17	0.52
3:F:137:MET:CE	3:F:155:MET:HA	2.40	0.52
3:I:39:GLU:O	3:I:43:THR:HG23	2.10	0.52
2:K:448:ASP:OD1	2:K:456:LYS:NZ	2.28	0.52
1:V:226:ARG:HD2	1:V:233:GLU:OE2	2.10	0.52
2:W:351:ARG:HB3	2:W:354:THR:HG21	1.91	0.52
1:A:65:THR:HG23	1:A:168:PHE:HD1	1.75	0.51
2:B:117:LYS:HB3	2:B:926:TRP:CD2	2.45	0.51
2:B:629:PRO:CG	2:B:874:GLY:O	2.58	0.51
2:E:613:GLU:HG3	2:E:615:ALA:H	1.75	0.51
2:H:389:THR:HG23	2:H:867:TYR:CE1	2.46	0.51
2:K:287:GLN:NE2	2:K:1090:ASP:O	2.38	0.51
3:L:84:GLN:NE2	3:L:89:PRO:O	2.42	0.51
1:M:188:PRO:HG2	3:O:302:ASN:CG	2.29	0.51
1:M:257:ARG:NH2	2:N:90:GLU:CG	2.60	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:177:HIS:NE2	1:P:237:ALA:HB2	2.25	0.51
2:Q:182:SER:O	2:Q:186:ILE:HD12	2.08	0.51
2:Q:862:VAL:HA	2:Q:892:LYS:O	2.10	0.51
3:R:165:TRP:CD1	3:R:252:VAL:HG21	2.45	0.51
2:T:117:LYS:HB3	2:T:926:TRP:CE2	2.45	0.51
2:T:395:VAL:HG23	2:T:432:VAL:HB	1.91	0.51
3:U:129:GLU:OE2	3:U:187:ARG:NH1	2.36	0.51
1:V:178:CYS:HB3	1:V:299:THR:O	2.10	0.51
1:V:212:ARG:CG	1:V:212:ARG:NH1	2.72	0.51
2:W:976:TYR:CD1	2:W:1000:ARG:NE	2.78	0.51
2:W:1057:GLN:HE22	6:W:5801:MD1:H162	1.57	0.51
1:A:245:ARG:O	2:H:790:ASN:ND2	2.40	0.51
2:H:33:PRO:HD2	3:I:239:GLU:OE2	2.10	0.51
2:K:654:VAL:HG12	6:K:5801:MD1:O2B	2.11	0.51
3:L:168:LYS:HE2	3:L:225:LEU:HD21	1.91	0.51
1:M:149:ALA:HA	1:M:168:PHE:HB3	1.92	0.51
2:N:273:HIS:HB3	6:N:5801:MD1:C13	2.40	0.51
3:O:289:PHE:CE1	3:O:312:HIS:HB2	2.45	0.51
1:P:302:ASN:HA	1:P:304:TYR:HE2	1.74	0.51
2:T:69:PRO:O	2:T:922:VAL:HG11	2.10	0.51
2:T:152:THR:CG2	2:T:154:GLU:HG2	2.40	0.51
3:U:229:ARG:HG2	3:U:231:ARG:HB2	1.92	0.51
1:V:68:TYR:CE1	2:W:1128:ALA:HA	2.45	0.51
1:V:275:ASN:O	1:V:281:THR:OG1	2.23	0.51
1:V:294:TYR:CE1	1:V:319:MET:HG3	2.44	0.51
3:X:168:LYS:HD2	3:X:171:TRP:CE2	2.45	0.51
1:A:256:THR:CG2	1:A:259:MET:HG2	2.40	0.51
2:B:130:ARG:NH1	2:B:702:GLU:OE1	2.35	0.51
2:B:665:GLN:NE2	2:B:669:ASN:HB2	2.24	0.51
3:F:238:ALA:HB2	3:F:244:LEU:HD12	1.92	0.51
1:G:20:SER:OG	1:G:196:LYS:NZ	2.38	0.51
1:G:311:ALA:HB3	1:G:316:LEU:HD11	1.92	0.51
2:H:301:LEU:HB3	2:H:521:VAL:HG22	1.92	0.51
3:I:154:ARG:HD2	8:I:401:HEM:CBB	2.41	0.51
1:J:218:CYS:O	1:J:221:LYS:HE2	2.10	0.51
3:L:110:TYR:CD1	3:L:268:CYS:HB2	2.46	0.51
1:P:241:ARG:NH1	2:Q:90:GLU:OE2	2.43	0.51
2:Q:857:LEU:HB2	2:Q:900:THR:CG2	2.23	0.51
2:T:261:ALA:O	2:T:608:ARG:HD3	2.10	0.51
2:T:485:TYR:HA	2:T:488:HIS:HB3	1.93	0.51
1:V:187:CYS:HA	5:V:504:F3S:S2	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:310:TRP:CZ2	2:W:342:GLN:HG3	2.45	0.51
1:D:33:ASN:OD1	1:D:308:PRO:HA	2.10	0.51
2:E:851:PRO:HA	2:E:858:PRO:HB2	1.93	0.51
2:K:937:ASN:HD21	2:K:953:GLY:CA	2.23	0.51
1:M:166:ARG:HD2	2:N:337:TYR:HB2	1.92	0.51
2:N:597:TYR:CZ	2:Q:49:TRP:HA	2.45	0.51
2:Q:388:ARG:HG3	2:Q:395:VAL:HG23	1.93	0.51
2:T:930:ASP:OD1	2:T:931:TRP:N	2.42	0.51
2:T:977:VAL:HB	2:T:1001:LEU:HD23	1.92	0.51
1:V:241:ARG:HD3	1:V:255:GLU:O	2.11	0.51
2:W:971:ASP:HB2	2:W:1007:TYR:CD2	2.45	0.51
2:W:996:TYR:CZ	2:W:1000:ARG:HG3	2.44	0.51
3:X:51:VAL:CG1	3:X:316:LEU:HA	2.41	0.51
2:B:449:VAL:CG2	10:B:5919:HOH:O	2.59	0.51
2:B:579:PRO:HB3	2:B:605:ILE:HG13	1.92	0.51
3:C:137:MET:HB3	3:C:164:LEU:HD13	1.93	0.51
1:D:190:LYS:HD3	2:E:40:PRO:HD3	1.93	0.51
2:E:959:ILE:HB	2:E:1016:THR:CG2	2.41	0.51
3:F:155:MET:HG3	8:F:401:HEM:C1C	2.46	0.51
2:H:1132:ASN:OD1	2:H:1135:MET:N	2.34	0.51
3:I:51:VAL:O	3:I:51:VAL:HG12	2.09	0.51
3:I:321:TRP:CD1	3:X:161:PRO:HD2	2.46	0.51
2:N:241:ARG:NH1	2:N:757:ASN:O	2.43	0.51
2:Q:223:LYS:NZ	2:Q:646:THR:OG1	2.39	0.51
2:Q:431:PHE:CE2	2:Q:825:THR:HG22	2.45	0.51
2:Q:625:ILE:HD12	2:Q:633:ARG:CG	2.41	0.51
2:T:577:SER:O	2:T:776:GLY:HA2	2.09	0.51
1:A:333:VAL:HG13	1:A:373:PHE:HB2	1.92	0.51
3:C:236:LEU:HB2	3:C:245:THR:O	2.10	0.51
2:E:177:ALA:HB1	2:E:695:PHE:HE2	1.75	0.51
2:E:208:LYS:O	2:E:212:ASP:N	2.35	0.51
2:E:468:LEU:HB3	2:E:476:ILE:H	1.74	0.51
2:E:1029:THR:HG21	2:E:1049:SER:CB	2.41	0.51
3:F:95:VAL:H	3:F:306:ASN:ND2	2.09	0.51
2:H:1119:TRP:CD2	2:H:1121:PRO:HD2	2.45	0.51
2:K:577:SER:O	2:K:781:LYS:NZ	2.34	0.51
2:K:611:ASP:HB3	2:K:1089:ALA:HB2	1.93	0.51
2:K:711:SER:HB3	2:K:714:ASN:OD1	2.11	0.51
1:M:291:LEU:HB2	1:M:320:PHE:HB3	1.93	0.51
1:M:311:ALA:HB3	1:M:316:LEU:HD11	1.93	0.51
2:N:1001:LEU:HA	2:N:1054:GLY:HA3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:193:ASP:N	3:O:197:THR:OG1	2.28	0.51
2:Q:355:ASP:HB3	2:Q:542:TYR:OH	2.10	0.51
1:S:311:ALA:HB3	1:S:316:LEU:HD11	1.93	0.51
2:T:527:GLU:HA	2:T:530:ASN:HB2	1.93	0.51
1:V:207:ARG:HG2	1:V:207:ARG:NH1	2.11	0.51
3:X:108:THR:HA	3:X:270:SER:HA	1.92	0.51
3:C:285:GLU:OE1	3:U:285:GLU:HG3	2.10	0.51
1:D:16:PRO:HG3	1:D:128:TRP:CE3	2.44	0.51
2:E:950:PRO:HD2	2:E:954:GLU:HB3	1.92	0.51
1:G:36:ILE:HG22	2:H:310:ILE:HG23	1.93	0.51
3:I:305:LYS:CD	3:I:307:ILE:CG2	2.73	0.51
2:K:909:TYR:CZ	2:K:1104:LYS:HD3	2.45	0.51
2:Q:445:THR:O	2:Q:448:ASP:HB2	2.11	0.51
2:E:131:LEU:HG	2:E:696:PRO:HB3	1.93	0.51
3:F:157:ASP:HA	3:F:240:GLY:CA	2.41	0.51
1:G:55:GLN:NE2	1:G:233:GLU:OE1	2.38	0.51
1:G:212:ARG:HD2	1:G:225:TYR:CD1	2.46	0.51
1:J:238:CYS:SG	1:J:257:ARG:HB2	2.50	0.51
2:N:476:ILE:HG13	2:N:478:VAL:CG1	2.40	0.51
1:P:313:ARG:O	1:P:317:ARG:HG2	2.11	0.51
2:Q:117:LYS:HD2	2:Q:922:VAL:HG23	1.93	0.51
2:Q:533:PHE:CE2	2:Q:1063:TRP:HB3	2.46	0.51
2:T:39:ASN:HB3	2:T:42:ASP:HB3	1.91	0.51
2:W:848:ARG:NH2	2:W:859:ASN:OD1	2.44	0.51
1:A:34:ARG:HB2	1:A:266:ILE:HG22	1.92	0.51
2:B:597:TYR:OH	2:H:52:VAL:HG22	2.11	0.51
1:G:177:HIS:NE2	1:G:237:ALA:HB2	2.25	0.51
3:I:51:VAL:HB	3:I:316:LEU:HA	1.93	0.51
3:I:53:TYR:HE1	3:I:319:ILE:HG12	1.76	0.51
3:I:98:ALA:HB3	3:I:291:MET:CE	2.41	0.51
3:I:114:ILE:HG12	3:I:264:THR:HG23	1.91	0.51
2:K:519:LYS:HG3	2:K:551:ASN:HD21	1.74	0.51
1:M:249:THR:HG21	1:M:254:MET:HB2	1.93	0.51
2:Q:140:TRP:HZ3	2:Q:180:TYR:HB3	1.76	0.51
2:T:885:ARG:HG2	2:T:888:ARG:HH21	1.75	0.51
2:T:1074:PHE:CE1	2:T:1083:PHE:HB3	2.46	0.51
2:W:307:LYS:HA	6:W:5802:MD1:H5'1	1.93	0.51
2:W:1124:THR:CG2	2:W:1126:TYR:HB2	2.40	0.51
1:A:195:ARG:NH2	1:A:243:GLU:OE2	2.44	0.51
1:A:375:MET:SD	2:B:326:ARG:HB3	2.51	0.51
2:B:250:ASP:OD2	2:B:254:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1088:GLU:HG2	2:B:1091:ASN:CB	2.38	0.51
1:D:67:PRO:HB3	1:D:315:TYR:CE1	2.46	0.51
2:E:34:ALA:HB1	3:F:243:THR:O	2.11	0.51
2:H:681:ASP:OD1	6:H:5801:MD1:H1'	2.11	0.51
2:K:1119:TRP:O	2:K:1122:VAL:HG22	2.11	0.51
2:N:143:TRP:CD1	2:N:149:PRO:HD2	2.46	0.51
1:P:149:ALA:HA	1:P:168:PHE:HB3	1.93	0.51
1:S:318:GLN:HA	2:T:1144:ILE:HG21	1.92	0.51
2:T:89:VAL:CG1	2:T:119:TYR:HA	2.41	0.51
2:T:101:LEU:HD21	2:T:802:LEU:HD11	1.92	0.51
2:T:985:PRO:HB2	2:T:999:SER:HB3	1.93	0.51
2:W:875:ILE:HG23	2:W:888:ARG:HG3	1.91	0.51
2:B:648:VAL:HG13	2:B:676:GLN:HB3	1.91	0.50
2:B:990:LYS:HB2	2:B:993:ASP:OD2	2.10	0.50
2:H:117:LYS:NZ	2:H:921:THR:O	2.44	0.50
2:H:447:ASP:O	2:H:449:VAL:N	2.44	0.50
3:I:137:MET:SD	3:I:162:VAL:HG11	2.51	0.50
2:N:355:ASP:OD2	6:N:5802:MD1:N2	2.44	0.50
2:Q:268:SER:OG	2:Q:613:GLU:OE1	2.23	0.50
2:W:406:LEU:HD21	2:W:429:GLY:HA2	1.93	0.50
2:W:500:MET:HA	2:W:894:TRP:CH2	2.45	0.50
1:A:377:ASN:OD1	1:A:396:GLU:HB3	2.11	0.50
2:B:99:SER:HB3	2:B:105:LYS:HG2	1.93	0.50
2:B:923:HIS:NE2	6:B:5801:MD1:S12	2.85	0.50
3:C:302:ASN:HB2	8:C:401:HEM:HAA1	1.92	0.50
2:E:923:HIS:HB3	6:E:5801:MD1:H101	1.93	0.50
2:E:957:ILE:N	2:E:1003:LEU:HD11	2.26	0.50
2:E:1008:ASN:OD1	2:E:1009:PRO:HD2	2.12	0.50
1:G:172:GLN:HB3	1:G:267:ARG:HH21	1.76	0.50
3:L:51:VAL:HG23	3:L:104:HIS:HD2	1.77	0.50
1:M:241:ARG:HG2	1:M:254:MET:SD	2.52	0.50
2:N:468:LEU:O	2:N:475:GLU:HG2	2.11	0.50
2:N:629:PRO:HG2	2:N:874:GLY:O	2.11	0.50
3:O:171:TRP:O	3:O:175:LEU:HG	2.11	0.50
3:O:282:VAL:HG23	3:O:285:GLU:HB2	1.93	0.50
2:Q:554:TYR:O	2:Q:555:PHE:C	2.46	0.50
2:Q:569:GLY:O	2:Q:572:GLN:HB2	2.11	0.50
3:R:131:ARG:NE	3:R:170:ASP:OD2	2.36	0.50
1:S:173:ARG:NH2	1:S:220:TYR:O	2.42	0.50
1:S:402:ARG:O	2:T:804:ARG:NH1	2.44	0.50
2:T:423:GLU:O	2:T:427:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:822:TYR:CD1	2:T:1076:LYS:HD2	2.46	0.50
2:T:916:PRO:HA	6:T:5802:MD1:O1A	2.10	0.50
2:W:359:PHE:HA	2:W:362:ILE:HG22	1.93	0.50
2:W:397:PRO:HB2	2:W:404:TYR:CE2	2.47	0.50
2:W:532:TYR:CZ	2:W:1099:LYS:HG2	2.46	0.50
3:X:244:LEU:HB3	8:X:401:HEM:O2A	2.11	0.50
1:A:216:GLU:HG2	1:A:217:GLN:HG3	1.92	0.50
1:A:262:CYS:HB2	1:A:267:ARG:HD2	1.93	0.50
2:B:536:THR:OG1	2:B:1068:HIS:NE2	2.41	0.50
1:D:167:TRP:HH2	1:D:315:TYR:CE1	2.30	0.50
1:D:234:LYS:NZ	4:D:502:SF4:S1	2.72	0.50
1:D:258:CYS:N	4:D:501:SF4:S2	2.84	0.50
2:E:964:ALA:O	2:E:969:ILE:N	2.27	0.50
3:I:53:TYR:CE1	3:I:319:ILE:CA	2.86	0.50
3:I:155:MET:HE1	3:I:241:PHE:HA	1.83	0.50
1:M:246:ASP:OD1	2:N:59:TYR:OH	2.20	0.50
2:N:33:PRO:HA	3:O:277:LEU:HD21	1.91	0.50
2:N:949:MET:HE2	2:N:953:GLY:HA2	1.93	0.50
2:Q:227:GLY:HA3	2:Q:654:VAL:HG13	1.92	0.50
2:Q:310:ILE:HG12	2:Q:340:SER:HA	1.92	0.50
2:Q:710:ASN:HD22	2:Q:801:LEU:HD21	1.77	0.50
1:S:4:VAL:O	1:S:13:MET:N	2.34	0.50
1:V:211:TYR:O	3:X:301:ARG:HD2	2.10	0.50
2:W:915:THR:OG1	6:W:5801:MD1:N17	2.44	0.50
2:B:113:ARG:HG2	2:B:113:ARG:O	2.11	0.50
2:B:271:THR:HG21	2:B:1093:CYS:SG	2.52	0.50
2:B:652:THR:HG22	2:B:680:THR:CB	2.41	0.50
3:C:43:THR:HG22	3:C:147:PRO:HG3	1.93	0.50
1:D:50:THR:HA	1:D:55:GLN:OE1	2.11	0.50
2:E:671:ASN:N	2:E:672:PRO:CD	2.73	0.50
2:K:596:PRO:HG3	2:K:760:PHE:HE1	1.76	0.50
3:O:193:ASP:O	3:O:197:THR:OG1	2.29	0.50
1:P:231:VAL:HG21	10:P:604:HOH:O	2.04	0.50
3:R:301:ARG:H	3:R:304:GLN:HB2	1.75	0.50
1:S:178:CYS:HB3	1:S:299:THR:O	2.11	0.50
2:T:250:ASP:OD2	2:T:254:ARG:NH1	2.44	0.50
1:V:15:TYR:HE2	1:V:185:ALA:CB	2.24	0.50
1:V:66:LYS:HG2	1:V:171:LEU:HB2	1.92	0.50
2:B:69:PRO:HB3	2:B:700:TRP:CH2	2.46	0.50
2:E:736:LYS:O	2:E:740:GLY:N	2.31	0.50
3:F:95:VAL:HG22	3:F:306:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:305:LYS:NZ	8:F:401:HEM:C1C	2.47	0.50
1:G:173:ARG:NH2	1:G:220:TYR:O	2.40	0.50
2:H:714:ASN:ND2	10:H:5912:HOH:O	2.45	0.50
2:K:196:GLU:OE1	2:K:196:GLU:N	2.35	0.50
2:N:201:LEU:HD13	2:N:645:PRO:HG2	1.94	0.50
2:N:435:ASP:HB3	2:N:438:SER:O	2.12	0.50
2:N:527:GLU:OE1	2:N:527:GLU:N	2.45	0.50
2:N:790:ASN:ND2	1:P:245:ARG:O	2.33	0.50
1:P:48:THR:HG1	1:P:257:ARG:HH21	1.60	0.50
1:S:16:PRO:HG2	1:S:185:ALA:HB1	1.93	0.50
1:S:400:HIS:H	2:T:806:TYR:HB3	1.75	0.50
1:V:15:TYR:CD2	1:V:16:PRO:CD	2.94	0.50
2:W:504:PRO:HG2	2:W:507:LEU:HB2	1.93	0.50
2:W:843:ASN:OD1	2:W:868:ILE:HD13	2.12	0.50
2:B:948:ARG:NH2	2:B:1112:GLY:O	2.44	0.50
2:B:984:ARG:HH11	2:B:1061:ARG:CB	2.25	0.50
2:E:69:PRO:HB3	2:E:700:TRP:CH2	2.45	0.50
2:E:356:THR:OG1	2:E:847:HIS:CA	2.58	0.50
2:K:241:ARG:NH2	2:K:587:GLU:OE1	2.44	0.50
2:Q:625:ILE:HD11	2:Q:633:ARG:HG3	1.93	0.50
2:T:69:PRO:HB2	2:T:922:VAL:HG11	1.94	0.50
2:W:113:ARG:CG	2:W:113:ARG:NH1	2.73	0.50
2:W:974:TYR:C	2:W:1108:ALA:HB3	2.32	0.50
2:E:814:GLN:O	2:E:819:LEU:N	2.42	0.50
3:F:171:TRP:CZ3	3:F:229:ARG:HD2	2.47	0.50
2:K:572:GLN:HB3	2:K:778:THR:HB	1.93	0.50
3:L:251:ASP:OD2	3:L:273:THR:HG21	2.12	0.50
1:P:11:ARG:NH2	1:P:118:GLU:OE2	2.45	0.50
1:P:166:ARG:HD3	2:Q:1010:ALA:HA	1.94	0.50
2:Q:71:ASP:O	2:Q:73:HIS:CD2	2.64	0.50
2:Q:72:THR:HG21	2:Q:713:SER:CB	2.40	0.50
2:Q:198:ALA:O	2:Q:202:ILE:HG13	2.11	0.50
2:Q:385:LEU:H	2:Q:385:LEU:HD12	1.77	0.50
3:R:139:PRO:HB3	3:R:151:PHE:CE2	2.45	0.50
1:S:16:PRO:HG3	1:S:128:TRP:CE3	2.47	0.50
2:T:72:THR:HG22	2:T:564:GLY:C	2.32	0.50
1:V:192:ILE:HD13	1:V:203:ILE:HG12	1.94	0.50
1:V:263:VAL:CG2	2:W:315:PRO:HA	2.41	0.50
2:W:435:ASP:OD2	2:W:442:LYS:HE2	2.11	0.50
2:W:1119:TRP:CZ2	2:W:1121:PRO:HG2	2.47	0.50
3:X:81:LEU:HD22	3:X:307:ILE:O	2.06	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:109:ILE:C	3:X:110:TYR:CD1	2.85	0.50
3:X:125:ILE:HD12	3:X:187:ARG:HB2	1.93	0.50
1:A:63:VAL:HG13	1:A:172:GLN:HG3	1.94	0.50
1:A:195:ARG:HD3	1:A:200:ILE:HB	1.94	0.50
2:B:72:THR:HG21	2:B:313:LYS:HE3	1.92	0.50
2:B:547:MET:HG2	2:B:828:LEU:HD13	1.93	0.50
2:B:698:ASN:OD1	2:B:731:SER:OG	2.24	0.50
3:C:35:LYS:HD3	3:C:86:LYS:HA	1.94	0.50
1:D:117:PHE:HZ	1:D:182:GLY:HA2	1.75	0.50
1:D:226:ARG:NH2	3:F:216:SER:OG	2.40	0.50
2:E:855:PRO:O	2:E:902:ASN:N	2.37	0.50
3:F:257:LYS:N	3:F:264:THR:O	2.45	0.50
2:H:640:THR:HB	2:H:1087:PHE:HB3	1.93	0.50
3:I:140:LEU:HD12	3:I:161:PRO:HB2	1.94	0.50
1:M:52:ASN:HD22	3:O:215:LEU:HA	1.76	0.50
2:N:294:ASN:HA	2:N:319:TRP:CD2	2.47	0.50
1:P:192:ILE:O	2:Q:40:PRO:HB3	2.12	0.50
1:S:193:TYR:OH	2:T:50:GLU:OE2	2.19	0.50
3:X:95:VAL:H	3:X:306:ASN:HD21	1.58	0.50
2:B:143:TRP:CD1	2:B:149:PRO:HD2	2.47	0.50
2:B:424:GLN:O	2:B:428:ILE:CG1	2.59	0.50
3:C:167:TRP:NE1	3:C:256:SER:OG	2.45	0.50
1:D:48:THR:HG23	2:E:88:ARG:HD3	1.94	0.50
1:D:228:LEU:O	1:D:230:ARG:NH2	2.45	0.50
2:E:553:GLY:O	2:E:812:TRP:HE3	1.95	0.50
1:G:273:ASP:OD2	1:G:278:ASN:ND2	2.45	0.50
1:J:200:ILE:HD12	1:J:237:ALA:HB3	1.93	0.50
2:K:91:GLN:NE2	2:K:114:MET:HB2	2.21	0.50
2:N:189:THR:O	2:N:193:SER:OG	2.27	0.50
2:N:267:TRP:CD2	2:N:614:VAL:HG22	2.47	0.50
2:T:487:ILE:O	2:T:490:ARG:HG3	2.10	0.50
2:W:456:LYS:HB2	2:W:458:ILE:CD1	2.41	0.50
2:B:681:ASP:OD1	6:B:5801:MD1:H1'	2.12	0.49
2:B:1087:PHE:CD1	2:B:1087:PHE:C	2.85	0.49
1:D:255:GLU:OE1	1:D:346:ARG:NH1	2.45	0.49
2:E:267:TRP:HA	2:E:612:GLU:O	2.12	0.49
2:E:655:ASN:O	2:E:659:ASN:N	2.39	0.49
2:H:284:HIS:HD2	2:H:543:TYR:CE2	2.30	0.49
2:N:917:LYS:CD	6:N:5802:MD1:H15	2.24	0.49
2:N:941:ASP:OD2	2:N:944:ARG:N	2.45	0.49
2:T:712:CYS:O	2:T:808:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:491:ASP:OD2	2:W:864:THR:N	2.44	0.49
2:W:681:ASP:OD1	6:W:5801:MD1:H1'	2.12	0.49
2:W:939:PHE:HE2	2:W:1004:ARG:CD	1.54	0.49
1:A:3:LEU:HD22	1:A:3:LEU:N	2.27	0.49
2:B:69:PRO:HB3	2:B:700:TRP:HH2	1.75	0.49
2:B:213:ARG:HH21	2:B:642:MET:HB3	1.78	0.49
1:D:129:ALA:HB3	1:D:217:GLN:HB3	1.93	0.49
2:E:126:TYR:O	3:F:195:PHE:HE1	1.94	0.49
2:E:707:GLU:OE1	2:E:707:GLU:HA	2.12	0.49
1:G:63:VAL:HG21	4:G:503:SF4:S4	2.52	0.49
2:H:514:ASP:O	2:H:518:ILE:HG13	2.12	0.49
1:J:149:ALA:HA	1:J:168:PHE:HB3	1.95	0.49
1:J:177:HIS:NE2	1:J:237:ALA:HB2	2.27	0.49
2:K:383:PHE:HA	2:K:481:LEU:HD23	1.93	0.49
1:P:149:ALA:HB2	1:P:168:PHE:CD2	2.44	0.49
1:P:373:PHE:CE2	1:P:375:MET:HB2	2.46	0.49
2:Q:213:ARG:NH2	2:Q:610:LEU:HD21	2.27	0.49
2:Q:390:ASP:OD1	2:Q:390:ASP:N	2.44	0.49
2:Q:923:HIS:ND1	6:Q:5801:MD1:H102	2.26	0.49
2:T:68:SER:OG	10:T:5903:HOH:O	2.20	0.49
1:V:63:VAL:HG21	4:V:503:SF4:S4	2.52	0.49
1:V:73:GLN:HG3	1:V:138:GLU:O	2.12	0.49
1:V:186:ALA:O	1:V:188:PRO:HD3	2.12	0.49
1:V:259:MET:HE2	1:V:269:GLN:CG	2.42	0.49
2:W:917:LYS:HG3	6:W:5802:MD1:H15	1.77	0.49
1:A:259:MET:HA	1:A:267:ARG:CD	2.42	0.49
2:B:463:GLU:HG2	2:B:486:LYS:HZ1	1.77	0.49
2:B:888:ARG:HD3	2:B:890:ILE:HD12	1.94	0.49
2:B:941:ASP:OD2	2:B:943:TYR:N	2.46	0.49
2:E:123:ARG:NH1	3:F:194:ASP:HB2	2.07	0.49
3:O:56:ILE:HD11	3:O:103:ILE:CG1	2.42	0.49
2:Q:449:VAL:HG23	2:Q:827:ARG:HD2	1.94	0.49
3:R:130:PHE:CE1	3:R:301:ARG:HD3	2.47	0.49
3:R:282:VAL:O	3:R:285:GLU:HG2	2.13	0.49
2:T:382:ASP:OD2	2:T:830:ALA:N	2.44	0.49
1:V:175:CYS:HA	1:V:222:LYS:HG3	1.94	0.49
2:W:917:LYS:NZ	6:W:5801:MD1:N15	2.60	0.49
2:B:971:ASP:HB2	2:B:1007:TYR:CD2	2.47	0.49
2:B:978:ASP:OD1	2:B:1000:ARG:NH2	2.32	0.49
1:G:240:PRO:HB3	2:H:54:ARG:HG2	1.95	0.49
2:H:511:LEU:HG	2:H:515:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:295:ASP:OD2	2:K:556:GLY:N	2.39	0.49
2:K:795:GLU:HB3	2:K:798:VAL:HG22	1.95	0.49
1:M:189:ARG:NE	1:M:209:ARG:HG3	2.26	0.49
2:Q:73:HIS:CE1	2:Q:315:PRO:HD2	2.48	0.49
2:Q:130:ARG:NH2	2:Q:702:GLU:OE2	2.40	0.49
2:Q:276:GLN:O	2:Q:1095:ASN:ND2	2.44	0.49
2:Q:1030:VAL:HG13	2:Q:1053:TYR:CE2	2.47	0.49
2:Q:1110:ASN:HB3	2:Q:1117:GLY:O	2.12	0.49
1:S:137:LYS:HG3	2:T:945:MET:HE1	1.93	0.49
2:T:228:MET:HB3	2:T:231:LEU:CD2	2.43	0.49
1:V:378:ASP:O	1:V:395:VAL:HG23	2.12	0.49
2:W:229:GLY:HA3	2:W:237:TYR:CD1	2.47	0.49
2:B:64:THR:HG23	2:B:76:ARG:HD2	1.93	0.49
2:B:302:LEU:CD2	2:B:320:VAL:HG23	2.43	0.49
1:G:225:TYR:OH	3:I:124:ALA:O	2.26	0.49
2:H:707:GLU:O	2:H:719:ILE:HA	2.12	0.49
2:H:834:GLU:HB2	2:H:837:ILE:HD12	1.93	0.49
1:J:66:LYS:NZ	1:J:76:ASP:OD2	2.45	0.49
2:K:95:HIS:NE2	2:K:113:ARG:HD3	2.27	0.49
2:N:446:ARG:NH2	2:N:823:THR:O	2.38	0.49
3:O:120:ASP:HB3	3:O:258:PHE:CD2	2.47	0.49
3:O:305:LYS:HE3	8:O:401:HEM:C4B	2.47	0.49
2:Q:425:ARG:HH11	2:Q:425:ARG:HG3	1.76	0.49
2:Q:711:SER:HB3	2:Q:714:ASN:OD1	2.12	0.49
1:S:71:PHE:HE1	1:S:139:TRP:O	1.96	0.49
1:S:255:GLU:HG2	1:S:351:ILE:HG12	1.94	0.49
2:T:527:GLU:OE1	6:T:5802:MD1:H101	2.13	0.49
1:V:137:LYS:O	1:V:140:ARG:HG2	2.12	0.49
2:W:704:GLN:HA	2:W:704:GLN:NE2	2.26	0.49
2:B:779:THR:HB	2:B:801:LEU:HB2	1.94	0.49
1:D:259:MET:CE	1:D:269:GLN:CB	2.91	0.49
2:E:126:TYR:HB3	3:F:205:HIS:CD2	2.47	0.49
2:E:941:ASP:OD2	2:E:945:MET:HG3	2.11	0.49
3:F:85:ASP:HA	3:F:90:ASN:OD1	2.12	0.49
2:H:284:HIS:HD1	2:H:286:LEU:HB3	1.78	0.49
2:H:513:LYS:O	2:H:517:THR:HG23	2.13	0.49
2:K:647:LYS:HE3	2:K:673:ASN:O	2.12	0.49
3:O:51:VAL:HB	3:O:316:LEU:HA	1.95	0.49
1:P:30:PHE:CE1	1:P:267:ARG:HG2	2.47	0.49
2:Q:265:ARG:NH1	2:Q:612:GLU:HB2	2.27	0.49
2:Q:533:PHE:HB2	2:Q:1100:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:575:LYS:HD3	2:Q:575:LYS:N	2.23	0.49
2:Q:924:SER:OG	6:Q:5801:MD1:O2A	2.30	0.49
1:S:48:THR:HG23	2:T:88:ARG:HD3	1.95	0.49
2:T:51:SER:HA	2:T:54:ARG:CG	2.43	0.49
2:T:531:HIS:CG	2:T:1098:PRO:HD2	2.48	0.49
2:T:566:TYR:CZ	2:T:567:LYS:HG3	2.47	0.49
2:W:276:GLN:HB3	2:W:1095:ASN:ND2	2.27	0.49
1:D:192:ILE:O	2:E:40:PRO:HB3	2.12	0.49
2:E:618:ASN:ND2	2:E:661:LYS:H	2.11	0.49
2:E:1064:SER:O	2:E:1066:PRO:HD3	2.12	0.49
3:F:130:PHE:CD1	3:F:301:ARG:HD3	2.48	0.49
1:G:175:CYS:HA	1:G:222:LYS:HG3	1.95	0.49
1:G:262:CYS:HA	4:G:503:SF4:S3	2.52	0.49
2:H:466:PHE:HB2	2:H:478:VAL:CG2	2.42	0.49
2:H:595:ASP:O	2:H:772:ARG:NH2	2.46	0.49
2:K:1059:ILE:O	2:K:1101:THR:HG21	2.11	0.49
2:Q:131:LEU:HB3	2:Q:696:PRO:HB3	1.95	0.49
2:Q:631:TYR:OH	2:Q:871:ASP:OD2	2.26	0.49
2:Q:937:ASN:HD22	2:Q:954:GLU:C	2.15	0.49
2:T:752:LYS:C	2:T:754:PHE:H	2.16	0.49
1:V:177:HIS:NE2	1:V:237:ALA:HB2	2.28	0.49
1:V:208:CYS:HB3	1:V:231:VAL:CG1	2.43	0.49
2:W:73:HIS:ND1	2:W:315:PRO:HG2	2.28	0.49
1:A:44:ALA:HB2	2:B:119:TYR:HE2	1.78	0.49
1:A:132:TYR:O	1:A:221:LYS:NZ	2.45	0.49
1:A:262:CYS:SG	1:A:266:ILE:HG12	2.52	0.49
2:B:60:ASP:OD1	2:B:83:ASN:N	2.26	0.49
2:B:504:PRO:HG2	2:B:507:LEU:HD12	1.94	0.49
2:H:213:ARG:O	2:H:220:ARG:NH1	2.45	0.49
3:I:285:GLU:HA	3:I:285:GLU:OE2	2.12	0.49
2:K:332:VAL:HG23	2:K:344:ALA:HB2	1.94	0.49
2:K:428:ILE:HD11	2:K:1074:PHE:CG	2.48	0.49
2:N:60:ASP:OD2	2:N:83:ASN:N	2.31	0.49
3:C:163:ASN:HD22	3:C:164:LEU:N	2.11	0.49
3:F:81:LEU:HB3	3:F:306:ASN:HB3	1.95	0.49
3:F:241:PHE:CB	8:F:401:HEM:CHB	2.91	0.49
2:K:445:THR:OG1	2:K:446:ARG:N	2.46	0.49
2:K:681:ASP:OD1	6:K:5801:MD1:H1'	2.13	0.49
2:K:1022:ALA:HB1	2:K:1050:SER:HB2	1.93	0.49
3:L:239:GLU:HB2	3:L:243:THR:HG21	1.95	0.49
1:M:284:ILE:HG22	1:M:285:ARG:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:225:ARG:HH22	2:N:273:HIS:CE1	2.31	0.49
2:N:882:TRP:CE3	2:N:983:ASP:OD1	2.65	0.49
2:Q:213:ARG:HE	2:Q:642:MET:HB3	1.78	0.49
2:Q:425:ARG:HG3	2:Q:425:ARG:O	2.13	0.49
2:W:286:LEU:HD23	2:W:287:GLN:N	2.28	0.49
2:W:708:ILE:HD12	2:W:719:ILE:HG12	1.94	0.49
2:W:760:PHE:HB2	2:W:769:TYR:CE2	2.48	0.49
1:D:175:CYS:SG	1:D:234:LYS:HE2	2.53	0.49
2:E:934:ILE:HD13	2:E:942:PRO:HD3	1.93	0.49
2:H:706:PHE:CZ	2:H:722:LYS:HD2	2.47	0.49
3:I:110:TYR:CD1	3:I:268:CYS:HB2	2.48	0.49
3:I:123:GLN:NE2	3:I:182:GLU:OE1	2.45	0.49
3:L:305:LYS:HG2	3:L:307:ILE:HG23	1.95	0.49
1:M:211:TYR:O	3:O:301:ARG:NE	2.44	0.49
2:N:71:ASP:OD2	2:N:73:HIS:CD2	2.63	0.49
2:N:462:LEU:O	2:N:480:THR:HG21	2.13	0.49
2:N:711:SER:HB3	2:N:714:ASN:OD1	2.13	0.49
1:P:175:CYS:HA	1:P:222:LYS:HG3	1.95	0.49
2:Q:96:GLN:HG2	2:Q:108:ARG:CG	2.36	0.49
2:Q:307:LYS:HZ3	2:Q:313:LYS:HE2	1.77	0.49
2:Q:909:TYR:CE1	2:Q:1104:LYS:HB2	2.48	0.49
1:S:78:LYS:HD3	1:S:132:TYR:CZ	2.48	0.49
2:T:63:PHE:HB2	2:T:723:THR:HG22	1.95	0.49
1:V:373:PHE:CZ	2:W:326:ARG:HA	2.48	0.49
2:W:312:ASN:O	6:W:5802:MD1:N8	2.46	0.49
2:W:950:PRO:HD3	2:W:954:GLU:HG3	1.95	0.49
2:W:1040:ARG:CZ	2:W:1042:LEU:HD13	2.43	0.49
1:A:262:CYS:HA	4:A:503:SF4:S3	2.53	0.48
2:B:497:VAL:HA	2:B:500:MET:HG3	1.95	0.48
1:G:408:ASN:N	2:H:813:GLU:OE2	2.27	0.48
2:K:760:PHE:HB2	2:K:769:TYR:CE2	2.48	0.48
2:N:531:HIS:CG	2:N:1098:PRO:HD2	2.48	0.48
3:O:303:GLY:O	3:O:305:LYS:N	2.41	0.48
2:Q:123:ARG:NH2	2:Q:930:ASP:OD2	2.46	0.48
2:T:229:GLY:HA3	2:T:237:TYR:CD1	2.47	0.48
2:T:232:GLY:O	2:T:236:LYS:HB2	2.13	0.48
3:U:43:THR:CG2	3:U:147:PRO:HG3	2.40	0.48
2:W:1029:THR:HB	2:W:1049:SER:OG	2.13	0.48
2:B:310:ILE:CD1	2:B:310:ILE:N	2.76	0.48
2:B:453:LEU:HD11	2:B:827:ARG:NH1	2.27	0.48
2:B:851:PRO:O	2:B:858:PRO:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:THR:O	2:E:156:LYS:N	2.40	0.48
2:H:71:ASP:OD2	2:H:73:HIS:ND1	2.45	0.48
6:H:5802:MD1:N15	6:H:5802:MD1:O11	2.46	0.48
3:I:81:LEU:HD11	3:I:291:MET:HE2	1.95	0.48
3:L:309:ILE:HG13	3:L:310:GLN:HG3	1.95	0.48
2:N:57:TYR:O	2:N:88:ARG:NH1	2.42	0.48
3:O:241:PHE:HB2	8:O:401:HEM:C3A	2.47	0.48
1:P:265:GLN:NE2	2:Q:111:ASN:O	2.29	0.48
1:P:309:ARG:HG3	1:P:310:TRP:HE3	1.78	0.48
2:Q:77:ILE:HD13	2:Q:114:MET:HE3	1.94	0.48
2:Q:94:ASP:OD2	2:Q:98:TYR:OH	2.25	0.48
2:Q:974:TYR:CE1	2:Q:1004:ARG:HD3	2.48	0.48
1:V:8:HIS:O	1:V:90:TRP:HH2	1.95	0.48
1:V:189:ARG:NH1	1:V:209:ARG:HD2	2.28	0.48
2:W:225:ARG:HH11	2:W:656:LEU:HD12	1.78	0.48
2:W:520:PRO:HD2	2:W:520:PRO:O	2.12	0.48
2:W:543:TYR:CE1	2:W:559:SER:HB3	2.48	0.48
2:W:882:TRP:O	2:W:886:THR:HG23	2.13	0.48
3:X:235:ASP:OD1	3:X:278:ASP:OD2	2.32	0.48
1:A:72:PRO:HG3	1:A:139:TRP:CZ3	2.47	0.48
1:A:252:ARG:HH12	1:A:388:LYS:HB3	1.78	0.48
2:E:272:TRP:CH2	2:E:618:ASN:ND2	2.82	0.48
2:E:587:GLU:C	2:E:606:LYS:O	2.52	0.48
2:E:1062:ASP:CA	2:E:1096:THR:CG2	2.91	0.48
2:H:67:CYS:HB2	2:H:77:ILE:HD12	1.95	0.48
2:K:123:ARG:NH1	2:K:930:ASP:OD2	2.46	0.48
2:K:595:ASP:HB3	2:K:598:ALA:HB2	1.95	0.48
2:Q:172:ALA:HB1	2:Q:176:GLU:HG2	1.95	0.48
2:Q:210:MET:SD	2:Q:623:PRO:HD3	2.54	0.48
3:U:130:PHE:CE2	3:U:301:ARG:HD3	2.48	0.48
1:V:150:LYS:CG	1:V:167:TRP:NE1	2.76	0.48
1:V:334:PRO:HG2	2:W:325:GLU:O	2.13	0.48
2:W:143:TRP:CD1	2:W:149:PRO:HD2	2.47	0.48
2:B:88:ARG:NH2	10:B:5913:HOH:O	2.43	0.48
3:C:305:LYS:HE2	8:C:401:HEM:C4A	2.47	0.48
1:D:166:ARG:HB2	1:D:166:ARG:NH1	2.29	0.48
1:D:200:ILE:HD13	1:D:237:ALA:HB3	1.94	0.48
1:D:311:ALA:HB3	1:D:316:LEU:HD11	1.95	0.48
2:E:651:PHE:HD2	2:E:653:ASN:O	1.97	0.48
2:E:658:ASN:OD1	2:E:1024:ILE:HG23	2.12	0.48
2:H:90:GLU:HG2	2:H:91:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:HIS:HB2	1:J:271:PHE:HB3	1.95	0.48
2:K:983:ASP:OD2	2:K:1061:ARG:NE	2.45	0.48
2:K:1003:LEU:HD23	2:K:1003:LEU:H	1.78	0.48
3:O:301:ARG:CG	3:O:301:ARG:NH1	2.71	0.48
3:O:305:LYS:HE2	8:O:401:HEM:C1B	2.48	0.48
3:R:81:LEU:HA	3:R:307:ILE:O	2.14	0.48
1:S:217:GLN:NE2	10:S:605:HOH:O	2.34	0.48
2:T:983:ASP:HB3	2:T:984:ARG:CD	2.43	0.48
2:W:73:HIS:CG	2:W:315:PRO:HG2	2.48	0.48
2:E:193:SER:O	2:E:217:ALA:O	2.31	0.48
3:F:157:ASP:C	3:F:239:GLU:C	2.71	0.48
1:G:149:ALA:O	2:H:1009:PRO:HG2	2.14	0.48
1:J:38:CYS:O	2:K:116:LEU:HD22	2.13	0.48
1:J:267:ARG:NH1	4:J:503:SF4:S1	2.86	0.48
2:K:948:ARG:NH1	2:K:1112:GLY:O	2.47	0.48
1:M:189:ARG:HH11	1:M:189:ARG:CG	2.25	0.48
2:N:822:TYR:HB3	2:N:1076:LYS:HB2	1.96	0.48
2:N:836:GLU:H	2:N:836:GLU:HG3	1.36	0.48
2:Q:451:GLU:O	2:Q:454:VAL:HG22	2.13	0.48
2:Q:814:GLN:HA	2:Q:819:LEU:HB2	1.95	0.48
2:Q:888:ARG:HG2	2:Q:888:ARG:HH21	1.79	0.48
1:S:292:PRO:HB2	1:S:301:PRO:HG2	1.94	0.48
2:T:377:VAL:O	2:T:381:THR:HB	2.13	0.48
1:V:65:THR:HG21	1:V:147:ASP:H	1.78	0.48
1:V:364:PHE:CZ	1:V:366:THR:HB	2.49	0.48
1:A:211:TYR:CE2	3:C:302:ASN:HB3	2.49	0.48
1:A:246:ASP:OD1	2:B:59:TYR:OH	2.20	0.48
3:C:275:ASP:OD1	3:C:277:LEU:N	2.37	0.48
2:E:71:ASP:O	2:E:72:THR:CB	2.60	0.48
2:H:571:PHE:CE1	2:H:773:LEU:HB3	2.48	0.48
3:I:307:ILE:CD1	8:I:401:HEM:HAB	2.43	0.48
2:N:189:THR:O	2:N:218:GLY:HA3	2.13	0.48
2:N:462:LEU:N	2:N:462:LEU:HD23	2.28	0.48
2:N:928:VAL:HG11	2:N:1048:GLN:HB3	1.95	0.48
2:Q:1011:TYR:CE2	2:Q:1017:MET:HB2	2.47	0.48
2:T:588:ASP:OD2	2:T:591:LYS:N	2.46	0.48
2:T:915:THR:OG1	6:T:5801:MD1:N17	2.40	0.48
1:M:62:ASN:HD22	1:M:71:PHE:HB3	1.78	0.48
2:N:760:PHE:HB2	2:N:769:TYR:CE2	2.49	0.48
1:P:397:GLU:OE2	2:Q:107:THR:OG1	2.24	0.48
2:Q:527:GLU:N	2:Q:527:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:811:PHE:HA	2:Q:814:GLN:CG	2.42	0.48
2:Q:950:PRO:CD	2:Q:954:GLU:HB3	2.38	0.48
2:Q:957:ILE:HG23	2:Q:957:ILE:O	2.14	0.48
1:S:76:ASP:N	1:S:76:ASP:OD1	2.46	0.48
2:T:780:MET:HG3	2:T:801:LEU:HD23	1.95	0.48
2:W:834:GLU:OE2	10:W:5903:HOH:O	2.20	0.48
2:B:784:THR:HG22	2:B:787:ASP:H	1.79	0.48
3:F:95:VAL:CG2	3:F:306:ASN:HD22	2.26	0.48
1:G:236:ILE:HB	1:G:239:TYR:CD1	2.49	0.48
3:I:241:PHE:CD1	3:I:241:PHE:N	2.82	0.48
2:K:388:ARG:HB3	2:K:390:ASP:OD1	2.13	0.48
2:K:803:PHE:CG	2:K:808:ARG:HG3	2.48	0.48
2:N:485:TYR:OH	2:N:830:ALA:O	2.22	0.48
2:N:991:PRO:HA	2:N:996:TYR:HD1	1.78	0.48
2:Q:543:TYR:O	2:Q:547:MET:HG3	2.13	0.48
1:S:65:THR:HG21	1:S:147:ASP:H	1.79	0.48
1:S:373:PHE:HE2	1:S:375:MET:HE2	1.79	0.48
3:U:145:ILE:CG1	3:U:288:TYR:CE2	2.97	0.48
1:V:15:TYR:CZ	1:V:185:ALA:HB2	2.46	0.48
2:W:937:ASN:OD1	2:W:953:GLY:HA3	2.13	0.48
1:D:44:ALA:HB2	2:E:119:TYR:HE2	1.79	0.48
1:D:292:PRO:O	1:D:320:PHE:HD1	1.97	0.48
2:E:479:MET:C	2:E:484:MET:HE1	2.34	0.48
2:H:379:LYS:HD3	2:H:450:GLY:HA2	1.96	0.48
1:J:267:ARG:HD2	4:J:503:SF4:S1	2.53	0.48
2:K:142:ARG:NH1	2:K:158:LYS:HE2	2.28	0.48
1:M:26:PHE:CE1	1:M:237:ALA:HB1	2.49	0.48
2:N:376:TYR:CD2	2:N:550:GLY:HA2	2.49	0.48
2:N:398:LYS:O	2:N:471:ILE:HD13	2.14	0.48
2:N:950:PRO:HD2	2:N:954:GLU:HB3	1.95	0.48
3:O:233:VAL:HG11	3:O:252:VAL:HG12	1.96	0.48
2:T:189:THR:O	2:T:193:SER:OG	2.23	0.48
2:T:273:HIS:HB3	6:T:5801:MD1:C13	2.44	0.48
2:T:1022:ALA:HB1	2:T:1050:SER:CB	2.41	0.48
2:W:521:VAL:H	2:W:551:ASN:ND2	2.12	0.48
2:W:531:HIS:HA	2:W:1097:VAL:HG12	1.96	0.48
3:X:228:PRO:O	3:X:228:PRO:HG2	2.14	0.48
1:D:258:CYS:CB	4:D:501:SF4:S2	3.02	0.48
1:D:264:GLY:O	1:D:266:ILE:N	2.43	0.48
2:E:322:GLU:HA	2:E:325:GLU:OE1	2.14	0.48
2:E:619:HIS:HD2	2:E:1062:ASP:OD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:671:ASN:N	2:E:672:PRO:HD2	2.28	0.48
2:H:376:TYR:CD2	2:H:550:GLY:HA2	2.48	0.48
2:H:382:ASP:HA	2:H:385:LEU:HD13	1.95	0.48
2:H:973:ASP:OD1	2:H:1111:GLY:N	2.43	0.48
2:K:706:PHE:CZ	2:K:722:LYS:HD2	2.49	0.48
2:K:1087:PHE:CD1	2:K:1093:CYS:HB3	2.47	0.48
1:M:266:ILE:HG13	1:M:267:ARG:HG3	1.94	0.48
3:O:152:SER:HB3	3:O:157:ASP:HB2	1.95	0.48
2:Q:577:SER:O	2:Q:776:GLY:HA2	2.14	0.48
2:Q:914:VAL:HG12	2:Q:1099:LYS:HD3	1.95	0.48
3:R:86:LYS:HE2	3:R:309:ILE:HD11	1.96	0.48
3:R:302:ASN:CG	3:R:303:GLY:N	2.67	0.48
2:T:99:SER:HB3	2:T:105:LYS:HG3	1.95	0.48
2:W:115:CYS:HB2	2:W:314:MET:CE	2.44	0.48
2:W:893:SER:OG	2:W:896:GLU:HG3	2.14	0.48
1:D:135:GLU:HG3	3:F:128:GLN:OE1	2.13	0.47
2:E:92:ASN:HB3	2:E:94:ASP:OD1	2.14	0.47
2:H:76:ARG:HH12	2:H:720:TRP:HB3	1.79	0.47
3:I:154:ARG:NH1	10:I:501:HOH:O	2.47	0.47
1:J:255:GLU:OE1	1:J:346:ARG:NH2	2.47	0.47
2:K:98:TYR:CD1	2:K:798:VAL:HG21	2.49	0.47
1:M:127:GLN:OE1	3:O:89:PRO:HB3	2.14	0.47
2:N:388:ARG:NH2	2:N:390:ASP:OD2	2.45	0.47
2:N:893:SER:O	2:N:897:THR:N	2.42	0.47
2:N:925:GLN:HB2	2:N:926:TRP:CE3	2.49	0.47
2:N:1069:GLN:NE2	2:N:1094:ILE:HD11	2.28	0.47
2:Q:79:ALA:HA	2:Q:89:VAL:HG23	1.95	0.47
2:Q:641:HIS:CG	2:Q:1087:PHE:HB2	2.49	0.47
3:R:48:VAL:HG22	3:R:313:PRO:HB2	1.96	0.47
3:R:95:VAL:HG22	3:R:306:ASN:ND2	2.29	0.47
1:S:90:TRP:HE1	2:T:1144:ILE:HD11	1.79	0.47
1:S:257:ARG:HH22	2:T:90:GLU:HB2	1.79	0.47
2:W:39:ASN:OD1	2:W:39:ASN:N	2.36	0.47
2:B:531:HIS:CG	2:B:1098:PRO:HD2	2.49	0.47
3:C:302:ASN:O	3:C:305:LYS:HG3	2.14	0.47
2:E:703:PHE:CB	2:E:722:LYS:H	2.27	0.47
3:F:37:VAL:HA	3:F:154:ARG:HH21	1.79	0.47
3:F:161:PRO:HG3	3:O:321:TRP:CD2	2.50	0.47
2:H:184:GLY:HA3	2:H:676:GLN:NE2	2.30	0.47
2:H:428:ILE:HD11	2:H:1074:PHE:CG	2.49	0.47
1:J:63:VAL:HG21	4:J:503:SF4:S4	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1119:TRP:CD2	2:K:1121:PRO:HD2	2.49	0.47
3:L:155:MET:CG	8:L:401:HEM:NC	2.77	0.47
1:M:89:ILE:HG12	2:N:1145:LYS:HB3	1.96	0.47
2:N:273:HIS:HB3	6:N:5801:MD1:S13	2.54	0.47
2:N:703:PHE:O	2:N:722:LYS:HA	2.14	0.47
2:Q:115:CYS:HB2	2:Q:314:MET:HE2	1.92	0.47
2:Q:260:GLN:HA	2:Q:260:GLN:OE1	2.13	0.47
2:Q:923:HIS:O	2:Q:1021:SER:HB3	2.14	0.47
2:Q:1020:HIS:CE1	6:Q:5801:MD1:C20	2.97	0.47
1:S:34:ARG:HB2	1:S:266:ILE:HG22	1.95	0.47
1:S:149:ALA:HA	1:S:168:PHE:HB3	1.95	0.47
2:T:533:PHE:HB2	2:T:1100:GLU:HG3	1.95	0.47
2:T:942:PRO:HA	2:T:952:VAL:HG12	1.95	0.47
1:V:66:LYS:HD2	1:V:66:LYS:HA	1.44	0.47
2:W:166:ASN:HD21	2:W:1027:ASP:HB3	1.78	0.47
2:B:957:ILE:HB	2:B:1003:LEU:HD11	1.97	0.47
3:C:111:PHE:O	3:C:266:VAL:HA	2.14	0.47
3:F:95:VAL:HG23	3:F:306:ASN:HD22	1.79	0.47
3:F:128:GLN:H	3:F:128:GLN:HG2	1.38	0.47
1:G:126:ASN:C	1:G:127:GLN:HG2	2.30	0.47
2:H:130:ARG:NH1	2:H:702:GLU:OE2	2.44	0.47
2:K:115:CYS:SG	2:K:117:LYS:HB2	2.55	0.47
3:O:109:ILE:HB	3:O:271:LEU:CD1	2.44	0.47
3:O:165:TRP:CE2	3:O:252:VAL:HG21	2.49	0.47
2:Q:213:ARG:O	2:Q:220:ARG:NH2	2.47	0.47
2:Q:379:LYS:HB3	2:Q:450:GLY:HA2	1.96	0.47
2:Q:537:LEU:HD11	2:Q:842:GLU:CD	2.34	0.47
3:U:68:GLU:OE2	10:U:501:HOH:O	2.20	0.47
3:X:64:VAL:HG21	3:X:257:LYS:HB2	1.96	0.47
3:X:81:LEU:O	3:X:96:ASN:CA	2.60	0.47
1:D:44:ALA:HB3	1:D:258:CYS:HA	1.96	0.47
1:D:227:GLY:O	1:D:230:ARG:HD3	2.14	0.47
2:E:1119:TRP:CD2	2:E:1121:PRO:HD2	2.49	0.47
1:G:256:THR:OG1	1:G:259:MET:HG2	2.14	0.47
2:H:917:LYS:HD3	6:H:5802:MD1:H102	1.95	0.47
1:J:36:ILE:HG22	2:K:310:ILE:HG23	1.95	0.47
3:L:85:ASP:OD1	3:L:85:ASP:N	2.46	0.47
2:N:213:ARG:NH1	2:N:610:LEU:HD21	2.30	0.47
2:N:435:ASP:OD1	2:N:436:ALA:N	2.48	0.47
2:N:1124:THR:CG2	2:N:1126:TYR:CG	2.96	0.47
2:N:1135:MET:HE3	2:N:1139:LEU:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:466:PHE:O	2:Q:477:GLU:HG2	2.14	0.47
1:S:302:ASN:HA	1:S:304:TYR:CE1	2.50	0.47
2:T:409:ILE:CG2	2:T:445:THR:HG21	2.44	0.47
2:T:496:SER:O	2:T:500:MET:HG3	2.15	0.47
2:T:654:VAL:HG23	6:T:5801:MD1:O2B	2.15	0.47
1:V:76:ASP:OD1	1:V:76:ASP:N	2.46	0.47
2:W:69:PRO:HD2	2:W:71:ASP:HB2	1.96	0.47
2:W:100:ASP:OD2	2:W:104:ASN:HB2	2.15	0.47
2:W:274:GLY:O	2:W:527:GLU:HG3	2.14	0.47
2:W:393:LYS:HA	2:W:833:ASP:OD2	2.13	0.47
2:W:434:TRP:HB3	2:W:461:VAL:CG2	2.41	0.47
2:B:80:PHE:HE1	2:B:90:GLU:HB2	1.77	0.47
2:B:307:LYS:HD3	2:B:562:TRP:HB2	1.97	0.47
1:D:192:ILE:HD11	1:D:214:CYS:SG	2.54	0.47
3:F:89:PRO:HD2	3:F:302:ASN:ND2	2.26	0.47
1:J:346:ARG:CZ	1:J:346:ARG:HA	2.44	0.47
2:K:31:LEU:HD11	3:R:107:ILE:CD1	2.37	0.47
2:K:117:LYS:HZ2	2:K:922:VAL:HG22	1.79	0.47
2:K:218:GLY:O	2:K:221:THR:OG1	2.30	0.47
2:N:977:VAL:CG1	2:N:1001:LEU:HD23	2.45	0.47
2:Q:959:ILE:HG13	2:Q:960:HIS:N	2.29	0.47
1:S:65:THR:HG21	1:S:147:ASP:N	2.29	0.47
1:V:34:ARG:NH1	1:V:342:MET:HB3	2.29	0.47
1:V:137:LYS:HG2	2:W:945:MET:SD	2.54	0.47
1:V:241:ARG:HH12	1:V:257:ARG:HD2	1.60	0.47
2:W:392:LEU:O	2:W:831:TYR:OH	2.20	0.47
2:W:857:LEU:CB	2:W:900:THR:CG2	2.81	0.47
2:E:278:PRO:HG2	2:E:535:ALA:HB3	1.96	0.47
1:G:238:CYS:SG	1:G:257:ARG:HB2	2.55	0.47
3:I:171:TRP:CG	3:I:229:ARG:NH1	2.83	0.47
2:K:917:LYS:HE2	2:K:923:HIS:HD2	1.79	0.47
2:K:1088:GLU:HB3	2:K:1091:ASN:HB3	1.96	0.47
2:Q:575:LYS:H	2:Q:575:LYS:CD	2.26	0.47
2:Q:668:LYS:HG2	2:Q:986:TYR:CD2	2.49	0.47
2:T:291:VAL:O	2:T:562:TRP:HH2	1.98	0.47
2:T:348:ILE:HG12	2:T:507:LEU:HB3	1.96	0.47
1:V:61:ASN:HD22	1:V:62:ASN:N	2.12	0.47
2:W:527:GLU:OE2	6:W:5802:MD1:H101	2.15	0.47
2:W:1065:MET:O	2:W:1069:GLN:HG3	2.15	0.47
3:X:84:GLN:HG2	3:X:86:LYS:H	1.78	0.47
1:A:150:LYS:HD2	1:A:167:TRP:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:LYS:HA	6:B:5802:MD1:H5'1	1.97	0.47
2:B:937:ASN:ND2	2:B:954:GLU:H	2.12	0.47
2:E:131:LEU:HD12	2:E:132:ARG:H	1.79	0.47
2:E:650:TRP:HB3	2:E:678:MET:CB	2.45	0.47
2:E:849:GLU:O	2:E:859:ASN:N	2.48	0.47
3:F:131:ARG:CD	3:F:168:LYS:HG2	2.45	0.47
1:G:189:ARG:HD2	1:G:209:ARG:HD3	1.97	0.47
1:G:236:ILE:HB	1:G:239:TYR:HD1	1.79	0.47
2:H:950:PRO:HD2	2:H:954:GLU:HB3	1.97	0.47
2:H:971:ASP:HB2	2:H:1007:TYR:CD2	2.50	0.47
2:K:914:VAL:HG11	6:K:5802:MD1:H8	1.96	0.47
2:N:116:LEU:HD21	2:N:919:ARG:O	2.14	0.47
2:N:824:PRO:HG3	2:N:1074:PHE:HB3	1.95	0.47
3:O:294:TRP:HE1	3:O:305:LYS:HB3	1.74	0.47
2:Q:267:TRP:CE3	2:Q:614:VAL:HG22	2.49	0.47
2:Q:301:LEU:HD23	2:Q:521:VAL:HG22	1.96	0.47
2:Q:338:SER:HB2	2:Q:339:PRO:CD	2.45	0.47
2:Q:379:LYS:O	2:Q:449:VAL:HG22	2.14	0.47
2:Q:923:HIS:CG	6:Q:5801:MD1:H102	2.49	0.47
2:Q:930:ASP:OD1	2:Q:931:TRP:N	2.44	0.47
2:Q:971:ASP:HB2	2:Q:1007:TYR:CD2	2.50	0.47
6:Q:5802:MD1:N15	6:Q:5802:MD1:O11	2.47	0.47
3:R:143:ILE:HD12	3:R:143:ILE:C	2.34	0.47
2:T:139:GLY:O	2:T:159:TYR:HB3	2.15	0.47
2:T:1131:GLU:HG2	2:T:1139:LEU:HD11	1.95	0.47
3:U:62:ILE:HD11	3:U:67:LEU:HD11	1.95	0.47
1:V:65:THR:HG23	1:V:170:TYR:CE1	2.50	0.47
1:V:181:PRO:HG2	1:V:184:LEU:HB3	1.95	0.47
1:V:229:THR:O	1:V:231:VAL:HG23	2.13	0.47
2:W:545:PRO:O	2:W:549:THR:CG2	2.62	0.47
2:W:551:ASN:O	2:W:557:SER:CB	2.60	0.47
2:W:661:LYS:HE3	6:W:5801:MD1:N8	2.29	0.47
2:W:684:ILE:O	2:W:1023:TRP:CZ3	2.68	0.47
2:W:934:ILE:CD1	2:W:952:VAL:CG1	2.89	0.47
3:X:98:ALA:HB3	3:X:291:MET:CE	2.45	0.47
1:A:177:HIS:NE2	1:A:237:ALA:HB2	2.29	0.47
2:B:206:TYR:HE1	2:B:621:GLU:HG2	1.80	0.47
3:C:55:GLN:HG3	3:C:55:GLN:O	2.15	0.47
3:C:223:ASN:OD1	3:C:225:LEU:N	2.47	0.47
1:D:192:ILE:HA	1:D:202:LEU:O	2.15	0.47
2:E:1020:HIS:O	2:E:1020:HIS:CG	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:611:ASP:HB3	2:H:1089:ALA:HB2	1.97	0.47
2:H:917:LYS:CE	6:H:5801:MD1:H15	2.27	0.47
2:K:70:ASN:OD1	2:K:923:HIS:HE1	1.98	0.47
2:K:408:ASP:OD2	2:K:410:SER:OG	2.32	0.47
1:M:177:HIS:NE2	1:M:237:ALA:HB2	2.30	0.47
2:N:72:THR:HG21	2:N:313:LYS:HE3	1.95	0.47
2:N:115:CYS:SG	2:N:117:LYS:HB2	2.54	0.47
2:N:763:GLU:HG2	2:N:765:ARG:HD2	1.97	0.47
2:N:985:PRO:HB2	2:N:999:SER:HB3	1.95	0.47
1:S:189:ARG:HD2	1:S:209:ARG:HD2	1.95	0.47
2:W:381:THR:CG2	2:W:382:ASP:N	2.76	0.47
2:W:900:THR:O	2:W:901:LYS:HD3	2.15	0.47
2:B:79:ALA:HA	2:B:89:VAL:HA	1.97	0.47
1:D:166:ARG:HB2	1:D:166:ARG:CZ	2.44	0.47
1:D:331:PHE:HD2	1:D:332:MET:SD	2.38	0.47
2:E:272:TRP:HH2	2:E:618:ASN:ND2	2.13	0.47
1:G:45:CYS:HB2	4:G:501:SF4:S2	2.54	0.47
1:G:90:TRP:HB2	2:H:1146:VAL:HG22	1.97	0.47
1:G:207:ARG:HD3	2:H:44:TYR:OH	2.15	0.47
2:H:93:TYR:CE1	2:H:112:PRO:HB3	2.50	0.47
3:I:163:ASN:HD22	3:I:164:LEU:H	1.60	0.47
2:N:174:TRP:HE1	2:N:730:GLU:HG2	1.79	0.47
2:N:1119:TRP:CD2	2:N:1121:PRO:HD2	2.50	0.47
3:O:81:LEU:O	10:O:501:HOH:O	2.20	0.47
3:O:252:VAL:HG22	3:O:269:ARG:CG	2.45	0.47
3:R:140:LEU:HD11	3:R:237:ASN:HD21	1.79	0.47
2:W:192:TYR:CE2	2:W:647:LYS:HE2	2.50	0.47
2:W:271:THR:HG23	2:W:1090:ASP:HA	1.96	0.47
2:W:406:LEU:HD23	2:W:429:GLY:HA2	1.95	0.47
1:D:188:PRO:HB3	3:F:302:ASN:ND2	2.30	0.47
2:E:857:LEU:CB	2:E:900:THR:HG21	2.45	0.47
3:F:244:LEU:HB2	8:F:401:HEM:O1A	2.15	0.47
1:G:207:ARG:NH2	2:H:44:TYR:OH	2.40	0.47
2:K:577:SER:O	2:K:776:GLY:HA2	2.15	0.47
1:P:36:ILE:HD12	2:Q:310:ILE:HG23	1.96	0.47
2:Q:115:CYS:CB	2:Q:314:MET:HE2	2.44	0.47
2:Q:233:VAL:HB	2:Q:708:ILE:HG23	1.97	0.47
2:T:113:ARG:NH2	2:T:714:ASN:HD22	2.13	0.47
1:V:379:THR:O	1:V:379:THR:HG22	2.14	0.47
2:W:361:GLY:HA3	2:W:497:VAL:HG11	1.97	0.47
2:W:864:THR:HG22	2:W:893:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:974:TYR:O	2:W:1108:ALA:N	2.43	0.47
3:X:241:PHE:CD2	8:X:401:HEM:HMB3	2.50	0.47
1:A:16:PRO:HG2	1:A:185:ALA:HB1	1.97	0.46
2:B:527:GLU:OE1	6:B:5802:MD1:H101	2.15	0.46
2:E:141:LYS:O	2:E:145:ASP:N	2.43	0.46
2:H:91:GLN:HG2	2:H:112:PRO:HB2	1.96	0.46
2:H:350:ILE:HG13	2:H:501:THR:HB	1.97	0.46
2:H:388:ARG:HG3	2:H:395:VAL:HG12	1.97	0.46
2:H:1040:ARG:NE	2:H:1048:GLN:OE1	2.47	0.46
3:I:172:GLU:OE2	3:I:255:CYS:HA	2.15	0.46
1:J:149:ALA:O	2:K:1009:PRO:HG2	2.15	0.46
2:K:117:LYS:HB3	2:K:926:TRP:CE2	2.50	0.46
2:K:287:GLN:OE1	2:K:1078:LYS:HB2	2.14	0.46
2:K:594:LEU:HD22	2:K:759:LYS:HD2	1.98	0.46
1:M:190:LYS:HB3	2:N:37:VAL:CG1	2.45	0.46
2:N:61:ARG:HG3	2:N:61:ARG:NH1	2.31	0.46
1:P:256:THR:OG1	1:P:259:MET:HG2	2.14	0.46
1:S:175:CYS:HA	1:S:222:LYS:HG3	1.97	0.46
2:T:567:LYS:HB2	2:T:712:CYS:HB3	1.97	0.46
2:T:917:LYS:NZ	6:T:5801:MD1:O14	2.45	0.46
2:W:114:MET:HG2	4:W:5804:SF4:S1	2.54	0.46
2:W:265:ARG:HH21	2:W:612:GLU:HB2	1.80	0.46
2:W:709:THR:CG2	2:W:718:GLN:HB2	2.44	0.46
2:W:1023:TRP:HE3	2:W:1047:TYR:CE1	2.33	0.46
1:A:408:ASN:OD1	2:B:803:PHE:HB3	2.14	0.46
2:E:320:VAL:O	2:E:323:VAL:HG22	2.15	0.46
1:J:39:GLN:NE2	1:J:63:VAL:HB	2.30	0.46
2:K:72:THR:HG21	2:K:313:LYS:NZ	2.30	0.46
2:K:397:PRO:HG2	2:K:430:ASP:HB2	1.97	0.46
3:L:137:MET:HG2	3:L:290:ASN:HB3	1.98	0.46
3:L:303:GLY:HA2	3:L:305:LYS:HD2	1.97	0.46
1:M:8:HIS:ND1	1:M:300:GLU:HA	2.30	0.46
1:M:126:ASN:CB	3:O:90:ASN:OD1	2.62	0.46
1:P:68:TYR:CE1	2:Q:1139:LEU:HD11	2.50	0.46
2:Q:228:MET:O	2:Q:231:LEU:HD23	2.15	0.46
2:Q:246:LEU:O	2:Q:249:VAL:HG22	2.15	0.46
1:S:249:THR:O	1:S:252:ARG:HG3	2.14	0.46
1:S:408:ASN:OD1	2:T:803:PHE:HB3	2.14	0.46
2:T:527:GLU:OE1	2:T:527:GLU:N	2.49	0.46
1:V:9:LEU:H	1:V:9:LEU:HD12	1.80	0.46
2:W:504:PRO:HG3	2:W:507:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:137:MET:HB3	3:X:164:LEU:HG	1.97	0.46
1:D:99:THR:HG21	1:D:286:HIS:HA	1.98	0.46
3:I:231:ARG:HH11	3:I:250:GLN:HB2	1.80	0.46
2:K:626:VAL:HG13	2:K:628:THR:HG23	1.97	0.46
1:M:30:PHE:CD2	1:M:172:GLN:HB2	2.50	0.46
1:M:115:THR:HG23	1:M:297:PHE:O	2.15	0.46
2:N:527:GLU:OE1	6:N:5802:MD1:H101	2.15	0.46
2:N:958:HIS:CD2	2:N:1006:LYS:HD3	2.51	0.46
1:P:257:ARG:HH11	2:Q:90:GLU:CG	2.28	0.46
2:Q:640:THR:HB	2:Q:1087:PHE:CB	2.39	0.46
1:S:262:CYS:HA	4:S:503:SF4:S3	2.55	0.46
2:W:1023:TRP:N	2:W:1023:TRP:HD1	2.13	0.46
3:X:95:VAL:H	3:X:306:ASN:ND2	2.14	0.46
2:B:776:GLY:H	2:B:781:LYS:NZ	2.13	0.46
2:H:381:THR:O	2:H:827:ARG:HD3	2.15	0.46
2:H:760:PHE:HB2	2:H:769:TYR:CE2	2.50	0.46
2:H:930:ASP:OD1	2:H:931:TRP:N	2.49	0.46
3:I:137:MET:SD	3:I:155:MET:HA	2.55	0.46
1:J:150:LYS:HE2	2:K:1139:LEU:HB3	1.97	0.46
1:J:242:ILE:HD11	1:J:256:THR:HG22	1.97	0.46
2:N:468:LEU:O	2:N:476:ILE:N	2.48	0.46
1:V:216:GLU:HG2	1:V:217:GLN:HG3	1.97	0.46
2:W:309:LEU:HD12	2:W:313:LYS:HG3	1.98	0.46
3:X:41:GLU:O	3:X:310:GLN:HA	2.15	0.46
3:X:43:THR:HG22	3:X:147:PRO:HD3	1.97	0.46
3:X:117:ASP:HB3	3:X:263:TRP:CD1	2.47	0.46
3:X:154:ARG:HD3	3:X:241:PHE:HE2	1.79	0.46
1:A:146:GLU:O	2:B:1006:LYS:NZ	2.46	0.46
2:B:930:ASP:OD1	2:B:931:TRP:N	2.47	0.46
2:B:1065:MET:O	2:B:1069:GLN:HG3	2.15	0.46
1:D:13:MET:HE3	1:D:115:THR:HG21	1.98	0.46
1:D:186:ALA:HB2	1:D:217:GLN:HB2	1.96	0.46
1:D:313:ARG:HH12	1:D:325:ASP:HA	1.80	0.46
2:E:582:TYR:HB3	2:E:586:ALA:HB3	1.96	0.46
2:E:664:TYR:CE1	2:E:999:SER:HA	2.51	0.46
2:H:123:ARG:HD2	3:I:194:ASP:HB2	1.97	0.46
2:H:466:PHE:HB2	2:H:478:VAL:HG22	1.98	0.46
1:J:189:ARG:CD	1:J:209:ARG:HG3	2.44	0.46
1:J:410:ILE:HB	2:K:572:GLN:HE21	1.80	0.46
2:K:822:TYR:HB3	2:K:1076:LYS:HB2	1.97	0.46
2:K:971:ASP:HB2	2:K:1007:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:110:TYR:HD1	3:L:268:CYS:HB2	1.81	0.46
2:Q:546:VAL:HG12	2:Q:551:ASN:HB2	1.97	0.46
3:R:295:ASN:H	3:R:300:ASP:HB2	1.81	0.46
2:T:305:THR:HG23	2:T:525:TYR:HB3	1.97	0.46
2:T:355:ASP:OD2	2:T:542:TYR:OH	2.34	0.46
2:T:960:HIS:ND1	2:T:961:PRO:HD2	2.31	0.46
1:V:259:MET:O	1:V:346:ARG:NH2	2.48	0.46
2:W:431:PHE:CE2	2:W:825:THR:HA	2.50	0.46
2:W:930:ASP:O	2:W:934:ILE:HG12	2.16	0.46
1:A:402:ARG:HB3	1:A:406:HIS:HD2	1.80	0.46
2:B:350:ILE:HD12	2:B:358:LEU:HD22	1.98	0.46
3:C:143:ILE:HD13	3:C:151:PHE:CD2	2.51	0.46
2:E:617:TRP:O	2:E:666:MET:CE	2.63	0.46
3:F:95:VAL:CG2	3:F:306:ASN:ND2	2.79	0.46
1:J:2:THR:N	1:J:14:GLU:OE2	2.49	0.46
2:K:117:LYS:HB3	2:K:926:TRP:CD2	2.51	0.46
2:K:937:ASN:CB	2:K:954:GLU:O	2.63	0.46
1:M:36:ILE:HG22	2:N:310:ILE:HG23	1.97	0.46
1:P:192:ILE:CD1	1:P:203:ILE:HG12	2.46	0.46
1:P:282:TRP:HE3	1:P:283:LEU:HD12	1.80	0.46
2:Q:131:LEU:HD13	2:Q:683:GLU:C	2.35	0.46
2:Q:974:TYR:CE1	2:Q:1052:ARG:HD2	2.50	0.46
3:R:236:LEU:HB3	3:R:246:SER:HA	1.97	0.46
2:T:130:ARG:NH1	2:T:702:GLU:OE2	2.46	0.46
2:T:291:VAL:CG1	2:T:295:ASP:HB3	2.46	0.46
1:V:31:ASN:ND2	1:V:34:ARG:HG3	2.31	0.46
2:W:538:MET:O	2:W:541:SER:HB3	2.15	0.46
2:B:421:LYS:HB2	2:B:424:GLN:HG3	1.96	0.46
2:B:441:PRO:HG3	2:B:468:LEU:HD11	1.97	0.46
2:B:446:ARG:NH1	2:B:446:ARG:CG	2.75	0.46
1:D:190:LYS:HD3	2:E:40:PRO:CG	2.46	0.46
2:E:619:HIS:ND1	2:E:619:HIS:O	2.49	0.46
2:E:729:TYR:OH	3:F:200:HIS:O	2.29	0.46
2:H:225:ARG:NH1	2:H:272:TRP:CD1	2.82	0.46
2:K:274:GLY:HA2	2:K:1095:ASN:OD1	2.16	0.46
3:L:237:ASN:OD1	3:L:247:GLN:NE2	2.49	0.46
2:N:234:ILE:N	2:N:707:GLU:OE2	2.49	0.46
2:N:381:THR:O	2:N:827:ARG:HD3	2.16	0.46
3:O:95:VAL:HG21	3:O:115:TRP:CD1	2.51	0.46
3:O:111:PHE:O	3:O:266:VAL:HA	2.16	0.46
1:P:229:THR:O	1:P:231:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:309:ARG:HG3	1:P:310:TRP:CE3	2.51	0.46
2:Q:384:PRO:HG2	2:Q:385:LEU:HD12	1.96	0.46
1:S:399:ILE:HD11	2:T:298:PHE:CE2	2.51	0.46
2:T:77:ILE:HG22	2:T:89:VAL:HG22	1.98	0.46
1:V:115:THR:O	1:V:119:VAL:HG12	2.15	0.46
2:W:822:TYR:HB3	2:W:1076:LYS:HB2	1.98	0.46
2:E:925:GLN:O	2:E:926:TRP:HB2	2.15	0.46
2:E:979:ALA:HB1	2:E:1103:VAL:HA	1.97	0.46
3:F:289:PHE:CD1	3:F:314:LEU:HB3	2.50	0.46
1:G:189:ARG:HG3	1:G:211:TYR:HE2	1.80	0.46
1:J:45:CYS:HB2	4:J:501:SF4:S2	2.55	0.46
1:J:211:TYR:O	3:L:301:ARG:NE	2.43	0.46
2:K:143:TRP:CD1	2:K:149:PRO:HD2	2.51	0.46
2:K:330:ILE:HB	2:K:344:ALA:HA	1.97	0.46
2:K:415:TYR:CE1	2:K:420:LEU:HD23	2.50	0.46
2:K:660:ALA:C	2:K:1057:GLN:HE21	2.18	0.46
1:M:193:TYR:HH	2:N:49:TRP:HE1	1.64	0.46
2:N:270:TYR:HB3	2:N:1090:ASP:HB3	1.97	0.46
3:O:235:ASP:CA	3:O:250:GLN:OE1	2.64	0.46
1:P:29:VAL:HG21	1:P:283:LEU:CD2	2.45	0.46
2:Q:117:LYS:HE2	2:Q:919:ARG:O	2.16	0.46
2:Q:132:ARG:NH2	2:Q:133:TYR:OH	2.46	0.46
2:Q:420:LEU:HD12	2:Q:424:GLN:OE1	2.16	0.46
1:S:42:THR:HA	1:S:61:ASN:HD22	1.81	0.46
2:T:124:ARG:HD2	2:T:926:TRP:CD1	2.51	0.46
2:T:658:ASN:OD1	2:T:1024:ILE:HG23	2.15	0.46
1:V:106:ALA:N	1:V:107:PRO:HD3	2.30	0.46
2:W:1029:THR:CB	2:W:1049:SER:OG	2.64	0.46
1:A:404:ASP:CA	2:B:804:ARG:NH2	2.78	0.46
2:B:236:LYS:HG2	2:B:653:ASN:HB2	1.98	0.46
2:B:760:PHE:HB2	2:B:769:TYR:CE2	2.51	0.46
3:C:130:PHE:CE2	3:C:299:GLU:HG2	2.51	0.46
2:E:1131:GLU:H	2:E:1131:GLU:CD	2.13	0.46
3:F:269:ARG:NH2	3:F:279:VAL:O	2.44	0.46
2:H:425:ARG:NH2	2:H:430:ASP:OD1	2.43	0.46
1:J:256:THR:OG1	1:J:259:MET:HG2	2.16	0.46
2:K:70:ASN:HA	2:K:231:LEU:HD11	1.97	0.46
3:L:165:TRP:CZ2	3:L:269:ARG:HD3	2.51	0.46
2:N:379:LYS:HD3	2:N:450:GLY:HA2	1.98	0.46
2:N:434:TRP:HB3	2:N:461:VAL:HG23	1.98	0.46
1:P:14:GLU:HG2	1:P:121:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:147:ASP:HA	1:P:168:PHE:CE1	2.51	0.46
2:Q:888:ARG:HG2	2:Q:888:ARG:NH2	2.30	0.46
2:T:378:LYS:HG2	2:T:462:LEU:CD1	2.46	0.46
1:V:61:ASN:HD22	1:V:61:ASN:C	2.19	0.46
1:V:181:PRO:HG2	1:V:184:LEU:CB	2.46	0.46
2:W:373:ASP:N	2:W:548:LEU:O	2.46	0.46
1:A:123:LYS:HB2	1:A:125:ILE:HG22	1.98	0.46
3:C:305:LYS:O	3:C:307:ILE:HG23	2.16	0.46
1:D:35:CYS:HA	1:D:266:ILE:CD1	2.43	0.46
1:D:226:ARG:HH22	3:F:216:SER:CB	2.29	0.46
2:E:155:ASN:O	2:E:159:TYR:HB2	2.15	0.46
2:E:257:GLY:O	2:E:261:ALA:HB3	2.16	0.46
2:E:663:VAL:CA	2:E:664:TYR:N	2.70	0.46
2:H:824:PRO:HG3	2:H:1074:PHE:HB3	1.98	0.46
3:I:290:ASN:OD1	3:I:308:SER:OG	2.33	0.46
2:K:138:LYS:HG3	2:K:170:LEU:CD1	2.44	0.46
3:O:271:LEU:HG	3:O:281:PHE:HB2	1.98	0.46
2:Q:467:LYS:O	2:Q:468:LEU:HD23	2.16	0.46
2:Q:759:LYS:O	2:Q:763:GLU:CG	2.54	0.46
2:T:294:ASN:HA	2:T:319:TRP:CD2	2.51	0.46
2:W:60:ASP:OD1	2:W:82:ARG:HA	2.16	0.46
2:W:658:ASN:C	2:W:658:ASN:HD22	2.18	0.46
2:W:676:GLN:NE2	2:W:678:MET:SD	2.87	0.46
2:W:937:ASN:CB	2:W:954:GLU:O	2.64	0.46
1:A:410:ILE:HB	2:B:572:GLN:HE21	1.81	0.45
2:B:594:LEU:HD11	2:B:756:ASP:HB3	1.97	0.45
2:B:659:ASN:OD1	2:B:1021:SER:OG	2.34	0.45
2:E:663:VAL:O	2:E:666:MET:HB2	2.16	0.45
1:G:398:PRO:O	1:G:399:ILE:HD13	2.16	0.45
3:I:154:ARG:CD	8:I:401:HEM:HBB1	2.44	0.45
3:I:306:ASN:N	3:I:306:ASN:ND2	2.63	0.45
2:K:213:ARG:HD3	2:K:642:MET:HB3	1.97	0.45
1:M:126:ASN:HB3	3:O:90:ASN:OD1	2.17	0.45
1:M:181:PRO:HG2	1:M:184:LEU:HB3	1.98	0.45
2:N:61:ARG:NH1	10:N:5913:HOH:O	2.49	0.45
2:N:296:VAL:HG11	2:N:320:VAL:HG22	1.97	0.45
2:N:851:PRO:O	2:N:858:PRO:HB3	2.16	0.45
2:T:56:GLN:HG3	3:U:214:GLU:HA	1.98	0.45
2:T:97:ASN:O	2:T:794:GLY:HA3	2.16	0.45
2:T:722:LYS:NZ	10:T:5905:HOH:O	2.24	0.45
3:U:51:VAL:HG12	3:U:102:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:164:HIS:HB2	1:V:167:TRP:HB3	1.97	0.45
1:V:236:ILE:HB	1:V:239:TYR:CD2	2.51	0.45
2:W:293:MET:HE3	2:W:313:LYS:HD2	1.98	0.45
2:W:318:HIS:HA	2:W:321:THR:OG1	2.15	0.45
2:W:1017:MET:SD	2:W:1019:LYS:HG2	2.56	0.45
2:W:1022:ALA:HB1	2:W:1050:SER:CB	2.46	0.45
1:A:13:MET:HG2	1:A:14:GLU:N	2.31	0.45
2:B:335:PRO:HG3	2:B:352:ASN:ND2	2.31	0.45
2:E:1014:ASN:O	2:E:1015:CYS:HB2	2.15	0.45
2:E:1062:ASP:HA	2:E:1096:THR:HG22	1.95	0.45
3:F:95:VAL:H	3:F:306:ASN:HD21	1.63	0.45
2:H:485:TYR:HA	2:H:488:HIS:HB3	1.97	0.45
1:M:62:ASN:OD1	1:M:173:ARG:HB2	2.16	0.45
1:M:161:LEU:HA	1:M:161:LEU:HD23	1.75	0.45
1:M:276:PRO:HB3	1:M:286:HIS:NE2	2.31	0.45
2:N:82:ARG:HB2	2:N:87:MET:HG3	1.98	0.45
2:N:229:GLY:HA3	2:N:237:TYR:CD1	2.51	0.45
1:P:16:PRO:HG2	1:P:185:ALA:HB1	1.98	0.45
1:P:159:SER:HB2	2:Q:347:TRP:HB3	1.98	0.45
2:Q:613:GLU:HG3	2:Q:615:ALA:H	1.81	0.45
3:U:44:PRO:HG3	3:U:145:ILE:HB	1.98	0.45
3:U:54:MET:O	3:U:56:ILE:HG13	2.16	0.45
1:V:238:CYS:SG	1:V:256:THR:HG23	2.56	0.45
1:V:239:TYR:OH	2:W:53:TYR:HB2	2.17	0.45
2:W:69:PRO:HB2	2:W:922:VAL:HG11	1.98	0.45
2:W:1124:THR:O	2:W:1126:TYR:CE2	2.68	0.45
3:X:51:VAL:HG23	3:X:103:ILE:N	2.31	0.45
1:A:377:ASN:ND2	1:A:377:ASN:O	2.49	0.45
2:B:379:LYS:HB3	2:B:450:GLY:HA2	1.98	0.45
2:B:410:SER:HA	2:B:415:TYR:CD2	2.51	0.45
2:B:606:LYS:HD3	2:B:608:ARG:HH21	1.81	0.45
2:B:1088:GLU:CB	2:B:1091:ASN:HB3	2.46	0.45
1:D:52:ASN:HD21	3:F:215:LEU:HA	1.81	0.45
1:D:135:GLU:HG3	1:D:136:ASP:N	2.32	0.45
1:G:65:THR:HG21	1:G:147:ASP:N	2.31	0.45
1:G:256:THR:HG23	1:G:269:GLN:OE1	2.16	0.45
2:H:213:ARG:CZ	2:H:610:LEU:HD21	2.47	0.45
2:H:504:PRO:HG2	2:H:507:LEU:HD12	1.97	0.45
1:J:208:CYS:SG	1:J:231:VAL:HB	2.57	0.45
2:K:31:LEU:HD13	2:K:31:LEU:H	1.75	0.45
2:K:321:THR:HG22	2:K:343:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:384:PRO:O	2:K:433:VAL:HG23	2.17	0.45
2:N:91:GLN:NE2	2:N:114:MET:HB2	2.30	0.45
2:N:173:SER:OG	2:N:176:GLU:HG2	2.16	0.45
1:P:408:ASN:OD1	2:Q:803:PHE:HB3	2.16	0.45
2:Q:543:TYR:CE1	2:Q:559:SER:HB3	2.52	0.45
3:U:95:VAL:HG22	3:U:306:ASN:CG	2.37	0.45
1:V:368:ILE:HG12	1:V:369:HIS:ND1	2.31	0.45
2:W:225:ARG:NE	2:W:269:ASN:OD1	2.35	0.45
2:W:336:GLU:OE2	6:W:5802:MD1:O3'	2.25	0.45
2:W:1023:TRP:CE3	2:W:1047:TYR:CE1	3.04	0.45
1:A:239:TYR:N	1:A:240:PRO:HD2	2.31	0.45
2:B:382:ASP:HA	2:B:385:LEU:HD13	1.99	0.45
2:E:37:VAL:HG12	2:E:45:PRO:HD3	1.98	0.45
2:E:658:ASN:ND2	2:E:1023:TRP:HA	2.29	0.45
2:E:690:TYR:OH	2:E:1027:ASP:OD2	2.32	0.45
3:F:104:HIS:O	3:F:104:HIS:CD2	2.70	0.45
3:F:305:LYS:HE2	8:F:401:HEM:C1D	2.52	0.45
2:H:759:LYS:O	2:H:763:GLU:CG	2.64	0.45
2:H:923:HIS:CG	6:H:5801:MD1:H102	2.51	0.45
1:J:13:MET:HE2	1:J:13:MET:HB3	1.90	0.45
1:J:293:LEU:HB2	1:J:305:TYR:CE2	2.51	0.45
2:K:313:LYS:HE3	2:K:562:TRP:HB3	1.98	0.45
2:K:527:GLU:O	2:K:1099:LYS:HE3	2.17	0.45
2:K:546:VAL:HG12	2:K:552:VAL:HG23	1.98	0.45
2:K:865:ASN:HB3	2:K:868:ILE:HG12	1.98	0.45
2:K:921:THR:HG21	2:K:1021:SER:HB3	1.99	0.45
1:M:149:ALA:O	2:N:1009:PRO:HG2	2.16	0.45
2:N:722:LYS:NZ	10:N:5915:HOH:O	2.45	0.45
3:O:241:PHE:HB2	8:O:401:HEM:HMA3	1.98	0.45
1:P:16:PRO:HG3	1:P:128:TRP:CE3	2.50	0.45
2:Q:225:ARG:HB2	2:Q:267:TRP:CB	2.45	0.45
2:Q:305:THR:O	2:Q:333:ILE:O	2.35	0.45
2:Q:488:HIS:CE1	2:Q:868:ILE:HD11	2.51	0.45
2:Q:616:TYR:CD2	2:Q:623:PRO:HA	2.52	0.45
2:Q:963:ALA:HA	2:Q:1013:TYR:CE1	2.52	0.45
2:T:82:ARG:HB3	2:T:87:MET:HG3	1.97	0.45
2:T:505:LYS:O	2:T:509:GLU:HG3	2.17	0.45
1:V:170:TYR:OH	2:W:339:PRO:HB3	2.16	0.45
2:W:372:TYR:HB3	2:W:548:LEU:HB3	1.98	0.45
2:W:415:TYR:CD1	2:W:420:LEU:HB3	2.50	0.45
2:W:848:ARG:NH1	2:W:889:ASN:OD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:O	1:A:267:ARG:HA	2.17	0.45
2:B:618:ASN:ND2	2:B:661:LYS:O	2.45	0.45
2:B:823:THR:HG21	2:B:829:GLN:HG3	1.97	0.45
3:C:287:THR:HG22	3:C:314:LEU:HD23	1.99	0.45
1:D:296:GLN:H	1:D:296:GLN:HG3	1.54	0.45
2:E:182:SER:HA	2:E:185:ILE:HG22	1.97	0.45
2:Q:553:GLY:H	2:Q:809:HIS:HE1	1.64	0.45
2:Q:618:ASN:HD21	2:Q:661:LYS:HB2	1.82	0.45
3:R:86:LYS:HE2	3:R:309:ILE:HD13	1.98	0.45
1:S:256:THR:OG1	1:S:259:MET:HG2	2.16	0.45
1:V:92:THR:HG22	2:W:1147:ASP:O	2.16	0.45
1:V:215:VAL:HG22	1:V:223:PRO:O	2.15	0.45
1:V:346:ARG:HB3	2:W:112:PRO:HD3	1.99	0.45
2:W:273:HIS:HB3	6:W:5801:MD1:C13	2.47	0.45
2:W:282:PHE:CE1	2:W:837:ILE:HD11	2.50	0.45
2:W:717:ILE:O	2:W:798:VAL:HG23	2.17	0.45
2:W:1057:GLN:HE22	6:W:5801:MD1:C17	2.29	0.45
2:W:1064:SER:OG	2:W:1069:GLN:NE2	2.47	0.45
2:B:1057:GLN:OE1	2:B:1060:THR:HG21	2.16	0.45
2:E:385:LEU:HA	2:E:433:VAL:CG1	2.42	0.45
2:E:1042:LEU:HD23	2:E:1043:SER:O	2.17	0.45
2:H:217:ALA:HB2	2:H:262:LEU:HD12	1.98	0.45
2:H:531:HIS:CG	2:H:1098:PRO:HD2	2.52	0.45
2:H:1057:GLN:OE1	2:H:1060:THR:HG21	2.15	0.45
1:J:257:ARG:NH1	2:K:119:TYR:HE2	2.13	0.45
2:K:91:GLN:HG3	2:K:114:MET:SD	2.57	0.45
2:K:334:THR:HG22	2:K:336:GLU:N	2.29	0.45
1:M:63:VAL:HG21	4:M:503:SF4:S4	2.56	0.45
1:M:190:LYS:CB	2:N:37:VAL:CG1	2.94	0.45
1:M:194:LYS:HG3	1:M:201:VAL:CG2	2.42	0.45
2:N:350:ILE:HD12	2:N:358:LEU:HD22	1.98	0.45
2:N:447:ASP:O	2:N:449:VAL:HG22	2.16	0.45
2:N:722:LYS:HB2	2:Q:83:ASN:HA	1.99	0.45
2:Q:164:ARG:NH2	2:Q:674:ILE:O	2.48	0.45
2:Q:232:GLY:O	2:Q:236:LYS:HB2	2.17	0.45
2:Q:371:TRP:HB3	2:Q:516:ALA:HB1	1.97	0.45
3:R:94:SER:HB2	3:R:298:ARG:HG3	1.99	0.45
1:S:140:ARG:HD3	2:T:945:MET:HE2	1.99	0.45
2:T:753:ARG:HA	2:T:756:ASP:CG	2.37	0.45
2:T:811:PHE:O	2:T:815:VAL:HG22	2.17	0.45
2:T:939:PHE:CZ	2:T:1004:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:294:TRP:CZ2	3:U:305:LYS:HE3	2.52	0.45
1:V:173:ARG:NH2	1:V:220:TYR:O	2.47	0.45
1:V:282:TRP:CE3	1:V:283:LEU:HD12	2.51	0.45
2:W:37:VAL:HG22	2:W:45:PRO:CD	2.47	0.45
2:W:116:LEU:HD21	2:W:919:ARG:O	2.17	0.45
2:W:265:ARG:NE	2:W:612:GLU:HB2	2.30	0.45
1:D:65:THR:HG23	1:D:170:TYR:HE1	1.81	0.45
2:E:916:PRO:O	2:E:1019:LYS:HA	2.17	0.45
2:E:1020:HIS:HD2	6:E:5801:MD1:C16	2.30	0.45
2:H:468:LEU:HD12	2:H:478:VAL:HG21	1.98	0.45
2:H:515:ILE:HG23	2:H:521:VAL:HG11	1.99	0.45
2:H:861:ILE:HB	2:H:891:LYS:HA	1.99	0.45
1:J:181:PRO:HG2	1:J:184:LEU:HB3	1.98	0.45
2:K:141:LYS:HE2	2:K:180:TYR:HE2	1.82	0.45
6:K:5801:MD1:H7	6:K:5801:MD1:H11	1.98	0.45
1:M:276:PRO:HB3	1:M:286:HIS:CE1	2.52	0.45
1:M:302:ASN:HA	1:M:304:TYR:CE1	2.52	0.45
3:O:51:VAL:HG12	3:O:104:HIS:CD2	2.52	0.45
1:P:314:ALA:HA	1:P:317:ARG:HG3	1.99	0.45
2:Q:338:SER:HB2	2:Q:339:PRO:HD2	1.98	0.45
1:S:90:TRP:NE1	2:T:1144:ILE:HD11	2.32	0.45
2:T:571:PHE:HB2	2:T:581:PHE:HB2	1.98	0.45
2:W:705:GLU:HG3	2:W:706:PHE:N	2.31	0.45
1:A:181:PRO:HG2	1:A:184:LEU:HB3	1.98	0.45
2:B:656:LEU:O	2:B:660:ALA:HB2	2.16	0.45
2:B:662:HIS:H	2:B:1060:THR:CG2	2.29	0.45
1:D:202:LEU:HD21	1:D:236:ILE:CB	2.47	0.45
2:E:377:VAL:HG22	2:E:547:MET:O	2.17	0.45
2:E:679:SER:O	2:E:694:ALA:HA	2.17	0.45
2:E:1033:HIS:CE1	2:E:1052:ARG:CG	2.99	0.45
3:F:52:LYS:HA	3:F:317:GLU:CD	2.37	0.45
2:H:276:GLN:O	2:H:278:PRO:HD3	2.17	0.45
3:I:321:TRP:CE2	3:X:161:PRO:CG	2.99	0.45
2:K:814:GLN:HA	2:K:819:LEU:HB2	1.98	0.45
1:M:173:ARG:NH2	1:M:220:TYR:O	2.50	0.45
1:M:256:THR:HG21	1:M:259:MET:CE	2.47	0.45
2:N:531:HIS:O	2:N:1099:LYS:HB2	2.16	0.45
2:N:971:ASP:HB2	2:N:1007:TYR:CD2	2.51	0.45
2:Q:872:ASP:OD2	2:Q:890:ILE:HG12	2.16	0.45
3:U:46:LYS:N	3:U:46:LYS:HD2	2.32	0.45
1:V:364:PHE:CZ	2:W:300:LYS:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:367:GLU:OE1	1:V:372:LYS:HD3	2.17	0.45
2:W:210:MET:SD	2:W:623:PRO:HD3	2.57	0.45
2:W:301:LEU:HB3	2:W:521:VAL:HG22	1.99	0.45
2:W:1124:THR:HG22	2:W:1126:TYR:H	1.82	0.45
2:B:596:PRO:HG3	2:B:760:PHE:HE1	1.82	0.45
3:C:168:LYS:HD2	3:C:171:TRP:CE2	2.51	0.45
1:D:64:GLU:HG2	1:D:70:GLY:HA2	1.98	0.45
1:D:64:GLU:OE2	1:D:75:TRP:NE1	2.50	0.45
3:F:280:GLN:HB2	3:O:282:VAL:CG1	2.46	0.45
3:I:171:TRP:HH2	3:I:234:GLU:HG3	1.81	0.45
2:K:537:LEU:HD22	2:K:846:VAL:H	1.82	0.45
2:K:543:TYR:CE1	2:K:559:SER:HB3	2.51	0.45
2:K:689:GLU:OE2	2:K:1045:SER:OG	2.27	0.45
3:L:131:ARG:NH1	3:L:170:ASP:OD2	2.50	0.45
1:M:408:ASN:OD1	2:N:803:PHE:HB3	2.17	0.45
2:N:124:ARG:CD	2:N:929:THR:HG21	2.47	0.45
2:N:571:PHE:CD1	2:N:780:MET:HE3	2.51	0.45
3:O:87:ALA:HB2	3:O:241:PHE:HE1	1.82	0.45
3:O:231:ARG:HB2	3:O:231:ARG:CZ	2.47	0.45
1:P:32:ILE:HG21	1:P:308:PRO:HG3	1.97	0.45
2:Q:69:PRO:O	2:Q:922:VAL:CG1	2.54	0.45
2:Q:1059:ILE:HD12	2:Q:1060:THR:HG23	1.99	0.45
2:T:813:GLU:H	2:T:813:GLU:HG3	1.38	0.45
1:V:187:CYS:HA	1:V:188:PRO:HD2	1.82	0.45
2:W:974:TYR:CD1	2:W:1002:MET:SD	3.06	0.45
2:E:223:LYS:O	2:E:649:LEU:HA	2.16	0.45
2:H:308:ASN:HD21	2:H:339:PRO:HD2	1.82	0.45
2:H:380:PHE:CZ	2:H:815:VAL:HA	2.52	0.45
2:K:271:THR:HG21	2:K:1093:CYS:SG	2.57	0.45
2:N:400:ILE:HG13	2:N:401:ILE:HG13	1.99	0.45
3:O:172:GLU:OE2	3:O:232:ALA:HB1	2.17	0.45
2:Q:388:ARG:O	2:Q:392:LEU:HA	2.16	0.45
2:Q:425:ARG:HH22	2:Q:430:ASP:CG	2.20	0.45
2:Q:930:ASP:O	2:Q:934:ILE:HG13	2.17	0.45
2:T:223:LYS:HG2	2:T:267:TRP:NE1	2.31	0.45
2:T:648:VAL:HG13	2:T:676:GLN:HB2	1.98	0.45
1:V:9:LEU:HD12	1:V:9:LEU:N	2.32	0.45
2:B:218:GLY:O	2:B:221:THR:OG1	2.29	0.44
2:B:655:ASN:HD22	2:B:924:SER:CB	2.28	0.44
2:E:126:TYR:O	3:F:195:PHE:CE1	2.70	0.44
2:E:849:GLU:O	2:E:860:ALA:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:284:HIS:ND1	2:H:286:LEU:HB3	2.32	0.44
2:H:361:GLY:HA3	2:H:497:VAL:HG21	1.97	0.44
1:J:23:LYS:HE3	1:J:24:HIS:NE2	2.32	0.44
1:J:189:ARG:HD2	1:J:209:ARG:HG3	2.00	0.44
2:K:917:LYS:C	2:K:1019:LYS:HE2	2.35	0.44
3:L:242:GLY:H	8:L:401:HEM:HBA1	1.82	0.44
2:N:80:PHE:CE1	2:N:90:GLU:HB2	2.50	0.44
2:N:469:LYS:HA	2:N:475:GLU:HA	1.99	0.44
2:N:705:GLU:OE2	2:N:766:ALA:HB2	2.17	0.44
6:N:5801:MD1:H11	6:N:5801:MD1:H7	1.98	0.44
3:O:35:LYS:O	3:O:154:ARG:NH1	2.42	0.44
3:O:164:LEU:HD11	3:O:238:ALA:CB	2.47	0.44
1:P:338:LEU:O	1:P:341:VAL:HG12	2.16	0.44
1:P:377:ASN:OD1	1:P:394:THR:OG1	2.34	0.44
2:Q:527:GLU:HA	2:Q:530:ASN:HB2	1.98	0.44
3:R:309:ILE:HD12	3:R:309:ILE:HA	1.74	0.44
1:S:239:TYR:OH	2:T:50:GLU:O	2.30	0.44
2:T:413:PRO:HD2	2:T:447:ASP:OD2	2.18	0.44
1:V:64:GLU:OE1	1:V:173:ARG:NH1	2.33	0.44
2:W:37:VAL:HG22	2:W:45:PRO:HD3	1.99	0.44
2:W:272:TRP:CZ3	2:W:618:ASN:HB2	2.51	0.44
2:W:396:SER:O	2:W:399:ASP:HB2	2.17	0.44
2:W:998:VAL:HG12	2:W:1030:VAL:HG21	1.99	0.44
3:X:137:MET:HE2	3:X:137:MET:HB2	1.68	0.44
1:A:211:TYR:O	3:C:301:ARG:NE	2.49	0.44
1:A:410:ILE:HD11	2:B:803:PHE:HE1	1.81	0.44
2:B:139:GLY:O	2:B:159:TYR:HB3	2.17	0.44
2:B:386:LEU:HD13	2:B:478:VAL:HG23	1.98	0.44
1:D:294:TYR:CE1	1:D:319:MET:HG3	2.53	0.44
2:E:413:PRO:HB2	2:E:820:PRO:HD2	1.99	0.44
2:E:664:TYR:N	2:E:664:TYR:CD2	2.84	0.44
3:F:215:LEU:HD13	3:F:219:TYR:HE1	1.82	0.44
2:H:390:ASP:OD1	2:H:390:ASP:N	2.47	0.44
2:H:434:TRP:HB3	2:H:461:VAL:HG22	1.98	0.44
2:H:922:VAL:CG2	2:H:926:TRP:HZ3	2.30	0.44
1:J:189:ARG:CZ	1:J:209:ARG:HD2	2.47	0.44
2:K:804:ARG:NH2	2:K:817:GLU:OE2	2.46	0.44
2:K:937:ASN:HB3	2:K:954:GLU:O	2.17	0.44
1:M:2:THR:O	1:M:3:LEU:HD23	2.18	0.44
2:N:124:ARG:NH2	2:N:925:GLN:OE1	2.42	0.44
3:O:258:PHE:HB2	3:O:263:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:70:ASN:ND2	6:Q:5801:MD1:S12	2.90	0.44
1:S:6:ASN:OD1	1:S:8:HIS:N	2.50	0.44
1:S:41:CYS:SG	1:S:61:ASN:ND2	2.82	0.44
2:T:151:LEU:HA	2:T:151:LEU:HD23	1.75	0.44
2:T:861:ILE:HB	2:T:891:LYS:HA	1.99	0.44
2:T:909:TYR:HE2	2:T:980:ASN:HA	1.82	0.44
1:V:77:VAL:HG22	2:W:1138:PHE:HE1	1.82	0.44
1:V:116:ILE:HA	1:V:119:VAL:CG1	2.47	0.44
1:A:256:THR:HG22	1:A:259:MET:HG2	1.98	0.44
2:B:970:GLU:HG2	2:B:1118:VAL:CG2	2.47	0.44
1:D:65:THR:HG23	1:D:170:TYR:CE1	2.51	0.44
2:H:498:VAL:HG21	2:H:505:LYS:HB2	1.99	0.44
2:H:533:PHE:HB2	2:H:1100:GLU:HG3	1.98	0.44
2:H:648:VAL:HG13	2:H:676:GLN:HB2	1.98	0.44
2:H:661:LYS:HA	2:H:1057:GLN:OE1	2.17	0.44
2:H:813:GLU:O	2:H:819:LEU:HG	2.18	0.44
1:J:141:SER:HB3	2:K:938:ASN:O	2.16	0.44
2:N:89:VAL:CG1	2:N:119:TYR:HA	2.47	0.44
2:N:398:LYS:O	2:N:471:ILE:CD1	2.66	0.44
2:N:712:CYS:O	2:N:808:ARG:NH2	2.49	0.44
2:N:825:THR:OG1	2:N:829:GLN:NE2	2.45	0.44
1:P:284:ILE:HD13	1:P:304:TYR:CD2	2.52	0.44
2:T:284:HIS:CE1	2:T:286:LEU:HB3	2.53	0.44
1:V:262:CYS:HB3	1:V:346:ARG:HD2	1.99	0.44
1:V:263:VAL:HG21	2:W:315:PRO:HA	1.99	0.44
2:W:121:PHE:HZ	2:W:699:SER:HB2	1.82	0.44
2:W:381:THR:HG21	2:W:383:PHE:CD2	2.52	0.44
2:W:500:MET:HA	2:W:894:TRP:CZ2	2.52	0.44
2:W:995:PHE:O	2:W:998:VAL:HG22	2.17	0.44
1:A:175:CYS:HA	1:A:222:LYS:HG3	1.99	0.44
2:B:309:LEU:HD12	2:B:309:LEU:HA	1.81	0.44
1:D:8:HIS:CD2	1:D:292:PRO:CG	3.01	0.44
2:E:663:VAL:O	2:E:664:TYR:CA	2.66	0.44
2:E:927:ALA:O	2:E:933:PHE:CD1	2.71	0.44
2:H:117:LYS:HB3	2:H:926:TRP:CD2	2.52	0.44
2:H:1057:GLN:OE1	6:H:5801:MD1:N16	2.46	0.44
3:I:84:GLN:HE21	3:I:84:GLN:HB3	1.64	0.44
1:J:239:TYR:N	1:J:240:PRO:HD2	2.33	0.44
2:K:814:GLN:HB3	2:K:821:PHE:HE1	1.83	0.44
2:K:949:MET:HG2	2:K:954:GLU:OE1	2.18	0.44
3:L:164:LEU:O	3:L:236:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:LYS:HD3	1:M:222:LYS:HA	1.76	0.44
2:N:74:ALA:O	10:N:5902:HOH:O	2.21	0.44
2:N:91:GLN:OE1	2:N:119:TYR:OH	2.35	0.44
2:N:301:LEU:HD23	2:N:521:VAL:HG22	1.99	0.44
2:Q:496:SER:C	2:Q:500:MET:HG3	2.37	0.44
2:Q:642:MET:SD	2:Q:643:PRO:HD2	2.58	0.44
2:Q:803:PHE:CE1	2:Q:808:ARG:HD3	2.53	0.44
2:Q:943:TYR:HB3	3:R:188:TYR:HB3	1.98	0.44
1:S:373:PHE:CE2	1:S:375:MET:HB2	2.53	0.44
2:T:164:ARG:NH2	2:T:674:ILE:O	2.49	0.44
3:U:236:LEU:N	3:U:236:LEU:CD2	2.80	0.44
1:V:29:VAL:HA	1:V:304:TYR:O	2.17	0.44
2:W:914:VAL:O	2:W:1017:MET:HA	2.18	0.44
2:W:1119:TRP:CD2	2:W:1121:PRO:HD2	2.52	0.44
2:B:133:TYR:CD2	2:B:171:ARG:HG3	2.52	0.44
2:B:192:TYR:OH	2:B:675:GLU:OE2	2.19	0.44
2:B:393:LYS:HA	2:B:833:ASP:HB2	2.00	0.44
3:F:171:TRP:O	3:F:174:ASP:HB2	2.18	0.44
2:H:1056:GLN:HG2	2:H:1057:GLN:HG2	1.98	0.44
1:J:175:CYS:HA	1:J:222:LYS:HG3	2.00	0.44
2:K:70:ASN:OD1	2:K:923:HIS:CE1	2.70	0.44
3:L:303:GLY:CA	3:L:305:LYS:HD2	2.47	0.44
1:M:313:ARG:HA	1:M:313:ARG:HD3	1.87	0.44
2:Q:229:GLY:HA3	2:Q:237:TYR:CG	2.52	0.44
3:R:111:PHE:O	3:R:266:VAL:HA	2.18	0.44
2:T:382:ASP:HB3	2:T:481:LEU:HD23	2.00	0.44
2:W:70:ASN:ND2	2:W:228:MET:HG3	2.33	0.44
2:W:91:GLN:HG2	2:W:112:PRO:O	2.16	0.44
2:E:126:TYR:HB3	3:F:205:HIS:HD2	1.82	0.44
3:F:51:VAL:HG12	3:F:102:ALA:HB3	1.99	0.44
3:F:67:LEU:HD11	3:F:110:TYR:CE1	2.52	0.44
2:H:964:ALA:HB1	2:H:969:ILE:HB	1.99	0.44
3:I:51:VAL:HB	3:I:315:SER:O	2.17	0.44
1:J:33:ASN:OD1	1:J:308:PRO:HA	2.18	0.44
1:J:271:PHE:O	1:J:278:ASN:ND2	2.51	0.44
2:K:1024:ILE:O	2:K:1047:TYR:OH	2.22	0.44
2:N:123:ARG:NH1	2:N:930:ASP:OD1	2.51	0.44
1:P:90:TRP:CG	1:P:322:PRO:HG3	2.53	0.44
1:P:92:THR:O	1:P:95:LYS:HG2	2.17	0.44
1:P:239:TYR:N	1:P:240:PRO:HD2	2.33	0.44
3:R:130:PHE:CE2	3:R:299:GLU:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:302:ASN:CG	3:U:303:GLY:N	2.71	0.44
1:V:289:ILE:HG12	1:V:306:ILE:HG12	2.00	0.44
2:W:70:ASN:HA	2:W:231:LEU:HD21	1.99	0.44
2:W:372:TYR:CB	2:W:548:LEU:HB3	2.47	0.44
3:X:63:THR:HG23	3:X:66:ALA:H	1.82	0.44
1:A:141:SER:OG	2:B:938:ASN:O	2.22	0.44
2:B:834:GLU:HB2	2:B:837:ILE:HD12	1.99	0.44
1:D:134:PRO:HB2	1:D:139:TRP:NE1	2.33	0.44
1:D:190:LYS:HD3	2:E:40:PRO:HG3	1.98	0.44
2:E:995:PHE:HD2	2:E:999:SER:OG	2.01	0.44
3:F:305:LYS:NZ	8:F:401:HEM:C4B	2.86	0.44
1:G:34:ARG:CB	1:G:266:ILE:HG22	2.47	0.44
1:G:173:ARG:HH21	1:G:220:TYR:HB3	1.82	0.44
1:J:85:SER:O	10:J:601:HOH:O	2.21	0.44
1:J:212:ARG:HD2	1:J:225:TYR:CD1	2.53	0.44
1:J:266:ILE:HG13	1:J:267:ARG:HG3	2.00	0.44
1:M:229:THR:O	1:M:231:VAL:HG23	2.18	0.44
2:N:917:LYS:NZ	2:N:1020:HIS:ND1	2.65	0.44
2:Q:475:GLU:HG2	2:Q:475:GLU:O	2.18	0.44
3:R:155:MET:HE3	3:R:241:PHE:HA	2.00	0.44
2:W:1069:GLN:HE21	2:W:1094:ILE:HG12	1.82	0.44
1:A:276:PRO:HB3	1:A:286:HIS:CE1	2.52	0.44
1:D:45:CYS:SG	1:D:60:TRP:HB2	2.58	0.44
2:H:330:ILE:HB	2:H:344:ALA:HA	1.99	0.44
2:K:301:LEU:HD23	2:K:521:VAL:HG22	1.98	0.44
2:K:641:HIS:CE1	2:K:1087:PHE:HB2	2.53	0.44
2:K:851:PRO:O	2:K:858:PRO:HB3	2.18	0.44
1:M:9:LEU:HD22	1:M:111:TYR:CD2	2.53	0.44
1:M:208:CYS:SG	1:M:231:VAL:HG13	2.57	0.44
2:Q:115:CYS:CB	2:Q:314:MET:CE	2.89	0.44
2:Q:359:PHE:HB2	2:Q:541:SER:OG	2.17	0.44
1:S:34:ARG:HB3	1:S:266:ILE:HG22	2.00	0.44
2:T:181:ALA:HB2	2:T:693:PHE:CE2	2.52	0.44
2:T:1036:ARG:NH2	2:T:1040:ARG:HB3	2.33	0.44
3:U:84:GLN:NE2	3:U:89:PRO:O	2.51	0.44
1:V:16:PRO:HG2	1:V:128:TRP:CD1	2.38	0.44
2:W:44:TYR:CD1	2:W:45:PRO:HD2	2.52	0.44
2:W:69:PRO:HG2	2:W:71:ASP:HB2	2.00	0.44
2:B:189:THR:O	2:B:218:GLY:HA3	2.18	0.44
2:B:449:VAL:HG23	10:B:5919:HOH:O	2.18	0.44
1:D:230:ARG:NH1	3:F:182:GLU:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:995:PHE:CD2	2:E:999:SER:OG	2.71	0.44
3:F:137:MET:HG2	3:F:290:ASN:O	2.18	0.44
2:H:113:ARG:CG	2:H:315:PRO:HB2	2.48	0.44
3:I:51:VAL:HG11	3:I:316:LEU:HD22	2.00	0.44
1:J:150:LYS:HD3	1:J:167:TRP:HE1	1.83	0.44
2:K:69:PRO:O	2:K:70:ASN:HB3	2.18	0.44
2:K:270:TYR:HE2	2:K:276:GLN:HG3	1.82	0.44
2:K:397:PRO:HB3	2:K:404:TYR:CE1	2.53	0.44
2:K:445:THR:HG22	2:K:448:ASP:CG	2.38	0.44
2:N:67:CYS:HB2	2:N:77:ILE:HD12	1.99	0.44
2:N:525:TYR:CE2	2:N:561:THR:HB	2.53	0.44
2:N:613:GLU:HG3	2:N:615:ALA:H	1.82	0.44
3:O:303:GLY:C	3:O:305:LYS:CD	2.86	0.44
1:P:150:LYS:HD3	2:Q:1139:LEU:HD13	2.00	0.44
2:Q:150:GLU:H	2:Q:150:GLU:CD	2.20	0.44
2:Q:273:HIS:HB3	6:Q:5801:MD1:C13	2.48	0.44
1:S:36:ILE:CD1	2:T:317:ALA:HB3	2.46	0.44
2:T:271:THR:HG23	2:T:1090:ASP:HA	1.99	0.44
2:W:711:SER:HB3	2:W:714:ASN:OD1	2.17	0.44
2:W:882:TRP:HD1	2:W:883:GLU:OE2	2.01	0.44
3:X:123:GLN:HG2	3:X:125:ILE:HG13	2.00	0.44
3:X:162:VAL:HG12	3:X:238:ALA:O	2.18	0.44
1:A:123:LYS:HB2	1:A:125:ILE:CG2	2.48	0.43
1:A:365:GLU:HB2	1:A:374:THR:HG22	2.00	0.43
2:B:189:THR:O	2:B:193:SER:HB3	2.18	0.43
2:B:973:ASP:OD1	2:B:1111:GLY:N	2.44	0.43
2:B:1057:GLN:OE1	6:B:5801:MD1:N16	2.45	0.43
3:C:193:ASP:H	3:C:197:THR:HG1	1.59	0.43
3:F:136:LEU:HD12	3:F:267:PHE:CD2	2.52	0.43
3:I:154:ARG:CD	8:I:401:HEM:HBB2	2.46	0.43
3:I:171:TRP:CH2	3:I:234:GLU:HG3	2.53	0.43
1:J:263:VAL:HG13	2:K:315:PRO:HA	2.00	0.43
2:K:297:ARG:HA	2:K:323:VAL:HG12	2.00	0.43
2:K:334:THR:HB	2:K:347:TRP:HE1	1.83	0.43
3:L:163:ASN:OD1	3:L:278:ASP:HA	2.18	0.43
3:L:302:ASN:O	3:L:305:LYS:CE	2.55	0.43
3:O:241:PHE:CD2	3:O:241:PHE:O	2.70	0.43
3:O:303:GLY:CA	3:O:305:LYS:HD3	2.46	0.43
2:Q:97:ASN:O	2:Q:794:GLY:HA3	2.18	0.43
1:S:317:ARG:NH1	1:S:325:ASP:OD2	2.51	0.43
2:T:332:VAL:HG23	2:T:344:ALA:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:841:GLY:HA3	2:T:870:PRO:HB3	1.99	0.43
2:T:868:ILE:HG22	2:T:870:PRO:HD3	2.00	0.43
2:T:1121:PRO:O	2:T:1124:THR:OG1	2.28	0.43
1:V:5:HIS:O	1:V:180:TYR:OH	2.22	0.43
1:V:100:SER:OG	1:V:104:THR:CG2	2.64	0.43
1:A:255:GLU:HG2	1:A:351:ILE:HG12	1.99	0.43
1:A:410:ILE:HB	2:B:572:GLN:NE2	2.33	0.43
2:B:69:PRO:O	2:B:922:VAL:HG11	2.19	0.43
3:F:115:TRP:CD1	3:F:293:VAL:HG11	2.52	0.43
3:F:166:HIS:CD2	8:F:401:HEM:HMD3	2.53	0.43
3:F:269:ARG:HG2	3:F:270:SER:N	2.33	0.43
2:H:351:ARG:O	2:H:354:THR:OG1	2.34	0.43
3:I:321:TRP:C	3:I:322:GLN:OXT	2.57	0.43
1:J:209:ARG:NH1	3:L:234:GLU:OE1	2.51	0.43
2:K:110:TRP:CZ3	2:K:316:GLU:OE1	2.62	0.43
2:K:225:ARG:NE	2:K:269:ASN:OD1	2.52	0.43
2:K:290:ASP:OD2	2:K:712:CYS:HB2	2.17	0.43
1:M:4:VAL:HG21	1:M:180:TYR:CE1	2.53	0.43
2:N:803:PHE:CG	2:N:808:ARG:HG3	2.53	0.43
2:N:1057:GLN:HE22	6:N:5801:MD1:C17	2.31	0.43
1:P:149:ALA:O	2:Q:1009:PRO:HG2	2.18	0.43
2:Q:469:LYS:HA	2:Q:475:GLU:HA	2.01	0.43
2:T:190:LYS:HA	2:T:193:SER:OG	2.17	0.43
2:T:977:VAL:HG12	2:T:1059:ILE:HG21	2.00	0.43
2:T:1065:MET:SD	2:T:1065:MET:N	2.91	0.43
3:U:51:VAL:HG21	3:U:316:LEU:HG	1.99	0.43
2:W:132:ARG:NH2	3:X:200:HIS:CE1	2.86	0.43
2:W:872:ASP:O	2:W:875:ILE:HG22	2.19	0.43
1:A:22:PRO:HG3	1:A:194:LYS:HE3	2.00	0.43
2:B:674:ILE:HB	2:B:677:ILE:HD11	2.00	0.43
2:E:914:VAL:O	2:E:1017:MET:HA	2.18	0.43
3:I:53:TYR:HE1	3:I:319:ILE:HA	1.71	0.43
3:I:84:GLN:NE2	3:I:89:PRO:O	2.50	0.43
1:J:262:CYS:HA	4:J:503:SF4:S3	2.58	0.43
2:K:824:PRO:HG3	2:K:1074:PHE:HB3	2.00	0.43
1:M:8:HIS:CE1	1:M:300:GLU:HG2	2.53	0.43
3:O:241:PHE:HB2	8:O:401:HEM:CMA	2.48	0.43
1:P:334:PRO:HG2	2:Q:325:GLU:O	2.18	0.43
2:Q:230:LEU:HD11	2:Q:710:ASN:OD1	2.18	0.43
2:Q:776:GLY:H	2:Q:781:LYS:HZ1	1.67	0.43
3:R:63:THR:HG23	3:R:66:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:39:GLN:NE2	1:S:63:VAL:HB	2.32	0.43
2:T:293:MET:HE1	2:T:313:LYS:HB3	1.99	0.43
1:V:283:LEU:HD11	1:V:341:VAL:HG11	1.99	0.43
1:V:402:ARG:HD2	2:W:803:PHE:O	2.16	0.43
2:W:1023:TRP:HE3	2:W:1047:TYR:CD1	2.36	0.43
1:A:21:ARG:HE	1:A:179:THR:HG21	1.83	0.43
2:B:213:ARG:NH1	2:B:610:LEU:HD21	2.34	0.43
2:B:311:GLU:HG2	2:B:919:ARG:NH2	2.33	0.43
2:B:856:TYR:HB3	2:B:900:THR:OG1	2.17	0.43
1:D:225:TYR:HA	1:D:232:SER:HA	2.00	0.43
2:E:49:TRP:O	2:E:52:VAL:HG22	2.18	0.43
2:E:959:ILE:HD13	2:E:1016:THR:CG2	2.45	0.43
2:E:1014:ASN:ND2	2:E:1014:ASN:N	2.64	0.43
2:H:915:THR:HA	2:H:1018:MET:O	2.19	0.43
3:I:53:TYR:HE1	3:I:319:ILE:CG2	2.26	0.43
1:J:263:VAL:HG21	2:K:114:MET:O	2.19	0.43
2:K:261:ALA:O	2:K:608:ARG:HD3	2.18	0.43
2:K:273:HIS:HB3	6:K:5801:MD1:S13	2.59	0.43
2:K:303:ILE:HB	2:K:523:ILE:HD13	2.01	0.43
3:L:199:PRO:CB	2:N:632:GLY:HA3	2.48	0.43
2:N:139:GLY:O	2:N:159:TYR:HB3	2.18	0.43
1:P:190:LYS:HB3	2:Q:40:PRO:HG3	2.01	0.43
2:Q:542:TYR:N	2:Q:542:TYR:CD2	2.85	0.43
1:S:38:CYS:HB3	2:T:314:MET:HE2	1.99	0.43
1:S:149:ALA:O	2:T:1009:PRO:HG2	2.19	0.43
1:S:239:TYR:N	1:S:240:PRO:HD2	2.34	0.43
2:T:143:TRP:CD1	2:T:149:PRO:HD2	2.54	0.43
2:T:753:ARG:HA	2:T:756:ASP:CB	2.47	0.43
2:T:1074:PHE:HB2	2:T:1085:PHE:CE1	2.54	0.43
1:V:213:LYS:CD	3:X:301:ARG:HH21	2.27	0.43
1:V:272:LEU:HD23	1:V:272:LEU:HA	1.93	0.43
1:V:310:TRP:CE2	2:W:342:GLN:HG3	2.54	0.43
1:V:353:TYR:HD2	1:V:384:GLY:HA2	1.83	0.43
2:W:113:ARG:O	2:W:113:ARG:HG2	2.19	0.43
2:W:300:LYS:CG	2:W:520:PRO:HD3	2.48	0.43
2:W:386:LEU:HD22	2:W:478:VAL:HG23	2.00	0.43
2:W:937:ASN:HB3	2:W:954:GLU:O	2.19	0.43
1:A:277:LYS:HB3	1:A:354:GLU:HG3	1.99	0.43
2:B:984:ARG:NH1	2:B:1061:ARG:HB3	2.33	0.43
1:D:66:LYS:O	1:D:168:PHE:HB2	2.19	0.43
2:E:182:SER:O	2:E:185:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:920:HIS:N	2:E:920:HIS:ND1	2.66	0.43
1:G:2:THR:HG21	1:G:18:PHE:CD2	2.53	0.43
2:K:121:PHE:HZ	2:K:699:SER:HB2	1.83	0.43
2:K:616:TYR:CG	2:K:643:PRO:HG3	2.53	0.43
2:K:917:LYS:HE2	2:K:923:HIS:CD2	2.53	0.43
3:L:58:VAL:HG21	3:L:62:ILE:HG23	2.00	0.43
1:M:178:CYS:HB3	1:M:299:THR:O	2.19	0.43
2:N:386:LEU:HD12	2:N:432:VAL:HG12	2.01	0.43
2:N:706:PHE:CD1	2:N:721:GLY:HA3	2.53	0.43
2:Q:225:ARG:HE	2:Q:227:GLY:HA2	1.84	0.43
2:Q:307:LYS:NZ	2:Q:313:LYS:HZ1	2.15	0.43
3:U:31:ALA:HB3	3:U:34:VAL:HG22	2.00	0.43
1:V:9:LEU:HD11	1:V:298:GLY:HA2	2.00	0.43
1:V:252:ARG:NH2	1:V:386:ASP:OD1	2.49	0.43
2:W:91:GLN:HG3	2:W:114:MET:SD	2.59	0.43
3:X:49:LEU:HD13	3:X:77:VAL:HG13	2.00	0.43
3:X:56:ILE:HD12	3:X:105:ASP:HB3	2.00	0.43
1:A:149:ALA:O	2:B:1009:PRO:HG2	2.17	0.43
2:B:861:ILE:HB	2:B:891:LYS:HA	2.00	0.43
1:D:71:PHE:HB2	1:D:142:PRO:HA	2.01	0.43
1:D:377:ASN:O	1:D:377:ASN:ND2	2.51	0.43
2:E:577:SER:O	2:E:776:GLY:HA2	2.18	0.43
2:H:297:ARG:HA	2:H:323:VAL:HG12	1.99	0.43
2:K:355:ASP:OD2	6:K:5802:MD1:N2	2.51	0.43
2:N:95:HIS:NE2	2:N:113:ARG:HD3	2.34	0.43
2:N:232:GLY:O	2:N:236:LYS:HB2	2.18	0.43
2:N:837:ILE:HG13	2:N:1070:LEU:HD21	2.00	0.43
2:N:983:ASP:HB3	2:N:984:ARG:HD3	2.01	0.43
3:O:110:TYR:HA	3:O:267:PHE:O	2.18	0.43
1:P:24:HIS:HB2	1:P:271:PHE:HB3	2.01	0.43
1:P:34:ARG:NH1	1:P:342:MET:HB3	2.34	0.43
1:P:107:PRO:CG	1:P:285:ARG:HH11	2.25	0.43
2:Q:284:HIS:CE1	2:Q:286:LEU:HB3	2.54	0.43
2:Q:425:ARG:NH2	2:Q:430:ASP:OD1	2.52	0.43
2:Q:723:THR:O	2:Q:723:THR:OG1	2.29	0.43
3:R:136:LEU:HG	3:R:267:PHE:CE2	2.54	0.43
2:T:223:LYS:HG2	2:T:267:TRP:CE2	2.53	0.43
3:U:231:ARG:NH2	3:U:250:GLN:HB2	2.34	0.43
3:U:236:LEU:HA	3:U:247:GLN:HG3	2.00	0.43
1:V:366:THR:HG23	1:V:367:GLU:N	2.34	0.43
2:B:554:TYR:O	2:B:809:HIS:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:923:HIS:O	2:B:1021:SER:CB	2.59	0.43
2:B:1022:ALA:HB3	2:B:1051:PHE:CZ	2.53	0.43
3:C:137:MET:HG2	3:C:290:ASN:HB3	1.99	0.43
1:D:115:THR:HB	1:D:297:PHE:O	2.19	0.43
1:D:211:TYR:O	3:F:301:ARG:NE	2.48	0.43
2:E:63:PHE:CD2	2:E:724:GLY:HA2	2.54	0.43
2:E:664:TYR:CZ	2:E:1054:GLY:O	2.71	0.43
2:E:849:GLU:O	2:E:859:ASN:CA	2.66	0.43
1:G:9:LEU:HD22	1:G:111:TYR:CD2	2.54	0.43
1:G:410:ILE:HB	2:H:572:GLN:HE21	1.82	0.43
2:H:1021:SER:OG	2:H:1022:ALA:N	2.52	0.43
3:I:168:LYS:HD2	3:I:171:TRP:CE2	2.54	0.43
2:K:492:TYR:OH	2:K:847:HIS:HB3	2.19	0.43
2:N:121:PHE:HZ	2:N:699:SER:HB2	1.83	0.43
2:N:579:PRO:HB3	2:N:605:ILE:HG13	2.01	0.43
3:O:168:LYS:HD2	3:O:171:TRP:CE2	2.53	0.43
1:P:348:THR:OG1	1:P:349:GLN:N	2.51	0.43
1:P:364:PHE:CZ	2:Q:300:LYS:HD2	2.54	0.43
2:Q:143:TRP:CE2	2:Q:151:LEU:HD11	2.54	0.43
2:Q:271:THR:HB	2:Q:1094:ILE:O	2.19	0.43
2:Q:376:TYR:CD2	2:Q:550:GLY:HA2	2.53	0.43
2:Q:388:ARG:CG	2:Q:476:ILE:HD12	2.48	0.43
2:Q:616:TYR:CZ	2:Q:1094:ILE:HD11	2.53	0.43
1:S:346:ARG:HA	1:S:346:ARG:NE	2.34	0.43
2:T:252:HIS:NE2	2:T:751:ASP:OD1	2.41	0.43
2:T:448:ASP:OD1	2:T:456:LYS:NZ	2.38	0.43
3:U:41:GLU:O	10:U:502:HOH:O	2.21	0.43
1:V:259:MET:CE	1:V:269:GLN:HB2	2.48	0.43
1:V:393:THR:OG1	2:W:109:ASN:OD1	2.27	0.43
2:W:36:VAL:HG11	3:X:158:ARG:HE	1.82	0.43
2:W:265:ARG:NH1	2:W:610:LEU:HD23	2.33	0.43
3:X:130:PHE:HE1	3:X:301:ARG:HD3	1.82	0.43
3:X:155:MET:HG2	8:X:401:HEM:NC	2.34	0.43
2:B:680:THR:HG22	6:B:5801:MD1:N2	2.34	0.43
2:B:1021:SER:H	2:B:1056:GLN:NE2	2.17	0.43
2:E:75:CYS:SG	2:E:114:MET:HA	2.59	0.43
2:E:964:ALA:HB3	2:E:1007:TYR:CE1	2.51	0.43
2:E:1063:TRP:N	2:E:1096:THR:CG2	2.74	0.43
2:H:91:GLN:NE2	2:H:114:MET:HB2	2.33	0.43
2:H:252:HIS:NE2	2:H:751:ASP:OD1	2.38	0.43
2:H:321:THR:O	2:H:324:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:661:LYS:HD3	2:H:661:LYS:N	2.34	0.43
2:H:948:ARG:NH1	2:H:1112:GLY:O	2.52	0.43
2:K:116:LEU:HG	2:K:117:LYS:N	2.33	0.43
2:K:476:ILE:HD13	2:K:478:VAL:HG23	2.00	0.43
2:N:365:ILE:HD11	2:N:494:ILE:HD13	2.00	0.43
1:P:408:ASN:OD1	2:Q:804:ARG:N	2.48	0.43
2:Q:332:VAL:HG21	2:Q:341:ALA:HA	2.00	0.43
1:S:196:LYS:HB2	1:S:196:LYS:HE3	1.77	0.43
1:S:409:SER:O	1:S:409:SER:OG	2.31	0.43
2:T:230:LEU:HD11	2:T:710:ASN:OD1	2.18	0.43
3:U:287:THR:CG2	3:U:314:LEU:HD23	2.49	0.43
1:V:8:HIS:HE1	1:V:301:PRO:O	2.01	0.43
1:V:11:ARG:NH2	1:V:113:GLY:O	2.52	0.43
1:V:77:VAL:HG21	2:W:1126:TYR:CD1	2.53	0.43
1:V:78:LYS:HD3	1:V:132:TYR:CZ	2.54	0.43
1:V:209:ARG:HH12	3:X:234:GLU:CD	2.22	0.43
2:W:397:PRO:HB2	2:W:404:TYR:CD2	2.53	0.43
3:X:95:VAL:HG22	3:X:306:ASN:ND2	2.34	0.43
2:E:663:VAL:O	2:E:664:TYR:HA	2.19	0.43
2:E:957:ILE:CB	2:E:1003:LEU:HD11	2.49	0.43
3:F:71:PHE:CE2	3:F:112:GLN:HB2	2.53	0.43
1:G:9:LEU:HD22	1:G:111:TYR:HB3	2.00	0.43
1:G:48:THR:HG1	1:G:257:ARG:HH11	1.66	0.43
1:G:149:ALA:HA	1:G:168:PHE:HB3	2.01	0.43
1:G:302:ASN:HA	1:G:304:TYR:CE1	2.54	0.43
2:H:125:VAL:HG21	2:H:701:VAL:HG21	2.01	0.43
2:H:223:LYS:HG2	2:H:267:TRP:CE2	2.54	0.43
2:H:430:ASP:HB3	2:H:444:ILE:O	2.19	0.43
3:I:49:LEU:HD13	3:I:77:VAL:HG23	1.99	0.43
1:M:36:ILE:HD12	2:N:314:MET:HB2	2.01	0.43
1:M:212:ARG:CZ	3:O:130:PHE:CE2	3.02	0.43
1:M:263:VAL:HG21	2:N:114:MET:O	2.18	0.43
2:N:120:THR:HG22	2:N:931:TRP:CE3	2.49	0.43
2:N:425:ARG:HG2	2:N:425:ARG:HH11	1.83	0.43
2:N:434:TRP:HD1	2:N:461:VAL:HG21	1.83	0.43
2:N:814:GLN:H	2:N:814:GLN:HG2	1.48	0.43
1:P:309:ARG:NH1	2:Q:324:MET:HB2	2.34	0.43
1:S:37:ALA:HB3	2:T:919:ARG:NH2	2.34	0.43
2:T:47:ARG:HE	2:T:47:ARG:HB3	1.52	0.43
1:V:36:ILE:CG1	2:W:310:ILE:HG23	2.44	0.43
1:V:82:LEU:HB3	1:V:130:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:208:CYS:HB3	1:V:231:VAL:HG13	2.01	0.43
2:W:276:GLN:O	2:W:1095:ASN:ND2	2.52	0.43
2:B:716:PHE:N	2:B:716:PHE:CD1	2.85	0.43
2:B:788:ILE:HG12	2:B:799:ALA:HB2	2.01	0.43
2:B:977:VAL:HG23	2:B:1001:LEU:HG	1.99	0.43
1:D:226:ARG:NH1	3:F:216:SER:OG	2.52	0.43
2:E:67:CYS:HB2	2:E:77:ILE:HD11	2.01	0.43
2:E:272:TRP:HH2	2:E:618:ASN:HB2	1.80	0.43
3:F:201:SER:HB2	3:F:206:LYS:HE3	2.01	0.43
2:H:525:TYR:CE2	2:H:561:THR:HB	2.54	0.43
2:H:709:THR:CG2	2:H:718:GLN:HB2	2.41	0.43
2:K:1069:GLN:CD	2:K:1094:ILE:HD11	2.39	0.43
1:M:132:TYR:O	1:M:221:LYS:HE3	2.19	0.43
1:M:149:ALA:HB2	1:M:168:PHE:CD2	2.42	0.43
1:M:151:SER:OG	1:M:157:GLU:OE1	2.35	0.43
2:N:113:ARG:NH1	2:N:714:ASN:ND2	2.66	0.43
2:N:305:THR:O	6:N:5802:MD1:N2	2.50	0.43
1:P:410:ILE:HA	2:Q:1076:LYS:NZ	2.34	0.43
2:Q:72:THR:CG2	2:Q:713:SER:CB	2.97	0.43
2:Q:929:THR:O	2:Q:933:PHE:N	2.48	0.43
2:Q:951:GLY:CA	2:Q:1048:GLN:NE2	2.82	0.43
3:R:165:TRP:HE3	3:R:267:PHE:HD2	1.67	0.43
1:S:63:VAL:HG21	4:S:503:SF4:S4	2.59	0.43
2:T:100:ASP:OD1	2:T:104:ASN:N	2.51	0.43
2:T:333:ILE:O	6:T:5802:MD1:N2	2.50	0.43
2:T:1132:ASN:H	2:T:1135:MET:HB3	1.83	0.43
1:V:149:ALA:CB	1:V:168:PHE:HD2	2.16	0.43
2:W:232:GLY:O	2:W:236:LYS:HB2	2.19	0.43
2:W:1076:LYS:NZ	2:W:1080:GLY:O	2.52	0.43
2:B:449:VAL:HA	10:B:5919:HOH:O	2.18	0.42
2:B:462:LEU:HB3	2:B:482:LEU:HD13	2.01	0.42
2:B:894:TRP:HA	2:B:897:THR:OG1	2.19	0.42
3:C:48:VAL:HG22	3:C:313:PRO:HB2	1.99	0.42
1:G:239:TYR:N	1:G:240:PRO:HD2	2.34	0.42
2:H:271:THR:HG1	2:H:1093:CYS:HG	1.64	0.42
2:H:760:PHE:HB3	2:H:765:ARG:O	2.19	0.42
2:H:882:TRP:CD1	2:H:1061:ARG:NH2	2.87	0.42
2:K:360:LEU:HD13	2:K:492:TYR:CE1	2.54	0.42
6:K:5802:MD1:N15	6:K:5802:MD1:O11	2.52	0.42
1:M:52:ASN:ND2	3:O:215:LEU:HA	2.34	0.42
1:M:356:LYS:HD3	1:M:383:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:625:ILE:HG12	2:N:635:VAL:HG22	2.00	0.42
3:O:33:GLY:O	3:O:88:PHE:N	2.52	0.42
1:P:48:THR:OG1	1:P:257:ARG:NH2	2.51	0.42
1:P:148:THR:HA	2:Q:1008:ASN:OD1	2.19	0.42
2:Q:91:GLN:HG2	2:Q:113:ARG:O	2.19	0.42
2:Q:361:GLY:HA3	2:Q:497:VAL:HG11	2.01	0.42
2:Q:404:TYR:CE2	2:Q:406:LEU:HD23	2.49	0.42
3:R:155:MET:HE1	8:R:401:HEM:C1A	2.54	0.42
1:S:30:PHE:HB2	1:S:305:TYR:CD2	2.54	0.42
2:W:282:PHE:HB3	2:W:832:ASN:ND2	2.34	0.42
2:W:699:SER:O	2:W:703:PHE:CD1	2.71	0.42
1:A:11:ARG:NH2	1:A:113:GLY:O	2.52	0.42
2:B:71:ASP:OD2	2:B:73:HIS:HD2	2.02	0.42
1:D:222:LYS:HB2	4:D:502:SF4:S2	2.59	0.42
2:E:55:ASP:O	2:E:58:GLN:NE2	2.49	0.42
2:E:253:ASN:C	2:E:253:ASN:OD1	2.57	0.42
3:F:155:MET:CG	8:F:401:HEM:C1C	3.02	0.42
1:G:80:LEU:HD11	1:G:294:TYR:CE1	2.54	0.42
2:H:901:LYS:HD2	2:H:906:GLU:OE2	2.18	0.42
3:I:155:MET:HE2	3:I:155:MET:HB2	1.93	0.42
3:I:237:ASN:HD22	3:I:237:ASN:HA	1.55	0.42
1:J:337:GLU:OE2	1:J:355:TYR:OH	2.30	0.42
2:K:307:LYS:NZ	2:K:313:LYS:HE2	2.34	0.42
2:K:903:PHE:CE2	2:K:904:LEU:HG	2.54	0.42
2:N:480:THR:HG23	2:N:483:GLU:H	1.83	0.42
2:N:848:ARG:NH1	2:N:859:ASN:OD1	2.52	0.42
1:P:170:TYR:OH	2:Q:339:PRO:HB3	2.19	0.42
2:Q:467:LYS:C	2:Q:468:LEU:HD23	2.39	0.42
2:Q:962:GLN:N	2:Q:965:ARG:HH11	2.17	0.42
3:R:91:GLY:HA3	3:R:304:GLN:HA	2.00	0.42
2:T:152:THR:HG23	2:T:153:PRO:HD2	2.01	0.42
2:T:657:ILE:O	2:T:663:VAL:HG23	2.19	0.42
3:U:193:ASP:H	3:U:197:THR:HB	1.84	0.42
2:W:301:LEU:HD23	2:W:521:VAL:HG22	2.02	0.42
1:A:410:ILE:HD11	2:B:803:PHE:CE1	2.53	0.42
2:B:249:VAL:HG13	2:B:749:LEU:HD11	2.01	0.42
2:B:446:ARG:HH11	2:B:446:ARG:HG2	1.84	0.42
2:B:717:ILE:HD11	2:B:801:LEU:HB3	2.01	0.42
2:E:123:ARG:HD2	2:E:931:TRP:CD2	2.54	0.42
1:G:65:THR:HG21	1:G:147:ASP:H	1.83	0.42
1:G:408:ASN:OD1	2:H:803:PHE:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:296:VAL:HG11	2:K:320:VAL:HG22	2.00	0.42
2:N:301:LEU:HB3	2:N:521:VAL:HG22	2.01	0.42
2:Q:68:SER:C	2:Q:231:LEU:HD12	2.40	0.42
2:T:225:ARG:NH1	2:T:656:LEU:HD12	2.34	0.42
2:T:228:MET:HB3	2:T:231:LEU:HD23	2.02	0.42
2:T:710:ASN:HB2	2:T:801:LEU:HD11	2.01	0.42
1:V:30:PHE:CE1	1:V:267:ARG:HG2	2.55	0.42
2:W:986:TYR:CE2	2:W:989:TRP:HA	2.55	0.42
1:A:190:LYS:HB3	2:B:40:PRO:HG3	2.00	0.42
2:B:121:PHE:O	2:B:125:VAL:HG23	2.19	0.42
2:B:445:THR:HG23	2:B:447:ASP:H	1.83	0.42
2:B:661:LYS:HZ3	2:B:1098:PRO:HG3	1.83	0.42
2:B:661:LYS:HE2	6:B:5801:MD1:N8	2.34	0.42
2:B:912:TYR:HA	2:B:1102:LEU:HD23	2.00	0.42
2:B:963:ALA:O	2:B:967:LEU:HD12	2.19	0.42
1:D:188:PRO:HG2	1:D:189:ARG:H	1.84	0.42
1:D:258:CYS:HB3	4:D:501:SF4:S2	2.59	0.42
2:E:177:ALA:HB1	2:E:695:PHE:CE2	2.53	0.42
2:E:958:HIS:O	2:E:1016:THR:HA	2.19	0.42
2:E:1033:HIS:CE1	2:E:1052:ARG:CD	3.02	0.42
2:E:1087:PHE:HA	2:E:1092:HIS:O	2.20	0.42
2:H:923:HIS:O	2:H:1021:SER:HA	2.20	0.42
2:K:34:ALA:HB1	3:L:243:THR:HG22	2.01	0.42
2:K:99:SER:HB3	2:K:105:LYS:HG2	2.01	0.42
2:K:231:LEU:HD22	2:K:653:ASN:ND2	2.34	0.42
1:M:179:THR:HA	1:M:194:LYS:HZ1	1.85	0.42
2:N:229:GLY:HA3	2:N:237:TYR:CG	2.54	0.42
2:N:852:GLU:OE2	2:N:984:ARG:NH1	2.51	0.42
2:Q:547:MET:HE3	2:Q:830:ALA:HB2	2.01	0.42
2:Q:707:GLU:O	2:Q:719:ILE:HA	2.20	0.42
2:T:94:ASP:OD2	2:T:94:ASP:N	2.47	0.42
2:T:229:GLY:HA3	2:T:237:TYR:CG	2.55	0.42
2:T:554:TYR:O	2:T:557:SER:OG	2.29	0.42
1:V:58:MET:HB3	1:V:58:MET:HE2	1.94	0.42
2:W:35:VAL:HG22	3:X:245:THR:CG2	2.49	0.42
2:W:359:PHE:HA	2:W:362:ILE:CG2	2.48	0.42
2:B:115:CYS:SG	2:B:117:LYS:HE2	2.60	0.42
2:B:278:PRO:HD2	2:B:539:ASN:OD1	2.19	0.42
2:B:425:ARG:HH21	2:B:425:ARG:HD2	1.67	0.42
1:D:7:TRP:CD1	1:D:103:GLY:HA2	2.54	0.42
1:D:259:MET:HE1	1:D:269:GLN:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:PHE:CZ	2:E:324:MET:HG3	2.54	0.42
2:E:979:ALA:CB	2:E:1103:VAL:HA	2.50	0.42
2:H:36:VAL:CG1	3:I:243:THR:HG21	2.40	0.42
2:H:449:VAL:HG21	2:H:820:PRO:HA	2.01	0.42
2:K:232:GLY:O	2:K:236:LYS:HB2	2.19	0.42
1:M:268:LEU:HD22	1:M:345:PHE:CE1	2.55	0.42
2:N:309:LEU:HD23	2:N:320:VAL:HG21	2.02	0.42
2:Q:61:ARG:HB3	2:Q:81:VAL:HB	2.01	0.42
2:Q:505:LYS:HA	2:Q:508:ILE:HG12	2.01	0.42
3:U:35:LYS:HD3	3:U:85:ASP:O	2.19	0.42
3:X:95:VAL:HG12	3:X:116:ASP:O	2.20	0.42
2:B:543:TYR:HA	2:B:546:VAL:HG12	2.00	0.42
2:B:923:HIS:NE2	6:B:5802:MD1:S13	2.91	0.42
2:B:983:ASP:HB3	2:B:984:ARG:CD	2.45	0.42
2:B:984:ARG:NH1	2:B:1061:ARG:CB	2.83	0.42
1:D:65:THR:HB	1:D:145:GLY:O	2.20	0.42
1:D:346:ARG:CZ	1:D:346:ARG:HA	2.49	0.42
2:E:140:TRP:CZ3	2:E:693:PHE:CD1	3.08	0.42
2:E:353:ASN:HD22	2:E:353:ASN:HA	1.66	0.42
2:E:527:GLU:OE2	2:E:527:GLU:N	2.53	0.42
3:F:51:VAL:HG12	3:F:102:ALA:CB	2.49	0.42
3:F:95:VAL:HG11	3:F:115:TRP:HD1	1.85	0.42
3:F:275:ASP:HB3	3:F:278:ASP:OD2	2.19	0.42
1:G:315:TYR:O	1:G:318:GLN:HG2	2.20	0.42
2:H:284:HIS:CE1	2:H:286:LEU:HB3	2.55	0.42
2:H:351:ARG:CZ	2:H:354:THR:HG21	2.50	0.42
2:H:974:TYR:CE1	2:H:1004:ARG:HD3	2.55	0.42
3:I:218:GLY:O	3:I:223:ASN:N	2.45	0.42
2:K:91:GLN:HG2	2:K:112:PRO:HB2	2.01	0.42
2:K:814:GLN:NE2	10:K:5918:HOH:O	2.52	0.42
2:N:404:TYR:C	2:N:405:LYS:HD2	2.40	0.42
2:N:930:ASP:OD2	2:N:931:TRP:N	2.52	0.42
2:N:937:ASN:ND2	2:N:954:GLU:H	2.18	0.42
3:O:51:VAL:HG12	3:O:104:HIS:HD2	1.83	0.42
2:Q:77:ILE:HG23	2:Q:114:MET:CE	2.50	0.42
2:Q:238:GLY:C	2:Q:738:LEU:HD21	2.40	0.42
2:Q:309:LEU:HD13	2:Q:320:VAL:HG21	2.01	0.42
2:Q:357:ALA:HB1	2:Q:500:MET:SD	2.59	0.42
2:Q:430:ASP:HB3	2:Q:444:ILE:O	2.18	0.42
2:Q:821:PHE:N	2:Q:821:PHE:CD1	2.87	0.42
3:R:300:ASP:HA	3:R:304:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:173:SER:OG	2:T:176:GLU:HB2	2.20	0.42
2:T:759:LYS:O	2:T:763:GLU:HG3	2.19	0.42
2:T:1119:TRP:CD2	2:T:1121:PRO:HD2	2.55	0.42
1:V:65:THR:HG21	1:V:147:ASP:HA	2.02	0.42
2:W:332:VAL:HG21	2:W:341:ALA:HA	2.01	0.42
2:W:415:TYR:HD1	2:W:420:LEU:HB3	1.85	0.42
2:B:73:HIS:CG	2:B:315:PRO:HG2	2.55	0.42
2:B:662:HIS:CE1	2:B:665:GLN:HB2	2.54	0.42
2:B:882:TRP:CD1	2:B:1061:ARG:NH2	2.88	0.42
2:E:917:LYS:CE	2:E:923:HIS:HD2	2.33	0.42
2:H:190:LYS:HA	2:H:193:SER:HB2	2.02	0.42
2:H:654:VAL:HG23	6:H:5801:MD1:O2B	2.19	0.42
3:I:53:TYR:HE1	3:I:319:ILE:CB	2.33	0.42
1:J:238:CYS:HB3	1:J:241:ARG:HD3	2.01	0.42
2:K:980:ASN:CB	2:K:984:ARG:HH21	2.32	0.42
3:L:168:LYS:HD2	3:L:171:TRP:CE2	2.54	0.42
2:N:503:SER:HB2	2:N:508:ILE:HD11	2.01	0.42
1:P:189:ARG:HH21	1:P:207:ARG:HB3	1.84	0.42
1:P:373:PHE:CZ	1:P:375:MET:HB2	2.54	0.42
2:Q:866:PRO:O	2:Q:869:ARG:HD2	2.19	0.42
2:T:278:PRO:HD2	2:T:539:ASN:OD1	2.19	0.42
2:T:301:LEU:HB3	2:T:521:VAL:HG22	2.01	0.42
2:T:423:GLU:H	2:T:423:GLU:HG3	1.60	0.42
3:U:142:LYS:NZ	10:U:507:HOH:O	2.52	0.42
3:U:301:ARG:HH21	3:U:301:ARG:CG	2.32	0.42
1:V:121:LYS:O	1:V:124:ASN:OD1	2.38	0.42
2:W:803:PHE:CD2	2:W:808:ARG:HB2	2.55	0.42
2:W:983:ASP:CG	2:W:984:ARG:HH21	2.23	0.42
3:X:302:ASN:CG	3:X:303:GLY:N	2.73	0.42
1:A:198:ASP:N	1:A:198:ASP:OD1	2.50	0.42
2:B:34:ALA:HB1	3:C:243:THR:HG22	2.02	0.42
2:B:789:LEU:HD23	2:B:789:LEU:HA	1.91	0.42
3:C:120:ASP:OD2	3:C:120:ASP:N	2.45	0.42
2:E:194:GLY:O	2:E:195:PRO:C	2.58	0.42
3:F:71:PHE:HE2	3:F:266:VAL:HG11	1.84	0.42
3:F:162:VAL:HG22	3:F:238:ALA:O	2.20	0.42
3:F:241:PHE:HB2	8:F:401:HEM:HMA2	2.01	0.42
1:G:25:GLN:CD	1:G:302:ASN:HD22	2.23	0.42
2:H:537:LEU:HD13	2:H:846:VAL:O	2.19	0.42
2:K:229:GLY:HA3	2:K:237:TYR:CD1	2.55	0.42
2:K:811:PHE:HA	2:K:814:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:814:GLN:HB3	2:K:821:PHE:CE1	2.55	0.42
2:K:964:ALA:HB1	2:K:969:ILE:HB	2.01	0.42
1:M:53:LYS:O	1:M:226:ARG:NH2	2.39	0.42
1:M:76:ASP:OD1	1:M:76:ASP:N	2.53	0.42
1:M:395:VAL:O	2:N:326:ARG:NH2	2.49	0.42
2:N:752:LYS:HE3	2:N:756:ASP:OD2	2.19	0.42
2:N:923:HIS:NE2	6:N:5801:MD1:S12	2.93	0.42
3:O:305:LYS:HE3	8:O:401:HEM:NB	2.27	0.42
1:P:63:VAL:HG21	4:P:503:SF4:S4	2.59	0.42
2:Q:209:GLU:OE2	2:Q:633:ARG:NH1	2.52	0.42
2:Q:1065:MET:SD	2:Q:1065:MET:N	2.93	0.42
1:S:315:TYR:O	1:S:318:GLN:HG2	2.19	0.42
2:T:692:ASP:C	2:T:693:PHE:HD1	2.23	0.42
1:V:11:ARG:NH2	1:V:118:GLU:OE2	2.53	0.42
1:V:13:MET:HE3	1:V:13:MET:HB3	1.68	0.42
1:V:65:THR:HG23	1:V:170:TYR:HE1	1.85	0.42
1:V:260:SER:HA	1:V:346:ARG:CZ	2.50	0.42
2:W:286:LEU:HD23	2:W:287:GLN:H	1.83	0.42
2:W:811:PHE:HA	2:W:814:GLN:OE1	2.19	0.42
3:X:117:ASP:O	3:X:261:LYS:O	2.37	0.42
1:A:245:ARG:CD	2:B:54:ARG:HD3	2.49	0.42
2:B:210:MET:SD	2:B:623:PRO:HD3	2.60	0.42
2:B:286:LEU:HD23	2:B:287:GLN:N	2.35	0.42
2:B:717:ILE:O	2:B:798:VAL:HA	2.20	0.42
2:B:913:CYS:HB2	2:B:1103:VAL:HG23	2.01	0.42
2:B:913:CYS:CB	2:B:1103:VAL:CG2	2.97	0.42
2:B:967:LEU:HD22	2:B:1105:ILE:O	2.19	0.42
2:B:1070:LEU:HB2	2:B:1092:HIS:NE2	2.34	0.42
1:D:175:CYS:HA	1:D:222:LYS:HG3	2.01	0.42
2:E:157:THR:C	2:E:160:MET:H	2.23	0.42
1:G:32:ILE:HG21	1:G:308:PRO:HG3	2.02	0.42
2:H:811:PHE:HA	2:H:814:GLN:OE1	2.20	0.42
3:I:64:VAL:HG22	3:I:266:VAL:HG13	2.01	0.42
3:I:302:ASN:CG	8:I:401:HEM:CAA	2.72	0.42
1:J:30:PHE:CD1	1:J:267:ARG:HG2	2.55	0.42
1:M:236:ILE:HG13	1:M:238:CYS:H	1.85	0.42
2:N:547[A]:MET:HG2	2:N:828:LEU:HD13	2.01	0.42
3:O:170:ASP:OD1	3:O:170:ASP:N	2.52	0.42
1:P:37:ALA:HA	1:P:63:VAL:HG11	2.01	0.42
2:Q:294:ASN:HA	2:Q:319:TRP:CD2	2.55	0.42
2:Q:358:LEU:CD1	2:Q:508:ILE:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:445:THR:HG23	2:Q:447:ASP:H	1.84	0.42
2:Q:628:THR:N	2:Q:632:GLY:O	2.53	0.42
2:Q:641:HIS:CD2	2:Q:1069:GLN:HA	2.55	0.42
2:Q:912:TYR:HD2	2:Q:1014:ASN:O	2.02	0.42
1:S:239:TYR:OH	2:T:53:TYR:HB2	2.20	0.42
1:S:271:PHE:O	1:S:278:ASN:ND2	2.53	0.42
2:T:400:ILE:HG13	2:T:401:ILE:HG13	2.00	0.42
2:W:333:ILE:HG12	2:W:348:ILE:HB	2.01	0.42
2:W:546:VAL:HG12	2:W:551:ASN:HB2	2.01	0.42
2:B:479:MET:HE3	2:B:484:MET:HE2	2.01	0.42
2:B:611:ASP:HB3	2:B:1089:ALA:HB2	2.01	0.42
2:B:903:PHE:CE2	2:B:904:LEU:HG	2.55	0.42
2:E:187:HIS:O	2:E:191:LYS:N	2.53	0.42
3:F:71:PHE:HE1	3:F:102:ALA:CA	2.32	0.42
1:G:296:GLN:HG2	2:H:1144:ILE:HD11	2.01	0.42
2:H:56:GLN:HG3	3:I:214:GLU:HA	2.00	0.42
2:H:121:PHE:HZ	2:H:699:SER:HB2	1.85	0.42
2:H:375:ASP:O	2:H:379:LYS:HG2	2.20	0.42
2:H:483:GLU:O	2:H:486:LYS:HB2	2.20	0.42
1:J:212:ARG:HD2	1:J:225:TYR:CG	2.54	0.42
2:K:973:ASP:OD1	2:K:1111:GLY:N	2.51	0.42
1:M:23:LYS:HE3	1:M:24:HIS:CD2	2.55	0.42
2:N:265:ARG:HH11	2:N:644:SER:N	2.18	0.42
2:N:784:THR:OG1	2:N:787:ASP:HB2	2.20	0.42
2:T:152:THR:HG22	2:T:154:GLU:H	1.85	0.42
3:U:49:LEU:HD23	3:U:314:LEU:HD13	2.01	0.42
1:V:46:LYS:NZ	1:V:55:GLN:O	2.53	0.42
2:W:974:TYR:OH	2:W:1052:ARG:HD2	2.20	0.42
2:W:1075:HIS:HE1	2:W:1086:GLY:O	2.03	0.42
3:X:99:GLU:O	3:X:113:VAL:HA	2.20	0.42
2:B:446:ARG:NH1	2:B:446:ARG:HG2	2.34	0.41
3:C:67:LEU:HD12	3:C:266:VAL:HG21	2.01	0.41
1:D:22:PRO:HG2	1:D:25:GLN:HB2	2.02	0.41
1:D:204:ASP:O	1:D:208:CYS:N	2.49	0.41
2:E:148:PHE:CD1	2:E:148:PHE:N	2.88	0.41
2:E:414:SER:HB3	2:E:420:LEU:HG	2.02	0.41
2:E:677:ILE:O	2:E:692:ASP:N	2.39	0.41
2:E:856:TYR:CE2	2:E:894:TRP:CH2	3.08	0.41
2:E:928:VAL:O	2:E:928:VAL:HG12	2.20	0.41
3:F:235:ASP:N	3:F:250:GLN:OE1	2.48	0.41
2:H:662:HIS:O	2:H:666:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:666:MET:HA	2:H:670:VAL:HB	2.01	0.41
3:I:146:SER:O	3:I:149:GLU:N	2.49	0.41
1:J:62:ASN:ND2	1:J:71:PHE:HB3	2.28	0.41
3:L:222:HIS:HA	3:L:227:LEU:HD11	2.02	0.41
3:L:247:GLN:OE1	3:L:278:ASP:OD2	2.38	0.41
2:N:641:HIS:CG	2:N:1087:PHE:HB2	2.55	0.41
2:N:661:LYS:HD2	6:N:5801:MD1:N8	2.35	0.41
2:Q:201:LEU:HD13	2:Q:645:PRO:HG2	2.01	0.41
2:Q:803:PHE:CD1	2:Q:808:ARG:HD3	2.55	0.41
2:Q:821:PHE:N	2:Q:821:PHE:HD1	2.17	0.41
2:Q:957:ILE:HG22	2:Q:1004:ARG:O	2.20	0.41
2:T:220:ARG:HG3	2:T:265:ARG:HD3	2.02	0.41
2:T:760:PHE:HB2	2:T:769:TYR:CE2	2.55	0.41
2:W:222:PHE:CD2	2:W:246:LEU:HD11	2.54	0.41
2:W:1061:ARG:HH11	2:W:1061:ARG:HG3	1.85	0.41
3:X:269:ARG:NH1	3:X:279:VAL:O	2.53	0.41
3:X:301:ARG:H	3:X:304:GLN:HB2	1.85	0.41
1:A:34:ARG:CB	1:A:266:ILE:HG22	2.50	0.41
2:B:229:GLY:HA3	2:B:237:TYR:CD1	2.55	0.41
2:B:536:THR:HG1	2:B:1068:HIS:HE2	1.63	0.41
2:B:1001:LEU:HA	2:B:1054:GLY:HA3	2.02	0.41
1:D:183:CYS:HB3	1:D:218:CYS:HB2	2.01	0.41
2:E:195:PRO:O	2:E:199:GLN:N	2.48	0.41
1:G:246:ASP:OD1	2:H:59:TYR:OH	2.29	0.41
2:H:151:LEU:HD23	2:H:151:LEU:HA	1.68	0.41
2:H:543:TYR:CE1	2:H:559:SER:HB3	2.55	0.41
1:J:257:ARG:NH1	2:K:119:TYR:CE2	2.88	0.41
2:K:220:ARG:CZ	2:K:610:LEU:HD22	2.50	0.41
2:K:392:LEU:HD21	2:K:869:ARG:NH1	2.34	0.41
2:K:882:TRP:CD1	2:K:883:GLU:HG2	2.55	0.41
2:N:983:ASP:HB3	2:N:984:ARG:NE	2.35	0.41
2:Q:73:HIS:ND1	2:Q:315:PRO:CG	2.83	0.41
2:Q:133:TYR:CD2	2:Q:171:ARG:HG3	2.55	0.41
2:Q:917:LYS:C	2:Q:1019:LYS:HZ2	2.20	0.41
3:R:229:ARG:N	3:R:229:ARG:HD2	2.34	0.41
2:T:900:THR:O	2:T:901:LYS:HG2	2.20	0.41
2:T:939:PHE:CE1	2:T:1004:ARG:HD2	2.55	0.41
3:U:236:LEU:HD23	3:U:236:LEU:H	1.84	0.41
1:V:181:PRO:HB3	4:V:502:SF4:S1	2.60	0.41
2:W:230:LEU:HD21	2:W:710:ASN:HB2	2.02	0.41
2:W:282:PHE:HB3	2:W:832:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:629:PRO:HG2	2:W:874:GLY:O	2.20	0.41
3:X:225:LEU:HA	10:X:501:HOH:O	2.20	0.41
2:B:70:ASN:N	2:B:231:LEU:HD21	2.35	0.41
2:B:914:VAL:HG23	2:B:1017:MET:HG2	2.03	0.41
2:E:126:TYR:CG	3:F:205:HIS:CD2	3.08	0.41
2:E:915:THR:OG1	6:E:5801:MD1:N16	2.54	0.41
3:F:305:LYS:HE2	8:F:401:HEM:ND	1.94	0.41
3:F:305:LYS:HD3	8:F:401:HEM:NA	2.35	0.41
1:G:16:PRO:HG2	1:G:185:ALA:HB1	2.02	0.41
2:H:613:GLU:OE1	2:H:614:VAL:N	2.52	0.41
2:H:1040:ARG:HH21	2:H:1042:LEU:HD22	1.84	0.41
2:K:301:LEU:HB3	2:K:521:VAL:HG22	2.02	0.41
2:K:358:LEU:HB2	2:K:501:THR:HG21	2.01	0.41
3:L:67:LEU:HD13	3:L:266:VAL:HG11	2.01	0.41
3:L:203:ASN:ND2	2:N:207:PRO:HA	2.35	0.41
1:M:333:VAL:HG13	1:M:373:PHE:HB2	2.02	0.41
2:N:515:ILE:HG22	2:N:549:THR:HG21	2.01	0.41
2:N:1040:ARG:NH1	2:N:1048:GLN:OE1	2.53	0.41
3:O:110:TYR:HD1	3:O:268:CYS:HB2	1.77	0.41
3:O:241:PHE:HB2	8:O:401:HEM:C4A	2.56	0.41
2:Q:124:ARG:HD3	2:Q:926:TRP:CD1	2.55	0.41
2:Q:296:VAL:HG11	2:Q:320:VAL:HG22	2.01	0.41
2:T:89:VAL:HG11	2:T:119:TYR:HA	2.01	0.41
2:T:94:ASP:OD1	2:T:98:TYR:OH	2.28	0.41
2:T:434:TRP:HB3	2:T:461:VAL:CG2	2.50	0.41
2:T:760:PHE:HB3	2:T:765:ARG:O	2.20	0.41
2:T:768:VAL:O	2:T:772:ARG:HG3	2.19	0.41
1:V:189:ARG:HH21	1:V:207:ARG:NH1	2.18	0.41
2:W:35:VAL:H	3:X:245:THR:CG2	2.31	0.41
2:B:359:PHE:HB2	2:B:541:SER:OG	2.20	0.41
2:B:862:VAL:HG22	2:B:897:THR:HG21	2.03	0.41
2:B:1064:SER:OG	2:B:1069:GLN:NE2	2.47	0.41
2:E:666:MET:HA	2:E:670:VAL:HG23	2.02	0.41
2:E:939:PHE:HD2	2:E:954:GLU:HG3	1.86	0.41
2:E:959:ILE:HD11	2:E:963:ALA:HB3	2.03	0.41
1:G:181:PRO:HG2	1:G:184:LEU:HB3	2.01	0.41
1:G:346:ARG:CZ	1:G:346:ARG:HA	2.50	0.41
2:K:93:TYR:O	2:K:96:GLN:NE2	2.53	0.41
2:K:359:PHE:HB2	2:K:541:SER:OG	2.21	0.41
3:L:145:ILE:HG12	3:L:151:PHE:HB3	2.03	0.41
2:N:425:ARG:HG2	2:N:425:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:168:LYS:HB3	3:O:170:ASP:OD1	2.20	0.41
1:P:132:TYR:O	1:P:221:LYS:NZ	2.35	0.41
2:Q:628:THR:HG21	2:Q:873:TYR:HB3	2.03	0.41
2:Q:916:PRO:O	2:Q:1020:HIS:N	2.52	0.41
2:T:230:LEU:HD23	2:T:565:ASN:CG	2.40	0.41
2:T:909:TYR:CD1	2:T:909:TYR:N	2.87	0.41
1:V:32:ILE:HG13	1:V:306:ILE:O	2.20	0.41
1:V:189:ARG:NH1	1:V:209:ARG:CB	2.60	0.41
1:V:257:ARG:CD	2:W:90:GLU:OE1	2.64	0.41
1:V:331:PHE:CD2	1:V:331:PHE:C	2.93	0.41
2:W:648:VAL:HG23	2:W:676:GLN:CB	2.46	0.41
2:W:663:VAL:HG21	2:W:1024:ILE:HD13	2.03	0.41
2:W:795:GLU:HA	2:W:796:PRO:HD3	1.93	0.41
2:W:1061:ARG:HG3	2:W:1061:ARG:NH1	2.36	0.41
1:D:15:TYR:HE1	1:D:180:TYR:CA	2.32	0.41
3:F:302:ASN:OD1	8:F:401:HEM:HAA1	2.20	0.41
10:J:601:HOH:O	2:K:1145:LYS:NZ	2.28	0.41
2:K:179:THR:HG22	2:K:744:LYS:HD2	2.02	0.41
2:K:533:PHE:HA	2:K:1065:MET:HE3	2.02	0.41
1:M:22:PRO:HA	1:M:196:LYS:O	2.21	0.41
1:M:164:HIS:HB2	1:M:167:TRP:HB3	2.01	0.41
1:M:213:LYS:HB2	5:M:504:F3S:S2	2.60	0.41
2:N:290:ASP:O	2:N:808:ARG:NH1	2.54	0.41
2:N:294:ASN:OD1	2:N:807:PRO:HB3	2.20	0.41
2:N:543:TYR:CE1	2:N:559:SER:HB3	2.55	0.41
2:N:1003:LEU:HD23	2:N:1003:LEU:H	1.86	0.41
1:P:29:VAL:HA	1:P:304:TYR:O	2.20	0.41
2:Q:393:LYS:HA	2:Q:833:ASP:HB2	2.03	0.41
2:Q:864:THR:CG2	2:Q:893:SER:HB2	2.50	0.41
1:S:402:ARG:HD2	2:T:803:PHE:O	2.21	0.41
2:T:70:ASN:ND2	2:T:228:MET:HG3	2.35	0.41
2:T:882:TRP:CD1	2:T:883:GLU:HG2	2.56	0.41
1:V:111:TYR:CZ	1:V:113:GLY:HA3	2.56	0.41
2:W:531:HIS:O	2:W:1097:VAL:HB	2.21	0.41
2:W:663:VAL:O	2:W:667:LEU:HG	2.20	0.41
2:W:923:HIS:ND1	6:W:5801:MD1:H102	2.35	0.41
3:X:54:MET:O	3:X:56:ILE:HG13	2.20	0.41
1:A:8:HIS:HE1	1:A:301:PRO:O	2.03	0.41
1:A:107:PRO:HG3	1:A:285:ARG:NH2	2.35	0.41
2:B:295:ASP:OD1	2:B:556:GLY:N	2.53	0.41
3:C:301:ARG:CG	3:C:301:ARG:NH2	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:LYS:C	2:E:140:TRP:H	2.23	0.41
1:G:128:TRP:CE2	3:I:88:PHE:HD2	2.38	0.41
2:H:71:ASP:OD2	2:H:73:HIS:HB2	2.21	0.41
2:H:286:LEU:HD12	2:H:287:GLN:H	1.85	0.41
2:H:456:LYS:NZ	10:H:5919:HOH:O	2.49	0.41
3:I:280:GLN:OE1	3:X:272:ASN:OD1	2.38	0.41
1:J:9:LEU:HD22	1:J:111:TYR:HB3	2.02	0.41
2:K:116:LEU:HD12	2:K:932:ASN:ND2	2.35	0.41
2:K:117:LYS:HE2	2:K:919:ARG:O	2.20	0.41
2:K:881:TYR:O	2:K:885:ARG:HG3	2.21	0.41
2:K:1094:ILE:H	2:K:1094:ILE:HD12	1.86	0.41
1:M:320:PHE:HB2	1:M:324:VAL:HG12	2.02	0.41
2:N:67:CYS:O	2:N:74:ALA:HA	2.21	0.41
2:N:116:LEU:HG	2:N:117:LYS:N	2.36	0.41
2:N:141:LYS:HE2	2:N:180:TYR:HE2	1.85	0.41
2:N:689:GLU:OE2	2:N:1045:SER:OG	2.36	0.41
2:N:705:GLU:HG3	2:N:706:PHE:H	1.85	0.41
3:O:151:PHE:CE1	3:O:160:LYS:HB3	2.56	0.41
1:P:181:PRO:HG2	1:P:184:LEU:HB3	2.02	0.41
1:S:140:ARG:HD3	2:T:945:MET:CE	2.51	0.41
1:S:291:LEU:HB2	1:S:320:PHE:HB3	2.02	0.41
1:V:150:LYS:HD3	1:V:167:TRP:HE1	1.86	0.41
2:W:117:LYS:HE2	2:W:921:THR:O	2.20	0.41
2:W:468:LEU:HD12	2:W:468:LEU:HA	1.64	0.41
2:W:618:ASN:OD1	2:W:661:LYS:HB2	2.20	0.41
1:A:309:ARG:NH1	2:B:343:LYS:O	2.52	0.41
2:B:533:PHE:HB2	2:B:1100:GLU:HG3	2.03	0.41
2:B:801:LEU:HD12	2:B:801:LEU:O	2.21	0.41
1:D:289:ILE:HG12	1:D:306:ILE:CG2	2.50	0.41
2:E:666:MET:CE	2:E:670:VAL:HG21	2.50	0.41
2:E:856:TYR:HE2	2:E:894:TRP:CH2	2.38	0.41
1:G:6:ASN:OD1	1:G:8:HIS:N	2.53	0.41
2:H:844:PHE:O	2:H:846:VAL:HG23	2.20	0.41
1:J:276:PRO:HB3	1:J:286:HIS:NE2	2.36	0.41
2:K:712:CYS:O	2:K:808:ARG:NH2	2.53	0.41
1:M:212:ARG:NH1	3:O:129:GLU:O	2.28	0.41
1:M:263:VAL:CG1	2:N:315:PRO:HA	2.50	0.41
2:N:348:ILE:HG12	2:N:507:LEU:HB3	2.02	0.41
2:N:397:PRO:HB2	2:N:404:TYR:CE2	2.56	0.41
1:P:410:ILE:HB	2:Q:572:GLN:OE1	2.21	0.41
2:T:77:ILE:CG2	2:T:89:VAL:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:302:LEU:HD23	2:T:320:VAL:HG13	2.01	0.41
2:T:382:ASP:CG	2:T:829:GLN:HA	2.41	0.41
2:T:547:MET:HG2	2:T:828:LEU:HD13	2.01	0.41
2:T:1024:ILE:HG22	2:T:1055:SER:HB2	2.01	0.41
3:U:163:ASN:HD22	3:U:164:LEU:H	1.68	0.41
1:V:42:THR:HG21	2:W:935:TRP:CZ2	2.56	0.41
2:W:192:TYR:HB3	2:W:201:LEU:HD21	2.03	0.41
3:X:172:GLU:O	3:X:176:LEU:HD12	2.20	0.41
2:B:626:VAL:HG11	2:B:887:VAL:HG21	2.03	0.41
3:C:105:ASP:HB2	3:C:108:THR:H	1.86	0.41
2:E:281:PRO:HA	2:E:285:GLY:HA2	2.01	0.41
2:E:497:VAL:O	2:E:501:THR:HG22	2.21	0.41
2:E:928:VAL:HG21	2:E:1023:TRP:CE3	2.55	0.41
2:E:1033:HIS:NE2	2:E:1052:ARG:HD3	2.35	0.41
2:H:914:VAL:HG12	2:H:916:PRO:HD3	2.03	0.41
2:K:133:TYR:CD2	2:K:171:ARG:HB2	2.56	0.41
1:M:410:ILE:HB	2:N:572:GLN:NE2	2.35	0.41
2:N:47:ARG:HG3	2:N:47:ARG:NH2	2.36	0.41
3:O:272:ASN:HD22	3:O:280:GLN:HB3	1.86	0.41
1:P:225:TYR:OH	3:R:124:ALA:O	2.31	0.41
1:P:346:ARG:HA	1:P:346:ARG:CZ	2.51	0.41
1:P:408:ASN:ND2	2:Q:805:THR:OG1	2.31	0.41
2:Q:72:THR:HG23	2:Q:711:SER:OG	2.20	0.41
2:Q:116:LEU:HD21	2:Q:919:ARG:O	2.21	0.41
2:Q:171:ARG:HG2	2:Q:172:ALA:N	2.35	0.41
2:Q:278:PRO:O	2:Q:281:PRO:HD2	2.21	0.41
3:R:295:ASN:H	3:R:300:ASP:CB	2.34	0.41
2:T:470:THR:HG23	2:T:474:LYS:O	2.21	0.41
2:T:923:HIS:CG	6:T:5801:MD1:H102	2.55	0.41
1:V:343:SER:OG	1:V:395:VAL:HG13	2.21	0.41
2:W:395:VAL:HG13	2:W:432:VAL:CG2	2.50	0.41
2:W:571:PHE:CD1	2:W:780:MET:HE1	2.56	0.41
2:W:666:MET:HA	2:W:670:VAL:HB	2.02	0.41
3:X:51:VAL:HG13	3:X:316:LEU:HA	2.02	0.41
3:X:291:MET:C	8:X:401:HEM:HAC	2.42	0.41
1:A:6:ASN:HD22	1:A:13:MET:CE	2.33	0.41
1:A:9:LEU:O	1:A:110:THR:HA	2.21	0.41
1:A:211:TYR:O	3:C:301:ARG:CD	2.69	0.41
2:B:305:THR:O	6:B:5802:MD1:N2	2.53	0.41
2:B:712:CYS:O	2:B:808:ARG:NH2	2.54	0.41
2:B:980:ASN:OD1	2:B:981:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1074:PHE:HB2	2:B:1085:PHE:HE1	1.86	0.41
2:B:1087:PHE:CD2	2:B:1093:CYS:HB3	2.56	0.41
1:D:140:ARG:H	1:D:140:ARG:HG3	1.76	0.41
1:G:399:ILE:HD11	2:H:298:PHE:HE2	1.85	0.41
2:H:271:THR:HB	2:H:1094:ILE:O	2.21	0.41
2:H:1017:MET:SD	2:H:1019:LYS:HD3	2.61	0.41
3:I:63:THR:HG23	3:I:66:ALA:H	1.85	0.41
3:I:193:ASP:HB3	3:I:196:SER:OG	2.21	0.41
3:I:256:SER:HB2	3:I:265:VAL:HG12	2.03	0.41
1:J:402:ARG:HD2	2:K:803:PHE:O	2.21	0.41
2:K:72:THR:O	2:K:711:SER:OG	2.29	0.41
2:K:94:ASP:OD1	2:K:94:ASP:N	2.54	0.41
2:K:151:LEU:HD23	2:K:151:LEU:HA	1.77	0.41
2:K:348:ILE:HG12	2:K:507:LEU:HB3	2.02	0.41
2:K:428:ILE:HD13	2:K:428:ILE:HA	1.91	0.41
2:K:462:LEU:HD23	2:K:462:LEU:HA	1.92	0.41
2:K:944:ARG:HA	2:K:949:MET:CE	2.51	0.41
2:K:984:ARG:HH11	2:K:1061:ARG:HB3	1.86	0.41
1:M:209:ARG:HH11	3:O:234:GLU:CD	2.23	0.41
2:N:91:GLN:HG2	2:N:112:PRO:HB2	2.02	0.41
2:N:515:ILE:HG23	2:N:521:VAL:HG11	2.03	0.41
2:N:903:PHE:CE2	2:N:904:LEU:HG	2.56	0.41
2:N:923:HIS:CG	6:N:5801:MD1:H102	2.56	0.41
3:O:237:ASN:OD1	10:O:502:HOH:O	2.22	0.41
3:O:269:ARG:NH1	3:O:278:ASP:HB3	2.36	0.41
3:O:303:GLY:HA2	3:O:305:LYS:HE2	2.02	0.41
3:O:321:TRP:HA	3:O:321:TRP:CE3	2.56	0.41
1:P:36:ILE:O	2:Q:919:ARG:NH2	2.54	0.41
1:P:393:THR:OG1	2:Q:109:ASN:OD1	2.37	0.41
2:Q:234:ILE:N	2:Q:707:GLU:OE2	2.52	0.41
2:Q:307:LYS:HZ3	2:Q:313:LYS:CE	2.33	0.41
2:Q:363:THR:HG23	2:Q:548:LEU:HD11	2.03	0.41
2:Q:531:HIS:C	2:Q:1097:VAL:CG2	2.89	0.41
2:Q:616:TYR:CG	2:Q:643:PRO:HG3	2.55	0.41
2:Q:625:ILE:HD11	2:Q:633:ARG:CG	2.50	0.41
2:Q:625:ILE:HB	2:Q:635:VAL:HG12	2.02	0.41
2:Q:1040:ARG:NE	2:Q:1048:GLN:OE1	2.46	0.41
3:R:143:ILE:C	3:R:143:ILE:CD1	2.89	0.41
1:S:2:THR:HG21	1:S:18:PHE:CD1	2.56	0.41
2:T:225:ARG:HB2	2:T:267:TRP:HB2	2.02	0.41
2:T:307:LYS:HE2	2:T:309:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:717:ILE:O	2:T:798:VAL:HA	2.20	0.41
3:U:53:TYR:CZ	3:U:319:ILE:HG23	2.56	0.41
1:V:211:TYR:CD1	3:X:302:ASN:HB3	2.56	0.41
2:W:77:ILE:CG2	2:W:89:VAL:HG21	2.51	0.41
2:W:155:ASN:O	2:W:159:TYR:HD1	2.04	0.41
2:W:229:GLY:HA3	2:W:237:TYR:CG	2.55	0.41
2:W:364:LYS:HA	2:W:489:LEU:HD13	2.03	0.41
2:W:389:THR:HG23	2:W:867:TYR:CE1	2.54	0.41
2:W:937:ASN:ND2	2:W:954:GLU:C	2.66	0.41
2:W:958:HIS:HB2	2:W:1017:MET:HB3	2.03	0.41
3:X:109:ILE:C	3:X:110:TYR:HD1	2.19	0.41
3:X:241:PHE:CE2	8:X:401:HEM:HMB3	2.56	0.41
3:X:280:GLN:HA	3:X:280:GLN:OE1	2.21	0.41
1:A:181:PRO:HG2	1:A:184:LEU:CB	2.51	0.41
2:B:285:GLY:HA3	2:B:822:TYR:O	2.20	0.41
2:B:356:THR:HG23	2:B:541:SER:HB2	2.03	0.41
2:B:431:PHE:CE2	2:B:825:THR:HA	2.56	0.41
1:D:402:ARG:HB2	2:E:804:ARG:HA	2.02	0.41
2:E:566:TYR:O	2:E:568:ALA:N	2.50	0.41
3:F:51:VAL:HG12	3:F:102:ALA:C	2.41	0.41
3:F:51:VAL:CG1	3:F:102:ALA:HB3	2.51	0.41
2:H:554:TYR:CZ	2:H:815:VAL:HG11	2.56	0.41
2:H:581:PHE:HB3	2:H:1079:ILE:HG23	2.03	0.41
3:I:305:LYS:C	3:I:306:ASN:HD22	2.25	0.41
1:J:33:ASN:O	2:K:343:LYS:NZ	2.50	0.41
1:J:181:PRO:HG2	1:J:184:LEU:CB	2.51	0.41
2:K:284:HIS:CE1	2:K:286:LEU:HB3	2.56	0.41
3:O:140:LEU:CG	3:O:161:PRO:HG2	2.51	0.41
1:P:311:ALA:HB3	1:P:316:LEU:HD11	2.02	0.41
2:Q:139:GLY:O	2:Q:159:TYR:HB3	2.22	0.41
2:Q:310:ILE:HG13	2:Q:340:SER:HA	2.02	0.41
2:Q:497:VAL:HA	2:Q:500:MET:CG	2.48	0.41
2:Q:1137:LYS:HE2	2:Q:1143:LEU:HD13	2.02	0.41
1:S:64:GLU:OE1	1:S:70:GLY:HA2	2.21	0.41
1:S:397:GLU:OE1	2:T:806:TYR:OH	2.26	0.41
1:V:259:MET:HE3	1:V:269:GLN:HB2	2.02	0.41
1:V:309:ARG:NH2	2:W:324:MET:HB2	2.35	0.41
2:W:192:TYR:OH	2:W:675:GLU:OE2	2.20	0.41
2:W:658:ASN:HD21	2:W:1024:ILE:HG23	1.84	0.41
2:W:952:VAL:CG1	2:W:952:VAL:O	2.69	0.41
2:B:380:PHE:CZ	2:B:815:VAL:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:PRO:HB2	2:B:404:TYR:CE2	2.56	0.40
2:B:849:GLU:O	2:B:859:ASN:HA	2.21	0.40
2:B:949:MET:HE2	2:B:953:GLY:HA2	2.03	0.40
2:B:977:VAL:HG12	2:B:1103:VAL:CG1	2.42	0.40
1:D:334:PRO:HG2	2:E:325:GLU:O	2.22	0.40
2:E:657:ILE:HD12	2:E:657:ILE:N	2.35	0.40
3:F:207:GLY:HA2	2:Q:208:LYS:HD2	2.03	0.40
1:G:291:LEU:HB2	1:G:320:PHE:HB3	2.03	0.40
2:H:261:ALA:O	2:H:608:ARG:HD3	2.20	0.40
2:H:424:GLN:HG2	2:H:1085:PHE:HE2	1.85	0.40
2:H:974:TYR:CE1	2:H:1052:ARG:HD2	2.55	0.40
3:I:160:LYS:HB3	3:I:160:LYS:HE3	1.74	0.40
3:I:281:PHE:HB3	3:I:316:LEU:HD11	2.03	0.40
1:J:410:ILE:HB	2:K:572:GLN:NE2	2.36	0.40
2:K:72:THR:HG21	2:K:313:LYS:HZ3	1.86	0.40
2:K:868:ILE:HG22	2:K:870:PRO:HD3	2.04	0.40
2:K:1121:PRO:O	2:K:1124:THR:OG1	2.29	0.40
1:M:189:ARG:HD2	1:M:209:ARG:HG3	2.03	0.40
2:N:390:ASP:OD1	2:N:391:THR:N	2.53	0.40
3:O:39:GLU:O	3:O:43:THR:N	2.52	0.40
2:Q:275:ASP:HB3	2:Q:563:ALA:CB	2.45	0.40
2:Q:417:ILE:O	2:Q:575:LYS:NZ	2.54	0.40
2:T:415:TYR:HE1	2:T:422:ASP:OD1	2.04	0.40
2:T:1137:LYS:HG2	2:T:1142:GLU:HB2	2.03	0.40
1:V:46:LYS:O	1:V:51:PHE:HB3	2.22	0.40
2:W:1059:ILE:H	2:W:1059:ILE:HG13	1.81	0.40
2:B:383:PHE:N	2:B:384:PRO:HD2	2.37	0.40
2:B:481:LEU:O	2:B:485:TYR:N	2.45	0.40
2:B:806:TYR:HB3	2:B:807:PRO:HD3	2.04	0.40
2:B:909:TYR:CD2	2:B:909:TYR:N	2.90	0.40
1:D:41:CYS:SG	1:D:61:ASN:ND2	2.88	0.40
2:E:531:HIS:HE1	6:E:5801:MD1:N15	2.19	0.40
2:E:998:VAL:O	2:E:1054:GLY:N	2.54	0.40
6:E:5801:MD1:O11	6:E:5801:MD1:C7	2.70	0.40
1:G:62:ASN:ND2	1:G:71:PHE:HB3	2.29	0.40
3:I:151:PHE:HA	3:I:160:LYS:HE2	2.04	0.40
2:K:640:THR:HG22	2:K:1087:PHE:HB3	2.02	0.40
2:N:248:ILE:HB	2:N:754:PHE:CZ	2.56	0.40
2:N:500:MET:HG2	2:N:894:TRP:CE2	2.56	0.40
1:P:318:GLN:OE1	2:Q:1141:GLY:HA2	2.21	0.40
1:P:362:LYS:HE3	1:P:374:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:719:ILE:HG22	2:Q:789:LEU:HD21	2.04	0.40
1:S:181:PRO:HG2	1:S:184:LEU:HB3	2.03	0.40
1:S:259:MET:SD	1:S:267:ARG:HD3	2.61	0.40
1:S:368:ILE:HG12	1:S:369:HIS:CE1	2.56	0.40
2:T:301:LEU:HD23	2:T:521:VAL:HG22	2.03	0.40
1:V:34:ARG:NH1	1:V:342:MET:O	2.45	0.40
1:V:77:VAL:HG22	2:W:1138:PHE:CE1	2.55	0.40
1:V:211:TYR:HD1	1:V:211:TYR:HA	1.80	0.40
2:W:641:HIS:HE1	2:W:1092:HIS:O	2.03	0.40
2:W:976:TYR:CE1	2:W:1000:ARG:CZ	3.04	0.40
2:B:276:GLN:HE22	2:B:1092:HIS:N	2.05	0.40
2:B:977:VAL:HG21	2:B:1001:LEU:HD23	2.03	0.40
2:E:922:VAL:O	2:E:922:VAL:HG12	2.20	0.40
1:G:399:ILE:HD12	2:H:807:PRO:HD3	2.03	0.40
2:H:201:LEU:HD13	2:H:645:PRO:HG2	2.03	0.40
2:H:577:SER:O	2:H:776:GLY:HA2	2.22	0.40
2:K:225:ARG:NH1	2:K:654:VAL:HG11	2.37	0.40
1:M:337:GLU:O	1:M:341:VAL:HG23	2.21	0.40
3:O:59:PRO:HD3	3:O:66:ALA:HB1	2.03	0.40
2:Q:527:GLU:OE1	6:Q:5802:MD1:H101	2.20	0.40
1:V:26:PHE:HA	1:V:271:PHE:CD2	2.56	0.40
1:V:33:ASN:ND2	1:V:331:PHE:CD2	2.89	0.40
1:V:61:ASN:HB2	4:V:501:SF4:S4	2.62	0.40
1:V:187:CYS:HB2	1:V:192:ILE:HG13	2.03	0.40
1:V:211:TYR:CZ	3:X:302:ASN:HB3	2.56	0.40
2:W:1023:TRP:CE3	2:W:1047:TYR:CD1	3.09	0.40
3:X:109:ILE:HD12	3:X:316:LEU:HD21	2.03	0.40
1:A:15:TYR:OH	1:A:181:PRO:O	2.29	0.40
2:B:332:VAL:HG23	2:B:344:ALA:HB2	2.03	0.40
2:B:624:LEU:HB2	2:B:1064:SER:OG	2.21	0.40
2:B:661:LYS:NZ	2:B:1096:THR:OG1	2.33	0.40
2:B:842:GLU:OE1	2:B:848:ARG:NH2	2.55	0.40
2:B:1061:ARG:CG	2:B:1062:ASP:N	2.85	0.40
3:C:305:LYS:HD3	3:C:307:ILE:CG2	2.52	0.40
2:E:413:PRO:HB2	2:E:820:PRO:CD	2.51	0.40
3:F:171:TRP:HZ3	3:F:233:VAL:O	2.04	0.40
3:F:256:SER:CB	3:F:265:VAL:HG12	2.52	0.40
1:G:184:LEU:HD21	2:H:40:PRO:HB2	2.03	0.40
2:H:271:THR:HA	2:H:1095:ASN:OD1	2.22	0.40
2:H:536:THR:HG1	2:H:1068:HIS:HE2	1.65	0.40
3:I:305:LYS:NZ	8:I:401:HEM:NC	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:641:HIS:CG	2:K:1087:PHE:HB2	2.56	0.40
2:K:1034:GLU:OE2	2:K:1053:TYR:OH	2.32	0.40
3:L:100:ILE:HB	3:L:291:MET:HE1	2.04	0.40
2:N:409:ILE:HG13	2:N:415:TYR:HE2	1.86	0.40
2:N:834:GLU:HB2	2:N:837:ILE:HD12	2.03	0.40
2:N:973:ASP:OD1	2:N:1111:GLY:N	2.47	0.40
2:Q:497:VAL:CA	2:Q:500:MET:HG3	2.49	0.40
2:Q:717:ILE:O	2:Q:798:VAL:HA	2.21	0.40
3:R:145:ILE:HD11	3:R:151:PHE:HD2	1.87	0.40
2:T:278:PRO:O	2:T:281:PRO:HD2	2.22	0.40
2:T:436:ALA:HB3	2:T:459:ASP:OD2	2.22	0.40
2:T:462:LEU:HA	2:T:462:LEU:HD12	1.75	0.40
1:V:36:ILE:HG13	2:W:310:ILE:HD12	2.02	0.40
1:V:237:ALA:HA	4:V:501:SF4:S1	2.61	0.40
2:W:760:PHE:HB3	2:W:765:ARG:O	2.22	0.40
3:X:237:ASN:OD1	3:X:247:GLN:NE2	2.51	0.40
1:A:404:ASP:HA	2:B:804:ARG:HH21	1.82	0.40
2:B:506:ASP:OD2	2:B:506:ASP:N	2.53	0.40
2:B:801:LEU:HD11	2:B:803:PHE:CE2	2.56	0.40
3:C:137:MET:HE1	3:C:153:PRO:O	2.21	0.40
1:D:34:ARG:NH2	2:E:318:HIS:ND1	2.70	0.40
1:D:55:GLN:NE2	1:D:233:GLU:OE1	2.54	0.40
2:E:1020:HIS:ND1	2:E:1020:HIS:C	2.71	0.40
3:F:153:PRO:HB3	3:F:311:TRP:CD1	2.56	0.40
2:H:160:MET:O	2:H:164:ARG:HG2	2.21	0.40
2:H:848:ARG:NH1	2:H:859:ASN:OD1	2.55	0.40
1:J:8:HIS:CD2	1:J:300:GLU:HA	2.56	0.40
2:K:417:ILE:HD13	2:K:417:ILE:HA	1.91	0.40
3:L:280:GLN:HB2	3:R:282:VAL:HG22	2.04	0.40
2:N:751:ASP:OD1	2:N:753:ARG:NH2	2.55	0.40
2:N:892:LYS:HG2	2:N:896:GLU:HB3	2.04	0.40
3:O:67:LEU:HD13	3:O:266:VAL:HG21	2.04	0.40
2:Q:456:LYS:HB2	2:Q:458:ILE:HD12	2.04	0.40
2:Q:970:GLU:HA	2:Q:1007:TYR:OH	2.21	0.40
1:S:32:ILE:HG21	1:S:308:PRO:HG3	2.03	0.40
2:T:920:HIS:CD2	2:T:936:ASN:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	D	406/410 (99%)	388 (96%)	18 (4%)	0	100	100
1	G	407/410 (99%)	399 (98%)	8 (2%)	0	100	100
1	J	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	M	407/410 (99%)	401 (98%)	6 (2%)	0	100	100
1	P	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	S	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	V	407/410 (99%)	395 (97%)	12 (3%)	0	100	100
2	B	1119/1148 (98%)	1078 (96%)	41 (4%)	0	100	100
2	E	1104/1148 (96%)	1034 (94%)	68 (6%)	2 (0%)	47	80
2	H	1117/1148 (97%)	1073 (96%)	43 (4%)	1 (0%)	51	83
2	K	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	N	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	Q	1113/1148 (97%)	1071 (96%)	39 (4%)	3 (0%)	41	74
2	T	1117/1148 (97%)	1079 (97%)	38 (3%)	0	100	100
2	W	1117/1148 (97%)	1072 (96%)	44 (4%)	1 (0%)	51	83
3	C	291/322 (90%)	282 (97%)	9 (3%)	0	100	100
3	F	290/322 (90%)	278 (96%)	12 (4%)	0	100	100
3	I	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
3	L	291/322 (90%)	288 (99%)	3 (1%)	0	100	100
3	O	289/322 (90%)	280 (97%)	9 (3%)	0	100	100
3	R	289/322 (90%)	279 (96%)	10 (4%)	0	100	100
3	U	290/322 (90%)	284 (98%)	6 (2%)	0	100	100
3	X	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
All	All	14498/15040 (96%)	13995 (96%)	496 (3%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	520	PRO
2	H	1021	SER
2	Q	69	PRO
2	Q	113	ARG
2	Q	1021	SER
2	W	72	THR
2	E	72	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/365 (98%)	352 (98%)	7 (2%)	57	82
1	D	229/365 (63%)	219 (96%)	10 (4%)	28	63
1	G	356/365 (98%)	348 (98%)	8 (2%)	52	80
1	J	362/365 (99%)	356 (98%)	6 (2%)	60	84
1	M	348/365 (95%)	337 (97%)	11 (3%)	39	72
1	P	350/365 (96%)	339 (97%)	11 (3%)	40	73
1	S	355/365 (97%)	350 (99%)	5 (1%)	67	86
1	V	324/365 (89%)	300 (93%)	24 (7%)	13	42
2	B	943/991 (95%)	902 (96%)	41 (4%)	29	64
2	E	373/991 (38%)	347 (93%)	26 (7%)	15	45
2	H	952/991 (96%)	930 (98%)	22 (2%)	50	79
2	K	956/991 (96%)	934 (98%)	22 (2%)	50	79
2	N	959/991 (97%)	933 (97%)	26 (3%)	44	75
2	Q	913/991 (92%)	868 (95%)	45 (5%)	25	59
2	T	953/991 (96%)	926 (97%)	27 (3%)	43	75
2	W	918/991 (93%)	864 (94%)	54 (6%)	19	52
3	C	238/265 (90%)	229 (96%)	9 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	175/265 (66%)	162 (93%)	13 (7%)	13	42
3	I	220/265 (83%)	205 (93%)	15 (7%)	16	46
3	L	236/265 (89%)	227 (96%)	9 (4%)	33	67
3	O	196/265 (74%)	178 (91%)	18 (9%)	9	32
3	R	235/265 (89%)	226 (96%)	9 (4%)	33	67
3	U	235/265 (89%)	222 (94%)	13 (6%)	21	55
3	X	223/265 (84%)	205 (92%)	18 (8%)	11	37
All	All	11408/12968 (88%)	10959 (96%)	449 (4%)	32	66

All (449) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	93	ASP
1	A	101	GLN
1	A	123	LYS
1	A	125	ILE
1	A	212	ARG
1	A	235	CYS
2	B	30	LEU
2	B	58	GLN
2	B	82	ARG
2	B	89	VAL
2	B	113	ARG
2	B	123	ARG
2	B	142[A]	ARG
2	B	142[B]	ARG
2	B	228	MET
2	B	262	LEU
2	B	267	TRP
2	B	276	GLN
2	B	307	LYS
2	B	309	LEU
2	B	310	ILE
2	B	370	LYS
2	B	387	ILE
2	B	425	ARG
2	B	442	LYS
2	B	445	THR
2	B	446	ARG

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Mol	Chain	Res	Type
2	B	506	ASP
2	B	618	ASN
2	B	628	THR
2	B	631	TYR
2	B	633	ARG
2	B	653	ASN
2	B	654	VAL
2	B	656	LEU
2	B	733	ASP
2	B	804	ARG
2	B	924	SER
2	B	977	VAL
2	B	983	ASP
2	B	984	ARG
2	B	993	ASP
2	B	1021	SER
2	B	1048	GLN
2	B	1087	PHE
2	B	1088	GLU
2	B	1105	ILE
3	C	105	ASP
3	C	123	GLN
3	C	151	PHE
3	C	163	ASN
3	C	216	SER
3	C	229	ARG
3	C	236	LEU
3	C	301	ARG
3	C	305	LYS
1	D	15	TYR
1	D	34	ARG
1	D	102	TYR
1	D	146	GLU
1	D	166	ARG
1	D	235	CYS
1	D	257	ARG
1	D	315	TYR
1	D	331	PHE
1	D	332	MET
2	E	73	HIS
2	E	110	TRP
2	E	114	MET

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Mol	Chain	Res	Type
2	E	170	LEU
2	E	174	TRP
2	E	239	MET
2	E	273	HIS
2	E	353	ASN
2	E	420	LEU
2	E	559	SER
2	E	651	PHE
2	E	666	MET
2	E	670	VAL
2	E	700	TRP
2	E	731	SER
2	E	872	ASP
2	E	920	HIS
2	E	930	ASP
2	E	957	ILE
2	E	1003	LEU
2	E	1014	ASN
2	E	1020	HIS
2	E	1047	TYR
2	E	1057	GLN
2	E	1096	THR
2	E	1110	ASN
3	F	71	PHE
3	F	84	GLN
3	F	104	HIS
3	F	172	GLU
3	F	205	HIS
3	F	206	LYS
3	F	219	TYR
3	F	229	ARG
3	F	231	ARG
3	F	249	HIS
3	F	251	ASP
3	F	286	SER
3	F	305	LYS
1	G	15	TYR
1	G	24	HIS
1	G	61	ASN
1	G	98	GLU
1	G	196	LYS
1	G	212	ARG

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Mol	Chain	Res	Type
1	G	235	CYS
1	G	247	SER
2	H	31	LEU
2	H	152	THR
2	H	154	GLU
2	H	156	LYS
2	H	228	MET
2	H	236	LYS
2	H	237	TYR
2	H	267	TRP
2	H	270	TYR
2	H	425	ARG
2	H	618	ASN
2	H	633	ARG
2	H	661	LYS
2	H	662	HIS
2	H	751	ASP
2	H	752	LYS
2	H	823	THR
2	H	895	GLU
2	H	917	LYS
2	H	922	VAL
2	H	955	HIS
2	H	984	ARG
3	I	32	GLU
3	I	48	VAL
3	I	72	LYS
3	I	84	GLN
3	I	121	ASN
3	I	155	MET
3	I	163	ASN
3	I	229	ARG
3	I	237	ASN
3	I	241	PHE
3	I	268	CYS
3	I	291	MET
3	I	301	ARG
3	I	305	LYS
3	I	321	TRP
1	J	11	ARG
1	J	34	ARG
1	J	141	SER

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Mol	Chain	Res	Type
1	J	212	ARG
1	J	235	CYS
1	J	257	ARG
2	K	31	LEU
2	K	32	LYS
2	K	36	VAL
2	K	101	LEU
2	K	241	ARG
2	K	345	ASP
2	K	405	LYS
2	K	421	LYS
2	K	425	ARG
2	K	449	VAL
2	K	510	ARG
2	K	577	SER
2	K	618	ASN
2	K	647	LYS
2	K	648	VAL
2	K	649	LEU
2	K	765	ARG
2	K	781	LYS
2	K	938	ASN
2	K	984	ARG
2	K	1003	LEU
2	K	1061	ARG
3	L	163	ASN
3	L	216	SER
3	L	229	ARG
3	L	268	CYS
3	L	270	SER
3	L	271	LEU
3	L	301	ARG
3	L	302	ASN
3	L	305	LYS
1	M	12	ARG
1	M	20	SER
1	M	21	ARG
1	M	61	ASN
1	M	76	ASP
1	M	125	ILE
1	M	189	ARG
1	M	235	CYS

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Mol	Chain	Res	Type
1	M	241	ARG
1	M	259	MET
1	M	375	MET
2	N	116	LEU
2	N	124	ARG
2	N	237	TYR
2	N	425	ARG
2	N	461	VAL
2	N	469	LYS
2	N	471	ILE
2	N	475	GLU
2	N	476	ILE
2	N	511	LEU
2	N	618	ASN
2	N	653	ASN
2	N	654	VAL
2	N	722	LYS
2	N	752	LYS
2	N	800	MET
2	N	814	GLN
2	N	897	THR
2	N	984	ARG
2	N	996	TYR
2	N	1021	SER
2	N	1035	THR
2	N	1061	ARG
2	N	1122	VAL
2	N	1133	ASP
2	N	1147	ASP
3	O	48	VAL
3	O	84	GLN
3	O	110	TYR
3	O	142	LYS
3	O	210	GLN
3	O	215	LEU
3	O	229	ARG
3	O	241	PHE
3	O	246	SER
3	O	250	GLN
3	O	253	ASP
3	O	268	CYS
3	O	269	ARG

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Mol	Chain	Res	Type
3	O	282	VAL
3	O	286	SER
3	O	301	ARG
3	O	305	LYS
3	O	308	SER
1	P	11	ARG
1	P	12	ARG
1	P	24	HIS
1	P	151	SER
1	P	230	ARG
1	P	235	CYS
1	P	257	ARG
1	P	283	LEU
1	P	285	ARG
1	P	309	ARG
1	P	346	ARG
2	Q	60	ASP
2	Q	69	PRO
2	Q	82	ARG
2	Q	96	GLN
2	Q	99	SER
2	Q	108	ARG
2	Q	196	GLU
2	Q	237	TYR
2	Q	267	TRP
2	Q	302	LEU
2	Q	314	MET
2	Q	331	VAL
2	Q	351	ARG
2	Q	382	ASP
2	Q	383	PHE
2	Q	394	ARG
2	Q	395	VAL
2	Q	425	ARG
2	Q	431	PHE
2	Q	445	THR
2	Q	446	ARG
2	Q	449	VAL
2	Q	465	SER
2	Q	469	LYS
2	Q	479	MET
2	Q	482	LEU

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Mol	Chain	Res	Type
2	Q	483	GLU
2	Q	567	LYS
2	Q	625	ILE
2	Q	640	THR
2	Q	661	LYS
2	Q	827	ARG
2	Q	829	GLN
2	Q	847	HIS
2	Q	861	ILE
2	Q	888	ARG
2	Q	897	THR
2	Q	901	LYS
2	Q	933	PHE
2	Q	937	ASN
2	Q	959	ILE
2	Q	993	ASP
2	Q	1003	LEU
2	Q	1021	SER
2	Q	1055	SER
3	R	51	VAL
3	R	84	GLN
3	R	163	ASN
3	R	216	SER
3	R	229	ARG
3	R	236	LEU
3	R	253	ASP
3	R	315	SER
3	R	316	LEU
1	S	24	HIS
1	S	78	LYS
1	S	212	ARG
1	S	235	CYS
1	S	375	MET
2	T	96	GLN
2	T	150	GLU
2	T	220	ARG
2	T	237	TYR
2	T	293	MET
2	T	316	GLU
2	T	422	ASP
2	T	425	ARG
2	T	438	SER

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Mol	Chain	Res	Type
2	T	445	THR
2	T	446	ARG
2	T	469	LYS
2	T	476	ILE
2	T	618	ASN
2	T	653	ASN
2	T	656	LEU
2	T	661	LYS
2	T	713	SER
2	T	718	GLN
2	T	813	GLU
2	T	924	SER
2	T	954	GLU
2	T	983	ASP
2	T	984	ARG
2	T	1021	SER
2	T	1061	ARG
2	T	1116	LYS
3	U	35	LYS
3	U	142	LYS
3	U	143	ILE
3	U	144	THR
3	U	145	ILE
3	U	163	ASN
3	U	183	GLU
3	U	229	ARG
3	U	236	LEU
3	U	262	LYS
3	U	269	ARG
3	U	301	ARG
3	U	305	LYS
1	V	13	MET
1	V	24	HIS
1	V	61	ASN
1	V	64	GLU
1	V	66	LYS
1	V	67	PRO
1	V	76	ASP
1	V	102	TYR
1	V	116	ILE
1	V	126	ASN
1	V	146	GLU

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Mol	Chain	Res	Type
1	V	150	LYS
1	V	189	ARG
1	V	192	ILE
1	V	207	ARG
1	V	212	ARG
1	V	235	CYS
1	V	259	MET
1	V	366	THR
1	V	371	LYS
1	V	375	MET
1	V	379	THR
1	V	386	ASP
1	V	392	ARG
2	W	35	VAL
2	W	39	ASN
2	W	41	LEU
2	W	71	ASP
2	W	72	THR
2	W	89	VAL
2	W	92	ASN
2	W	124	ARG
2	W	130	ARG
2	W	157	THR
2	W	220	ARG
2	W	237	TYR
2	W	244	ASN
2	W	302	LEU
2	W	313	LYS
2	W	342	GLN
2	W	352	ASN
2	W	379	LYS
2	W	425	ARG
2	W	433	VAL
2	W	438	SER
2	W	442	LYS
2	W	468	LEU
2	W	470	THR
2	W	479	MET
2	W	491	ASP
2	W	496	SER
2	W	500	MET
2	W	502	ASN

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Mol	Chain	Res	Type
2	W	599	SER
2	W	618	ASN
2	W	633	ARG
2	W	654	VAL
2	W	656	LEU
2	W	658	ASN
2	W	666	MET
2	W	767	SER
2	W	801	LEU
2	W	892	LYS
2	W	924	SER
2	W	955	HIS
2	W	984	ARG
2	W	1000	ARG
2	W	1001	LEU
2	W	1042	LEU
2	W	1048	GLN
2	W	1049	SER
2	W	1061	ARG
2	W	1099	LYS
2	W	1107	LYS
2	W	1118	VAL
2	W	1124	THR
2	W	1138	PHE
2	W	1147	ASP
3	X	39	GLU
3	X	72	LYS
3	X	79	VAL
3	X	80	LYS
3	X	84	GLN
3	X	137	MET
3	X	142	LYS
3	X	146	SER
3	X	154	ARG
3	X	201	SER
3	X	227	LEU
3	X	229	ARG
3	X	259	GLU
3	X	278	ASP
3	X	279	VAL
3	X	305	LYS
3	X	308	SER

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Mol	Chain	Res	Type
3	X	309	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	GLN
2	B	276	GLN
2	B	304	GLN
2	B	655	ASN
2	B	790	ASN
1	D	143	ASN
2	E	1014	ASN
2	E	1020	HIS
3	F	302	ASN
3	F	306	ASN
1	G	302	ASN
3	I	104	HIS
3	I	302	ASN
2	K	551	ASN
2	K	653	ASN
2	K	923	HIS
2	K	937	ASN
2	K	1057	GLN
2	N	1020	HIS
2	Q	96	GLN
2	Q	342	GLN
2	Q	618	ASN
2	Q	814	GLN
2	Q	829	GLN
2	Q	932	ASN
2	Q	937	ASN
2	Q	1057	GLN
1	V	31	ASN
2	W	244	ASN
2	W	704	GLN
2	W	1048	GLN
3	X	163	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 88 ligands modelled in this entry, 24 are monoatomic - leaving 64 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	SF4	A	501	1	0,12,12	0.00	-	-		
4	SF4	Q	5804	2	0,12,12	0.00	-	-		
5	F3S	S	504	1	0,9,9	0.00	-	-		
4	SF4	J	503	1	0,12,12	0.00	-	-		
6	MD1	H	5802	7	38,51,51	6.87	21 (55%)	35,78,78	1.78	11 (31%)
5	F3S	J	504	1	0,9,9	0.00	-	-		
6	MD1	T	5801	7	38,51,51	6.81	21 (55%)	35,78,78	1.44	4 (11%)
4	SF4	V	501	1	0,12,12	0.00	-	-		
4	SF4	A	503	1	0,12,12	0.00	-	-		
4	SF4	N	5804	2	0,12,12	0.00	-	-		
8	HEM	R	401	3	27,50,50	1.89	5 (18%)	17,82,82	1.52	4 (23%)
8	HEM	L	401	3	27,50,50	1.88	5 (18%)	17,82,82	1.43	3 (17%)
8	HEM	I	401	3	27,50,50	1.96	9 (33%)	17,82,82	1.95	5 (29%)
4	SF4	W	5804	2	0,12,12	0.00	-	-		
4	SF4	D	503	1	0,12,12	0.00	-	-		
4	SF4	P	501	1	0,12,12	0.00	-	-		
6	MD1	Q	5801	7	38,51,51	6.66	21 (55%)	35,78,78	1.65	7 (20%)
8	HEM	F	401	-	27,50,50	1.95	5 (18%)	17,82,82	2.23	7 (41%)
4	SF4	G	502	1	0,12,12	0.00	-	-		
8	HEM	C	401	3	27,50,50	1.86	5 (18%)	17,82,82	1.52	4 (23%)
4	SF4	E	5804	2	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	F3S	M	504	1	0,9,9	0.00	-	-		
4	SF4	A	502	1	0,12,12	0.00	-	-		
4	SF4	D	502	1	0,12,12	0.00	-	-		
4	SF4	J	501	1	0,12,12	0.00	-	-		
5	F3S	V	504	1	0,9,9	0.00	-	-		
6	MD1	E	5801	7,6	38,51,51	6.61	22 (57%)	35,78,78	1.68	8 (22%)
6	MD1	K	5802	7	38,51,51	6.89	21 (55%)	35,78,78	1.64	13 (37%)
6	MD1	N	5801	7	38,51,51	6.78	21 (55%)	35,78,78	1.52	7 (20%)
4	SF4	M	503	1	0,12,12	0.00	-	-		
4	SF4	G	501	1	0,12,12	0.00	-	-		
6	MD1	T	5802	7	38,51,51	6.91	21 (55%)	35,78,78	1.79	12 (34%)
6	MD1	E	5802	7,6	38,51,51	6.93	21 (55%)	35,78,78	1.80	10 (28%)
6	MD1	W	5801	7	38,51,51	6.78	21 (55%)	35,78,78	1.51	5 (14%)
4	SF4	D	501	1	0,12,12	0.00	-	-		
4	SF4	M	501	1	0,12,12	0.00	-	-		
8	HEM	U	401	3	27,50,50	1.88	4 (14%)	17,82,82	1.63	3 (17%)
4	SF4	P	503	1	0,12,12	0.00	-	-		
4	SF4	V	502	1	0,12,12	0.00	-	-		
4	SF4	G	503	1	0,12,12	0.00	-	-		
4	SF4	S	503	1	0,12,12	0.00	-	-		
6	MD1	B	5801	7	38,51,51	6.80	21 (55%)	35,78,78	1.45	5 (14%)
8	HEM	O	401	3	27,50,50	1.83	5 (18%)	17,82,82	1.77	5 (29%)
6	MD1	Q	5802	7	38,51,51	6.87	21 (55%)	35,78,78	1.80	11 (31%)
4	SF4	S	501	1	0,12,12	0.00	-	-		
4	SF4	H	5804	2	0,12,12	0.00	-	-		
4	SF4	S	502	1	0,12,12	0.00	-	-		
4	SF4	P	502	1	0,12,12	0.00	-	-		
5	F3S	G	504	1	0,9,9	0.00	-	-		
6	MD1	N	5802	7	38,51,51	6.89	21 (55%)	35,78,78	1.76	12 (34%)
6	MD1	W	5802	7	38,51,51	6.90	21 (55%)	35,78,78	1.83	11 (31%)
4	SF4	J	502	1	0,12,12	0.00	-	-		
5	F3S	P	504	1	0,9,9	0.00	-	-		
6	MD1	H	5801	7	38,51,51	6.80	21 (55%)	35,78,78	1.52	6 (17%)
6	MD1	B	5802	7	38,51,51	6.89	21 (55%)	35,78,78	1.84	9 (25%)
5	F3S	D	504	1	0,9,9	0.00	-	-		
4	SF4	M	502	1	0,12,12	0.00	-	-		
4	SF4	B	5804	2	0,12,12	0.00	-	-		
4	SF4	T	5804	2	0,12,12	0.00	-	-		
4	SF4	K	5804	2	0,12,12	0.00	-	-		
4	SF4	V	503	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MD1	K	5801	7	38,51,51	6.78	21 (55%)	35,78,78	1.56	7 (20%)
8	HEM	X	401	3	27,50,50	1.95	4 (14%)	17,82,82	1.48	2 (11%)
5	F3S	A	504	1	0,9,9	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	A	501	1	-	-	0/6/5/5
4	SF4	Q	5804	2	-	-	0/6/5/5
5	F3S	S	504	1	-	-	0/3/3/3
4	SF4	J	503	1	-	-	0/6/5/5
6	MD1	H	5802	7	-	3/21/59/59	0/5/5/5
5	F3S	J	504	1	-	-	0/3/3/3
6	MD1	T	5801	7	-	11/21/59/59	0/5/5/5
4	SF4	V	501	1	-	-	0/6/5/5
8	HEM	R	401	3	-	1/6/54/54	-
4	SF4	A	503	1	-	-	0/6/5/5
4	SF4	N	5804	2	-	-	0/6/5/5
8	HEM	L	401	3	-	0/6/54/54	-
8	HEM	I	401	3	-	3/6/54/54	-
4	SF4	W	5804	2	-	-	0/6/5/5
8	HEM	F	401	-	-	2/6/54/54	-
6	MD1	Q	5801	7	-	10/21/59/59	0/5/5/5
4	SF4	D	503	1	-	-	0/6/5/5
4	SF4	P	501	1	-	-	0/6/5/5
8	HEM	C	401	3	-	1/6/54/54	-
4	SF4	G	502	1	-	-	0/6/5/5
4	SF4	E	5804	2	-	-	0/6/5/5
5	F3S	M	504	1	-	-	0/3/3/3
6	MD1	T	5802	7	-	3/21/59/59	0/5/5/5
6	MD1	E	5801	7,6	1/1/10/12	9/21/59/59	0/5/5/5
4	SF4	A	502	1	-	-	0/6/5/5
6	MD1	K	5802	7	-	3/21/59/59	0/5/5/5
6	MD1	N	5801	7	-	11/21/59/59	0/5/5/5
4	SF4	D	502	1	-	-	0/6/5/5
4	SF4	J	501	1	-	-	0/6/5/5
4	SF4	M	503	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	G	501	1	-	-	0/6/5/5
6	MD1	E	5802	7,6	-	4/21/59/59	0/5/5/5
4	SF4	D	501	1	-	-	0/6/5/5
4	SF4	M	501	1	-	-	0/6/5/5
8	HEM	U	401	3	-	1/6/54/54	-
4	SF4	P	503	1	-	-	0/6/5/5
4	SF4	V	502	1	-	-	0/6/5/5
4	SF4	G	503	1	-	-	0/6/5/5
4	SF4	S	503	1	-	-	0/6/5/5
6	MD1	B	5801	7	-	10/21/59/59	0/5/5/5
8	HEM	O	401	3	-	0/6/54/54	-
6	MD1	Q	5802	7	-	9/21/59/59	0/5/5/5
4	SF4	S	501	1	-	-	0/6/5/5
4	SF4	H	5804	2	-	-	0/6/5/5
5	F3S	V	504	1	-	-	0/3/3/3
4	SF4	S	502	1	-	-	0/6/5/5
4	SF4	P	502	1	-	-	0/6/5/5
5	F3S	G	504	1	-	-	0/3/3/3
6	MD1	N	5802	7	-	3/21/59/59	0/5/5/5
6	MD1	W	5802	7	-	6/21/59/59	0/5/5/5
4	SF4	J	502	1	-	-	0/6/5/5
6	MD1	H	5801	7	-	11/21/59/59	0/5/5/5
5	F3S	P	504	1	-	-	0/3/3/3
6	MD1	B	5802	7	-	3/21/59/59	0/5/5/5
5	F3S	D	504	1	-	-	0/3/3/3
4	SF4	M	502	1	-	-	0/6/5/5
4	SF4	V	503	1	-	-	0/6/5/5
4	SF4	B	5804	2	-	-	0/6/5/5
4	SF4	T	5804	2	-	-	0/6/5/5
4	SF4	K	5804	2	-	-	0/6/5/5
6	MD1	W	5801	7	-	10/21/59/59	0/5/5/5
6	MD1	K	5801	7	-	11/21/59/59	0/5/5/5
8	HEM	X	401	3	-	0/6/54/54	-
5	F3S	A	504	1	-	-	0/3/3/3

All (379) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5802	MD1	C7-N8	28.72	1.61	1.27
6	T	5802	MD1	C7-N8	28.42	1.61	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	5802	MD1	C7-N8	28.38	1.61	1.27
6	W	5802	MD1	C7-N8	28.25	1.61	1.27
6	N	5802	MD1	C7-N8	28.22	1.61	1.27
6	B	5802	MD1	C7-N8	28.13	1.61	1.27
6	Q	5802	MD1	C7-N8	28.10	1.60	1.27
6	H	5802	MD1	C7-N8	28.06	1.60	1.27
6	H	5801	MD1	C7-N8	27.80	1.60	1.27
6	T	5801	MD1	C7-N8	27.79	1.60	1.27
6	K	5801	MD1	C7-N8	27.66	1.60	1.27
6	W	5801	MD1	C7-N8	27.64	1.60	1.27
6	B	5801	MD1	C7-N8	27.59	1.60	1.27
6	N	5801	MD1	C7-N8	27.39	1.60	1.27
6	Q	5801	MD1	C7-N8	26.08	1.58	1.27
6	E	5801	MD1	C7-N8	25.24	1.57	1.27
6	E	5801	MD1	C4-N9	-11.41	1.32	1.47
6	B	5801	MD1	C4-N9	-11.30	1.32	1.47
6	K	5802	MD1	C17-N17	11.19	1.55	1.35
6	B	5802	MD1	C17-N17	11.09	1.55	1.35
6	W	5802	MD1	C17-N17	11.09	1.55	1.35
6	Q	5802	MD1	C17-N17	11.08	1.55	1.35
6	H	5802	MD1	C17-N17	11.07	1.55	1.35
6	Q	5801	MD1	C17-N17	11.06	1.55	1.35
6	N	5802	MD1	C17-N17	11.06	1.55	1.35
6	N	5801	MD1	C4-N9	-11.04	1.33	1.47
6	E	5801	MD1	C17-N17	11.04	1.55	1.35
6	T	5802	MD1	C17-N17	11.01	1.55	1.35
6	E	5802	MD1	C17-N17	10.99	1.54	1.35
6	W	5801	MD1	C4-N9	-10.92	1.33	1.47
6	T	5801	MD1	C17-N17	10.91	1.54	1.35
6	H	5802	MD1	C4-N9	-10.90	1.33	1.47
6	H	5801	MD1	C17-N17	10.90	1.54	1.35
6	B	5801	MD1	C17-N17	10.90	1.54	1.35
6	K	5801	MD1	C4-N9	-10.87	1.33	1.47
6	K	5802	MD1	C4-N9	-10.87	1.33	1.47
6	Q	5802	MD1	C4-N9	-10.87	1.33	1.47
6	N	5801	MD1	C17-N17	10.84	1.54	1.35
6	T	5801	MD1	C4-N9	-10.82	1.33	1.47
6	H	5801	MD1	C4-N9	-10.81	1.33	1.47
6	B	5802	MD1	C4-N9	-10.80	1.33	1.47
6	N	5802	MD1	C4-N9	-10.80	1.33	1.47
6	T	5802	MD1	C4-N9	-10.79	1.33	1.47
6	W	5802	MD1	C4-N9	-10.74	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	5801	MD1	C4-N9	-10.74	1.33	1.47
6	E	5802	MD1	C4-N9	-10.66	1.33	1.47
6	W	5801	MD1	C17-N17	10.63	1.54	1.35
6	K	5801	MD1	C17-N17	10.55	1.54	1.35
6	E	5801	MD1	C3'-C4'	-9.82	1.27	1.53
6	Q	5801	MD1	C15-N17	9.77	1.50	1.33
6	W	5802	MD1	C3'-C4'	-9.69	1.28	1.53
6	H	5801	MD1	C3'-C4'	-9.69	1.28	1.53
6	Q	5801	MD1	C3'-C4'	-9.69	1.28	1.53
6	B	5801	MD1	C3'-C4'	-9.66	1.28	1.53
6	E	5802	MD1	C3'-C4'	-9.66	1.28	1.53
6	T	5801	MD1	C3'-C4'	-9.61	1.28	1.53
6	N	5802	MD1	C3'-C4'	-9.61	1.28	1.53
6	B	5802	MD1	C3'-C4'	-9.58	1.28	1.53
6	H	5802	MD1	C3'-C4'	-9.56	1.28	1.53
6	K	5801	MD1	C3'-C4'	-9.56	1.28	1.53
6	T	5802	MD1	C3'-C4'	-9.55	1.28	1.53
6	N	5801	MD1	C3'-C4'	-9.55	1.28	1.53
6	W	5801	MD1	C3'-C4'	-9.54	1.28	1.53
6	Q	5802	MD1	C3'-C4'	-9.53	1.28	1.53
6	K	5802	MD1	C3'-C4'	-9.53	1.28	1.53
6	E	5802	MD1	C17-N18	9.40	1.52	1.35
6	K	5801	MD1	C17-N18	9.34	1.52	1.35
6	B	5802	MD1	C15-N17	9.32	1.49	1.33
6	T	5802	MD1	C17-N18	9.31	1.51	1.35
6	W	5802	MD1	C15-N17	9.26	1.49	1.33
6	E	5801	MD1	C15-N17	9.26	1.49	1.33
6	B	5801	MD1	C15-N17	9.25	1.49	1.33
6	Q	5802	MD1	C15-N17	9.24	1.49	1.33
6	T	5802	MD1	C15-N17	9.23	1.49	1.33
6	W	5802	MD1	C17-N18	9.22	1.51	1.35
6	K	5802	MD1	C15-N17	9.20	1.49	1.33
6	N	5802	MD1	C15-N17	9.19	1.49	1.33
6	E	5802	MD1	C15-N17	9.18	1.49	1.33
6	N	5801	MD1	C15-N17	9.15	1.49	1.33
6	N	5802	MD1	C17-N18	9.14	1.51	1.35
6	H	5801	MD1	C15-N17	9.13	1.48	1.33
6	H	5802	MD1	C15-N17	9.13	1.48	1.33
6	W	5801	MD1	C17-N18	9.13	1.51	1.35
6	N	5801	MD1	C17-N18	9.11	1.51	1.35
6	B	5802	MD1	C17-N18	9.10	1.51	1.35
6	T	5801	MD1	C17-N18	9.10	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	5801	MD1	C15-N17	9.09	1.48	1.33
6	H	5802	MD1	C17-N18	9.04	1.51	1.35
6	H	5801	MD1	C17-N18	9.01	1.51	1.35
6	W	5801	MD1	C15-N17	8.99	1.48	1.33
6	B	5801	MD1	C17-N18	8.96	1.51	1.35
6	Q	5802	MD1	C17-N18	8.93	1.51	1.35
6	K	5801	MD1	C15-N17	8.86	1.48	1.33
6	K	5802	MD1	C17-N18	8.85	1.51	1.35
6	E	5801	MD1	O11-C11	8.72	1.61	1.42
6	E	5801	MD1	C17-N18	8.67	1.50	1.35
6	Q	5801	MD1	O11-C11	8.55	1.61	1.42
6	B	5801	MD1	O11-C11	8.49	1.61	1.42
6	Q	5801	MD1	C17-N18	8.47	1.50	1.35
6	W	5802	MD1	O11-C11	8.46	1.61	1.42
6	E	5802	MD1	O11-C11	8.45	1.61	1.42
6	W	5801	MD1	O11-C11	8.45	1.61	1.42
6	T	5801	MD1	O11-C11	8.45	1.61	1.42
6	K	5802	MD1	O11-C11	8.43	1.61	1.42
6	H	5801	MD1	O11-C11	8.42	1.61	1.42
6	K	5801	MD1	O11-C11	8.41	1.61	1.42
6	N	5801	MD1	O11-C11	8.41	1.61	1.42
6	H	5802	MD1	O11-C11	8.40	1.60	1.42
6	N	5802	MD1	O11-C11	8.37	1.60	1.42
6	B	5802	MD1	O11-C11	8.37	1.60	1.42
6	T	5802	MD1	O11-C11	8.36	1.60	1.42
6	Q	5802	MD1	O11-C11	8.36	1.60	1.42
6	W	5802	MD1	C2'-C1'	-8.16	1.27	1.53
6	Q	5802	MD1	C2'-C1'	-8.15	1.27	1.53
6	N	5802	MD1	C2'-C1'	-8.12	1.27	1.53
6	K	5802	MD1	C2'-C1'	-8.12	1.27	1.53
6	T	5802	MD1	C2'-C1'	-8.10	1.27	1.53
6	B	5802	MD1	C2'-C1'	-8.10	1.27	1.53
6	H	5802	MD1	C2'-C1'	-8.08	1.27	1.53
6	E	5802	MD1	C2'-C1'	-8.05	1.27	1.53
6	B	5801	MD1	C2'-C1'	-8.04	1.27	1.53
6	E	5801	MD1	C2'-C1'	-8.04	1.27	1.53
6	W	5801	MD1	C2'-C1'	-8.02	1.27	1.53
6	K	5801	MD1	C2'-C1'	-8.00	1.27	1.53
6	N	5801	MD1	C2'-C1'	-7.99	1.27	1.53
6	T	5801	MD1	C2'-C1'	-7.99	1.27	1.53
6	H	5801	MD1	C2'-C1'	-7.98	1.28	1.53
6	Q	5801	MD1	C2'-C1'	-7.97	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	5801	MD1	C13-C12	7.43	1.57	1.34
6	K	5801	MD1	C20-N18	7.14	1.44	1.34
6	E	5801	MD1	C13-C12	7.12	1.56	1.34
6	N	5801	MD1	C13-C12	7.09	1.56	1.34
6	W	5801	MD1	C13-C12	7.06	1.56	1.34
6	W	5802	MD1	C20-N18	7.01	1.44	1.34
6	E	5802	MD1	C20-N18	7.00	1.44	1.34
6	T	5802	MD1	C20-N18	7.00	1.44	1.34
6	B	5801	MD1	C13-C12	6.99	1.56	1.34
6	T	5801	MD1	C13-C12	6.98	1.56	1.34
6	H	5802	MD1	C14-C13	-6.97	1.43	1.51
6	N	5801	MD1	C20-N18	6.97	1.44	1.34
6	W	5801	MD1	C20-N18	6.96	1.44	1.34
6	K	5801	MD1	C13-C12	6.93	1.56	1.34
6	T	5801	MD1	C20-N18	6.92	1.44	1.34
6	B	5802	MD1	C20-N18	6.88	1.44	1.34
6	Q	5802	MD1	C13-C12	6.87	1.55	1.34
6	H	5801	MD1	C13-C12	6.85	1.55	1.34
6	H	5802	MD1	C20-N18	6.85	1.44	1.34
6	N	5802	MD1	C13-C12	6.83	1.55	1.34
6	N	5802	MD1	C20-N18	6.83	1.44	1.34
6	B	5802	MD1	C13-C12	6.82	1.55	1.34
6	H	5801	MD1	C20-N18	6.82	1.44	1.34
6	K	5802	MD1	C13-C12	6.82	1.55	1.34
6	Q	5802	MD1	C14-C13	-6.81	1.43	1.51
6	B	5801	MD1	C20-N18	6.81	1.44	1.34
6	T	5802	MD1	C13-C12	6.77	1.55	1.34
6	N	5802	MD1	C14-C13	-6.76	1.44	1.51
6	H	5802	MD1	C13-C12	6.75	1.55	1.34
6	W	5802	MD1	C13-C12	6.71	1.55	1.34
6	K	5802	MD1	C14-C13	-6.64	1.44	1.51
6	E	5802	MD1	C13-C12	6.61	1.55	1.34
6	Q	5802	MD1	C20-N18	6.60	1.44	1.34
6	E	5801	MD1	C20-N18	6.56	1.44	1.34
6	B	5802	MD1	C14-C13	-6.55	1.44	1.51
6	E	5801	MD1	C14-C13	-6.52	1.44	1.51
6	Q	5801	MD1	C15-C16	6.46	1.50	1.41
6	W	5801	MD1	C6-N1	6.46	1.43	1.33
6	Q	5802	MD1	C6-N1	6.44	1.43	1.33
6	K	5802	MD1	C20-N18	6.44	1.43	1.34
6	W	5802	MD1	C14-C13	-6.42	1.44	1.51
6	N	5801	MD1	C6-N1	6.42	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	5802	MD1	C6-N1	6.42	1.43	1.33
6	T	5801	MD1	C6-N1	6.41	1.43	1.33
6	B	5802	MD1	C6-N1	6.40	1.43	1.33
6	T	5802	MD1	C14-C13	-6.38	1.44	1.51
6	N	5802	MD1	C6-N1	6.37	1.43	1.33
6	T	5802	MD1	C6-N1	6.36	1.43	1.33
6	K	5801	MD1	C6-N1	6.35	1.43	1.33
6	H	5801	MD1	C6-N1	6.35	1.43	1.33
6	H	5802	MD1	C6-N1	6.34	1.43	1.33
6	Q	5801	MD1	C6-N1	6.31	1.43	1.33
6	B	5801	MD1	C6-N1	6.26	1.43	1.33
6	E	5801	MD1	C6-N1	6.25	1.43	1.33
6	E	5802	MD1	C6-N1	6.24	1.43	1.33
6	W	5802	MD1	C6-N1	6.18	1.43	1.33
6	Q	5801	MD1	C20-N18	6.13	1.43	1.34
6	T	5801	MD1	O4'-C1'	6.06	1.56	1.42
6	B	5801	MD1	O4'-C1'	6.04	1.56	1.42
6	Q	5801	MD1	O4'-C1'	6.01	1.56	1.42
6	W	5801	MD1	O4'-C1'	6.00	1.56	1.42
6	K	5801	MD1	O4'-C1'	5.98	1.56	1.42
6	N	5801	MD1	O4'-C1'	5.96	1.56	1.42
6	E	5802	MD1	C14-C13	-5.95	1.44	1.51
6	E	5801	MD1	O4'-C1'	5.93	1.56	1.42
6	W	5802	MD1	O4'-C1'	5.91	1.56	1.42
6	H	5801	MD1	O4'-C1'	5.91	1.56	1.42
6	W	5801	MD1	C15-C16	5.86	1.49	1.41
6	E	5802	MD1	O4'-C1'	5.85	1.55	1.42
6	N	5802	MD1	O4'-C1'	5.85	1.55	1.42
6	H	5802	MD1	O4'-C1'	5.84	1.55	1.42
6	B	5802	MD1	O4'-C1'	5.84	1.55	1.42
6	N	5801	MD1	C17-N16	5.84	1.45	1.33
6	T	5802	MD1	C17-N16	5.83	1.45	1.33
6	W	5802	MD1	C17-N16	5.83	1.45	1.33
6	E	5801	MD1	C17-N16	5.83	1.45	1.33
6	N	5802	MD1	C17-N16	5.82	1.45	1.33
6	K	5802	MD1	O4'-C1'	5.82	1.55	1.42
6	B	5801	MD1	C17-N16	5.81	1.45	1.33
6	H	5801	MD1	C17-N16	5.81	1.45	1.33
6	W	5801	MD1	C17-N16	5.81	1.45	1.33
6	K	5801	MD1	C17-N16	5.80	1.45	1.33
6	T	5802	MD1	O4'-C1'	5.80	1.55	1.42
6	E	5802	MD1	C17-N16	5.80	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5802	MD1	C17-N16	5.80	1.45	1.33
6	Q	5802	MD1	O4'-C1'	5.79	1.55	1.42
6	E	5801	MD1	C15-C16	5.76	1.49	1.41
6	T	5801	MD1	C17-N16	5.71	1.45	1.33
6	T	5801	MD1	C15-C16	5.70	1.49	1.41
6	H	5801	MD1	C15-C16	5.70	1.49	1.41
8	I	401	HEM	C3B-C2B	-5.67	1.32	1.40
6	H	5802	MD1	C17-N16	5.67	1.45	1.33
6	B	5801	MD1	C15-C16	5.66	1.49	1.41
6	Q	5801	MD1	C14-C13	-5.65	1.45	1.51
6	B	5802	MD1	C15-C16	5.64	1.49	1.41
6	Q	5802	MD1	C17-N16	5.64	1.45	1.33
6	N	5801	MD1	C15-C16	5.59	1.49	1.41
6	E	5802	MD1	C15-C16	5.58	1.49	1.41
6	T	5802	MD1	C15-C16	5.57	1.49	1.41
6	Q	5801	MD1	C17-N16	5.57	1.45	1.33
6	K	5801	MD1	C15-C16	5.57	1.49	1.41
6	W	5802	MD1	C15-C16	5.50	1.49	1.41
6	K	5802	MD1	C15-C16	5.50	1.49	1.41
6	Q	5802	MD1	C15-C16	5.46	1.48	1.41
6	N	5802	MD1	C15-C16	5.45	1.48	1.41
6	K	5802	MD1	C17-N16	5.41	1.44	1.33
6	H	5802	MD1	C15-C16	5.28	1.48	1.41
6	W	5802	MD1	O4'-C4'	5.25	1.56	1.45
6	K	5802	MD1	O4'-C4'	5.19	1.56	1.45
6	B	5802	MD1	O4'-C4'	5.18	1.56	1.45
6	E	5802	MD1	O4'-C4'	5.17	1.56	1.45
6	Q	5802	MD1	O4'-C4'	5.16	1.56	1.45
6	T	5802	MD1	O4'-C4'	5.15	1.56	1.45
6	N	5802	MD1	O4'-C4'	5.14	1.56	1.45
6	H	5801	MD1	C14-C13	-5.13	1.45	1.51
6	H	5802	MD1	O4'-C4'	5.11	1.56	1.45
6	N	5801	MD1	C14-C13	-5.05	1.45	1.51
6	Q	5801	MD1	O4'-C4'	5.05	1.56	1.45
6	T	5801	MD1	O4'-C4'	5.05	1.56	1.45
6	T	5801	MD1	C14-C13	-5.03	1.45	1.51
6	H	5801	MD1	O4'-C4'	5.02	1.56	1.45
6	K	5801	MD1	O4'-C4'	4.99	1.56	1.45
6	N	5801	MD1	O4'-C4'	4.98	1.56	1.45
8	F	401	HEM	C3B-C2B	-4.95	1.33	1.40
6	W	5801	MD1	O4'-C4'	4.92	1.56	1.45
6	B	5801	MD1	O4'-C4'	4.92	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	5801	MD1	C14-C13	-4.88	1.46	1.51
6	B	5801	MD1	C14-C13	-4.87	1.46	1.51
6	B	5802	MD1	C3'-C2'	4.79	1.66	1.53
6	Q	5801	MD1	C3'-C2'	4.77	1.66	1.53
6	H	5802	MD1	C3'-C2'	4.77	1.66	1.53
6	T	5802	MD1	C3'-C2'	4.77	1.66	1.53
6	E	5801	MD1	O4'-C4'	4.76	1.55	1.45
6	W	5801	MD1	C3'-C2'	4.76	1.66	1.53
6	K	5802	MD1	C3'-C2'	4.75	1.66	1.53
6	N	5801	MD1	C3'-C2'	4.75	1.66	1.53
6	H	5801	MD1	C3'-C2'	4.75	1.66	1.53
6	T	5801	MD1	C3'-C2'	4.74	1.66	1.53
6	Q	5802	MD1	C3'-C2'	4.74	1.66	1.53
6	N	5802	MD1	C3'-C2'	4.73	1.66	1.53
6	K	5801	MD1	C3'-C2'	4.72	1.66	1.53
8	X	401	HEM	C3B-C2B	-4.71	1.33	1.40
8	R	401	HEM	C3C-C2C	-4.69	1.33	1.40
6	B	5801	MD1	C3'-C2'	4.68	1.66	1.53
6	W	5802	MD1	C3'-C2'	4.67	1.66	1.53
6	E	5802	MD1	C3'-C2'	4.65	1.66	1.53
8	L	401	HEM	C3C-C2C	-4.64	1.33	1.40
6	E	5801	MD1	C3'-C2'	4.61	1.66	1.53
8	X	401	HEM	C3C-C2C	-4.58	1.34	1.40
8	C	401	HEM	C3C-C2C	-4.51	1.34	1.40
8	U	401	HEM	C3C-C2C	-4.51	1.34	1.40
6	W	5801	MD1	C14-C13	-4.45	1.46	1.51
8	F	401	HEM	C3C-CAC	4.32	1.56	1.47
8	F	401	HEM	C3C-C2C	-4.17	1.34	1.40
8	U	401	HEM	C3B-CAB	3.82	1.55	1.47
8	O	401	HEM	C3C-CAC	3.78	1.55	1.47
8	O	401	HEM	C3B-CAB	3.78	1.55	1.47
8	C	401	HEM	C3B-CAB	3.78	1.55	1.47
8	R	401	HEM	C3B-CAB	3.76	1.55	1.47
8	L	401	HEM	C3B-CAB	3.73	1.55	1.47
8	U	401	HEM	C3B-C2B	-3.71	1.35	1.40
8	R	401	HEM	C3B-C2B	-3.70	1.35	1.40
8	R	401	HEM	C3C-CAC	3.65	1.55	1.47
8	X	401	HEM	C3C-CAC	3.64	1.55	1.47
8	O	401	HEM	C3C-C2C	-3.64	1.35	1.40
8	L	401	HEM	C3C-CAC	3.61	1.55	1.47
8	L	401	HEM	C3B-C2B	-3.59	1.35	1.40
8	X	401	HEM	C3B-CAB	3.59	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	401	HEM	C3B-C2B	-3.55	1.35	1.40
8	C	401	HEM	C3C-CAC	3.54	1.55	1.47
8	O	401	HEM	C3B-C2B	-3.49	1.35	1.40
8	U	401	HEM	C3C-CAC	3.46	1.54	1.47
8	I	401	HEM	CAA-C2A	-3.40	1.47	1.52
8	F	401	HEM	C3B-CAB	3.23	1.54	1.47
6	W	5802	MD1	C8-N9	-3.08	1.35	1.45
6	E	5802	MD1	C8-N9	-3.08	1.35	1.45
6	N	5802	MD1	C8-N9	-3.07	1.35	1.45
6	E	5801	MD1	C8-N9	-3.07	1.35	1.45
6	W	5801	MD1	C8-N9	-3.07	1.35	1.45
6	B	5801	MD1	C8-N9	-3.07	1.35	1.45
6	T	5802	MD1	C8-N9	-3.06	1.35	1.45
6	Q	5802	MD1	C8-N9	-3.06	1.35	1.45
6	K	5802	MD1	C8-N9	-3.06	1.35	1.45
6	H	5802	MD1	C8-N9	-3.06	1.35	1.45
6	N	5801	MD1	C8-N9	-3.06	1.35	1.45
6	Q	5801	MD1	C8-N9	-3.05	1.35	1.45
6	T	5801	MD1	C8-N9	-3.05	1.35	1.45
6	K	5801	MD1	C8-N9	-3.05	1.35	1.45
6	B	5802	MD1	C8-N9	-3.04	1.35	1.45
6	H	5801	MD1	C8-N9	-3.03	1.35	1.45
8	I	401	HEM	C1D-ND	-2.72	1.30	1.36
6	E	5801	MD1	C5-C4	-2.69	1.36	1.53
6	B	5802	MD1	C5-C4	-2.67	1.36	1.53
6	B	5801	MD1	C5-C4	-2.66	1.36	1.53
6	Q	5802	MD1	C5-C4	-2.65	1.36	1.53
6	H	5802	MD1	C5-C4	-2.65	1.36	1.53
6	T	5802	MD1	C5-C4	-2.65	1.36	1.53
6	W	5801	MD1	C5-C4	-2.65	1.36	1.53
6	W	5802	MD1	C5-C4	-2.65	1.36	1.53
6	K	5802	MD1	C5-C4	-2.64	1.36	1.53
6	N	5801	MD1	C5-C4	-2.64	1.36	1.53
6	E	5802	MD1	C5-C4	-2.64	1.36	1.53
6	Q	5801	MD1	C5-C4	-2.64	1.36	1.53
6	K	5801	MD1	C5-C4	-2.63	1.36	1.53
6	N	5802	MD1	C5-C4	-2.63	1.36	1.53
6	T	5801	MD1	C5-C4	-2.63	1.36	1.53
6	H	5801	MD1	C5-C4	-2.62	1.36	1.53
6	W	5802	MD1	O6-C6	-2.50	1.18	1.23
8	I	401	HEM	C1C-C2C	-2.45	1.37	1.42
8	O	401	HEM	CAA-C2A	2.43	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5801	MD1	O6-C6	-2.39	1.18	1.23
6	E	5802	MD1	O6-C6	-2.33	1.18	1.23
6	B	5802	MD1	O6-C6	-2.32	1.18	1.23
6	Q	5801	MD1	O6-C6	-2.31	1.18	1.23
6	W	5801	MD1	O6-C6	-2.31	1.18	1.23
6	N	5802	MD1	O6-C6	-2.31	1.18	1.23
6	K	5801	MD1	O14-C15	-2.31	1.18	1.24
8	I	401	HEM	C4A-CHB	-2.30	1.34	1.41
6	W	5801	MD1	O14-C15	-2.28	1.18	1.24
8	L	401	HEM	CAA-C2A	2.28	1.55	1.52
6	N	5801	MD1	O6-C6	-2.28	1.18	1.23
6	Q	5802	MD1	O6-C6	-2.28	1.18	1.23
8	F	401	HEM	CAA-C2A	2.28	1.55	1.52
6	H	5802	MD1	O6-C6	-2.27	1.18	1.23
6	B	5801	MD1	O6-C6	-2.27	1.18	1.23
6	T	5802	MD1	O6-C6	-2.27	1.18	1.23
6	K	5802	MD1	O6-C6	-2.27	1.18	1.23
6	T	5801	MD1	O6-C6	-2.27	1.18	1.23
6	K	5801	MD1	O6-C6	-2.26	1.18	1.23
6	N	5801	MD1	O14-C15	-2.25	1.18	1.24
6	T	5801	MD1	O14-C15	-2.25	1.18	1.24
6	H	5801	MD1	O6-C6	-2.25	1.18	1.23
6	B	5801	MD1	O14-C15	-2.24	1.18	1.24
6	H	5801	MD1	O14-C15	-2.24	1.18	1.24
6	B	5802	MD1	O14-C15	-2.22	1.19	1.24
6	T	5802	MD1	O14-C15	-2.22	1.19	1.24
6	W	5802	MD1	O14-C15	-2.22	1.19	1.24
6	N	5802	MD1	O14-C15	-2.21	1.19	1.24
6	E	5802	MD1	O14-C15	-2.21	1.19	1.24
6	H	5802	MD1	O14-C15	-2.20	1.19	1.24
6	E	5801	MD1	O14-C15	-2.19	1.19	1.24
6	Q	5801	MD1	O14-C15	-2.19	1.19	1.24
6	Q	5802	MD1	O14-C15	-2.17	1.19	1.24
6	E	5801	MD1	C16-N15	2.17	1.42	1.38
8	I	401	HEM	C2A-C3A	-2.16	1.31	1.37
6	K	5802	MD1	O14-C15	-2.12	1.19	1.24
8	R	401	HEM	CAA-C2A	2.10	1.55	1.52
8	I	401	HEM	C3C-C2C	-2.07	1.37	1.40
8	I	401	HEM	C1A-CHA	-2.07	1.35	1.41
8	I	401	HEM	CAD-C3D	-2.06	1.48	1.52
8	C	401	HEM	CAA-C2A	2.06	1.55	1.52

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	5801	MD1	C4-C5-N7	4.25	108.09	102.46
6	H	5801	MD1	C4-C5-N7	4.24	108.08	102.46
6	E	5802	MD1	C4-C5-N7	4.21	108.05	102.46
6	W	5802	MD1	C4-C5-N7	4.21	108.03	102.46
8	F	401	HEM	CMA-C3A-C4A	-4.17	122.06	128.46
6	T	5801	MD1	C4-C5-N7	4.16	107.98	102.46
6	B	5802	MD1	C4-C5-N7	4.16	107.97	102.46
6	H	5802	MD1	C4-C5-N7	4.15	107.95	102.46
6	W	5801	MD1	C4-C5-N7	4.12	107.92	102.46
8	I	401	HEM	CBD-CAD-C3D	-4.12	104.89	112.48
6	T	5802	MD1	C4-C5-N7	4.10	107.90	102.46
6	N	5802	MD1	C4-C5-N7	4.10	107.90	102.46
6	N	5801	MD1	C4-C5-N7	4.10	107.89	102.46
6	K	5801	MD1	C4-C5-N7	4.09	107.88	102.46
6	E	5801	MD1	C4-C5-N7	4.02	107.79	102.46
6	Q	5802	MD1	C4-C5-N7	4.00	107.77	102.46
6	E	5802	MD1	O11-C11-C12	3.99	118.24	111.05
6	E	5801	MD1	O11-C11-C12	3.98	118.22	111.05
6	K	5802	MD1	C4-C5-N7	3.97	107.72	102.46
6	W	5802	MD1	O11-C11-C12	3.96	118.18	111.05
6	H	5802	MD1	O11-C11-C12	3.94	118.14	111.05
8	F	401	HEM	CBD-CAD-C3D	-3.93	105.24	112.48
6	B	5802	MD1	O11-C11-C12	3.87	118.03	111.05
6	B	5802	MD1	C15-C16-N15	3.85	122.35	119.12
6	B	5801	MD1	C4-C5-N7	3.81	107.51	102.46
6	T	5802	MD1	O11-C11-C12	3.64	117.60	111.05
6	E	5802	MD1	PA-O3B-PB	-3.62	120.41	132.83
8	U	401	HEM	CAA-CBA-CGA	-3.60	106.63	112.67
6	Q	5802	MD1	C4'-O4'-C1'	-3.59	101.55	109.47
6	Q	5802	MD1	O11-C11-C12	3.56	117.47	111.05
8	F	401	HEM	C4A-C3A-C2A	3.51	109.44	107.00
6	N	5802	MD1	O11-C11-C12	3.47	117.31	111.05
8	O	401	HEM	CAA-CBA-CGA	-3.47	106.85	112.67
6	N	5801	MD1	PA-O3B-PB	-3.46	120.97	132.83
6	T	5802	MD1	C4'-O4'-C1'	-3.32	102.14	109.47
6	Q	5801	MD1	N16-C17-N17	3.27	122.34	117.25
6	K	5802	MD1	C4'-O4'-C1'	-3.25	102.31	109.47
6	B	5801	MD1	N17-C17-N18	-3.24	120.34	125.42
8	F	401	HEM	CAA-CBA-CGA	-3.23	107.25	112.67
8	X	401	HEM	CBD-CAD-C3D	-3.22	106.55	112.48
6	Q	5801	MD1	C15-C16-N15	3.21	121.81	119.12
6	Q	5801	MD1	N17-C17-N18	-3.20	120.39	125.42
6	K	5801	MD1	PA-O3B-PB	-3.19	121.86	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	5801	MD1	N17-C17-N18	-3.16	120.47	125.42
6	H	5802	MD1	C4'-O4'-C1'	-3.16	102.51	109.47
6	H	5801	MD1	PA-O3B-PB	-3.13	122.09	132.83
6	N	5802	MD1	C15-C16-N15	3.13	121.75	119.12
8	I	401	HEM	CBA-CAA-C2A	-3.12	106.73	112.49
6	B	5802	MD1	N17-C17-N18	-3.10	120.55	125.42
6	W	5801	MD1	PA-O3B-PB	-3.10	122.18	132.83
6	W	5801	MD1	N17-C17-N18	-3.06	120.62	125.42
6	W	5802	MD1	C15-C16-N15	3.03	121.67	119.12
6	K	5801	MD1	N16-C17-N18	3.01	121.93	117.25
6	B	5802	MD1	C4'-O4'-C1'	-3.00	102.86	109.47
6	N	5801	MD1	N17-C17-N18	-2.99	120.73	125.42
6	W	5802	MD1	N17-C17-N18	-2.99	120.73	125.42
6	Q	5802	MD1	O4'-C1'-N9	2.98	113.48	109.04
6	K	5801	MD1	N17-C17-N18	-2.98	120.75	125.42
6	T	5801	MD1	PA-O3B-PB	-2.97	122.65	132.83
6	E	5801	MD1	C15-N17-C17	2.96	120.63	115.93
6	E	5801	MD1	N17-C17-N18	-2.94	120.81	125.42
6	T	5802	MD1	N17-C17-N18	-2.92	120.83	125.42
6	Q	5802	MD1	C15-C16-N15	2.90	121.56	119.12
6	N	5802	MD1	C4'-O4'-C1'	-2.90	103.08	109.47
6	N	5802	MD1	N17-C17-N18	-2.88	120.90	125.42
8	O	401	HEM	CMA-C3A-C4A	-2.87	124.05	128.46
6	W	5802	MD1	C4'-O4'-C1'	-2.87	103.14	109.47
6	Q	5801	MD1	PA-O3B-PB	-2.85	123.05	132.83
6	H	5802	MD1	C15-C16-N15	2.84	121.50	119.12
6	T	5801	MD1	N17-C17-N18	-2.82	120.99	125.42
6	H	5802	MD1	C15-N17-C17	2.82	120.41	115.93
6	W	5802	MD1	PA-O3B-PB	-2.81	123.17	132.83
8	I	401	HEM	CMD-C2D-C1D	-2.81	124.15	128.46
6	T	5802	MD1	C15-C16-N15	2.80	121.47	119.12
6	H	5802	MD1	N17-C17-N18	-2.80	121.03	125.42
6	B	5801	MD1	PA-O3B-PB	-2.78	123.29	132.83
6	K	5802	MD1	O11-C11-C12	2.77	116.04	111.05
6	E	5801	MD1	PA-O3B-PB	-2.77	123.33	132.83
6	B	5802	MD1	C15-N17-C17	2.76	120.32	115.93
8	X	401	HEM	CAA-CBA-CGA	-2.75	108.05	112.67
6	W	5802	MD1	C15-N17-C17	2.75	120.30	115.93
8	O	401	HEM	CBD-CAD-C3D	-2.74	107.42	112.48
6	E	5802	MD1	N17-C17-N18	-2.74	121.13	125.42
6	T	5802	MD1	C15-N17-C17	2.72	120.25	115.93
6	E	5802	MD1	C15-C16-N15	2.67	121.36	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	5802	MD1	O4'-C1'-N9	2.67	113.02	109.04
8	R	401	HEM	CBD-CAD-C3D	-2.67	107.56	112.48
6	T	5802	MD1	N18-C20-N8	2.65	122.36	116.00
8	I	401	HEM	C4C-C3C-C2C	-2.64	105.06	106.90
6	B	5801	MD1	C15-N17-C17	2.63	120.11	115.93
6	Q	5802	MD1	N17-C17-N18	-2.63	121.29	125.42
6	E	5802	MD1	N18-C20-N8	2.63	122.32	116.00
6	K	5801	MD1	C15-N17-C17	2.62	120.10	115.93
6	N	5802	MD1	C15-N17-C17	2.62	120.10	115.93
8	F	401	HEM	CBA-CAA-C2A	-2.61	107.67	112.49
8	I	401	HEM	CMD-C2D-C3D	2.61	129.86	124.94
6	W	5802	MD1	N18-C20-N8	2.60	122.25	116.00
6	W	5801	MD1	C15-N17-C17	2.60	120.06	115.93
6	Q	5802	MD1	PA-O3B-PB	-2.59	123.92	132.83
6	T	5802	MD1	O4'-C1'-N9	2.59	112.89	109.04
6	N	5801	MD1	C15-N17-C17	2.57	120.02	115.93
6	B	5802	MD1	N18-C20-N8	2.56	122.16	116.00
6	Q	5801	MD1	C3'-C2'-C1'	2.56	106.29	101.43
6	H	5801	MD1	C15-N17-C17	2.55	119.98	115.93
6	W	5801	MD1	N16-C17-N18	2.55	121.22	117.25
6	E	5802	MD1	C4'-O4'-C1'	-2.55	103.85	109.47
6	N	5802	MD1	O4'-C1'-N9	2.55	112.83	109.04
6	Q	5802	MD1	O4'-C1'-C2'	-2.53	101.11	106.64
8	R	401	HEM	CMA-C3A-C4A	-2.50	124.61	128.46
6	Q	5802	MD1	C15-N17-C17	2.50	119.90	115.93
6	E	5802	MD1	C15-N17-C17	2.47	119.86	115.93
6	E	5801	MD1	O3A-C10-C11	-2.47	100.82	107.94
6	W	5802	MD1	O4'-C1'-C2'	-2.46	101.28	106.64
6	Q	5801	MD1	C15-N17-C17	2.45	119.81	115.93
8	C	401	HEM	CMA-C3A-C4A	-2.44	124.71	128.46
6	H	5801	MD1	C3'-C2'-C1'	2.43	106.04	101.43
6	H	5802	MD1	PA-O3B-PB	-2.42	124.52	132.83
6	K	5802	MD1	O4'-C1'-C2'	-2.40	101.40	106.64
6	T	5801	MD1	C15-N17-C17	2.38	119.71	115.93
6	B	5802	MD1	PA-O3B-PB	-2.37	124.68	132.83
6	H	5802	MD1	N18-C20-N8	2.36	121.67	116.00
6	N	5802	MD1	PA-O3B-PB	-2.36	124.73	132.83
6	B	5801	MD1	O6-C6-N1	-2.35	119.53	122.69
6	K	5802	MD1	C15-C16-N15	2.35	121.09	119.12
6	E	5801	MD1	C4'-O4'-C1'	-2.34	104.31	109.47
6	E	5802	MD1	O4'-C1'-N9	2.33	112.50	109.04
8	L	401	HEM	CMB-C2B-C3B	2.31	129.01	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	401	HEM	CMB-C2B-C3B	2.31	129.00	124.68
6	B	5802	MD1	O4'-C1'-C2'	-2.30	101.63	106.64
6	N	5802	MD1	N18-C20-N8	2.29	121.50	116.00
8	C	401	HEM	CMB-C2B-C3B	2.29	128.96	124.68
6	Q	5802	MD1	N18-C20-N8	2.29	121.49	116.00
6	W	5802	MD1	O6-C6-N1	-2.28	119.63	122.69
6	T	5802	MD1	O4'-C1'-C2'	-2.26	101.71	106.64
8	L	401	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
6	K	5802	MD1	N18-C20-N8	2.25	121.39	116.00
8	U	401	HEM	CMB-C2B-C3B	2.24	128.88	124.68
8	U	401	HEM	CMA-C3A-C4A	-2.23	125.04	128.46
8	R	401	HEM	CAA-CBA-CGA	-2.22	108.94	112.67
6	H	5802	MD1	O4'-C1'-C2'	-2.20	101.85	106.64
8	F	401	HEM	CMB-C2B-C3B	2.20	128.78	124.68
8	F	401	HEM	C1D-C2D-C3D	2.19	108.52	107.00
6	T	5802	MD1	PA-O3B-PB	-2.19	125.32	132.83
6	N	5802	MD1	C2'-C3'-C4'	2.16	106.84	102.64
6	K	5802	MD1	O6-C6-N1	-2.15	119.81	122.69
6	H	5802	MD1	O6-C6-N1	-2.14	119.82	122.69
6	E	5802	MD1	O6-C6-N1	-2.13	119.83	122.69
8	R	401	HEM	CMB-C2B-C3B	2.12	128.65	124.68
6	K	5802	MD1	N16-C17-N17	2.12	120.55	117.25
6	N	5801	MD1	C3'-C2'-C1'	2.12	105.45	101.43
6	W	5802	MD1	O4'-C1'-N9	2.11	112.19	109.04
8	L	401	HEM	C3C-C4C-NC	-2.09	107.00	110.94
6	Q	5802	MD1	O6-C6-N1	-2.08	119.90	122.69
6	T	5802	MD1	O6-C6-N1	-2.07	119.91	122.69
6	N	5802	MD1	O4'-C1'-C2'	-2.07	102.13	106.64
8	C	401	HEM	C4C-C3C-C2C	2.06	108.34	106.90
6	K	5801	MD1	O6-C6-N1	-2.06	119.93	122.69
6	K	5802	MD1	PA-O3B-PB	-2.05	125.80	132.83
6	N	5801	MD1	O6-C6-N1	-2.04	119.95	122.69
6	K	5802	MD1	C15-N17-C17	2.04	119.16	115.93
8	O	401	HEM	CMC-C2C-C3C	2.03	128.48	124.68
6	K	5802	MD1	N17-C17-N18	-2.03	122.23	125.42
6	K	5801	MD1	C3'-C2'-C1'	2.03	105.28	101.43
6	E	5801	MD1	O6-C6-N1	-2.02	119.97	122.69
6	K	5802	MD1	C2'-C3'-C4'	2.02	106.57	102.64
6	N	5801	MD1	C2'-C3'-C4'	2.02	106.56	102.64
6	H	5801	MD1	O4'-C1'-N9	2.02	112.04	109.04
6	T	5802	MD1	C2'-C3'-C4'	2.02	106.56	102.64
6	N	5802	MD1	O6-C6-N1	-2.02	119.98	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	401	HEM	CAA-CBA-CGA	-2.01	109.29	112.67
6	H	5802	MD1	C2'-C3'-C4'	2.01	106.54	102.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	5801	MD1	C14

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	5801	MD1	C10-O3A-PB-O3B
6	B	5801	MD1	O3A-C10-C11-O11
6	B	5801	MD1	O3A-C10-C11-C12
6	B	5801	MD1	C3'-C4'-C5'-O5'
6	E	5801	MD1	O3A-C10-C11-O11
6	E	5801	MD1	O3A-C10-C11-C12
6	E	5801	MD1	C5'-O5'-PA-O3B
6	E	5802	MD1	O3A-C10-C11-C12
6	H	5801	MD1	C10-O3A-PB-O3B
6	H	5801	MD1	C10-O3A-PB-O2B
6	H	5801	MD1	O3A-C10-C11-O11
6	H	5801	MD1	O3A-C10-C11-C12
6	H	5801	MD1	C5'-O5'-PA-O2A
6	H	5802	MD1	O3A-C10-C11-O11
6	K	5801	MD1	C10-O3A-PB-O3B
6	K	5801	MD1	O3A-C10-C11-O11
6	K	5801	MD1	O3A-C10-C11-C12
6	K	5801	MD1	C5'-O5'-PA-O2A
6	K	5801	MD1	C3'-C4'-C5'-O5'
6	N	5801	MD1	C10-O3A-PB-O3B
6	N	5801	MD1	O3A-C10-C11-O11
6	N	5801	MD1	O3A-C10-C11-C12
6	N	5801	MD1	C5'-O5'-PA-O2A
6	N	5801	MD1	O4'-C4'-C5'-O5'
6	N	5801	MD1	C3'-C4'-C5'-O5'
6	Q	5801	MD1	C10-O3A-PB-O3B
6	Q	5801	MD1	C10-O3A-PB-O2B
6	Q	5801	MD1	O3A-C10-C11-C12
6	Q	5801	MD1	C5'-O5'-PA-O3B
6	Q	5801	MD1	C5'-O5'-PA-O2A
6	Q	5802	MD1	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	T	5801	MD1	C10-O3A-PB-O3B
6	T	5801	MD1	O3A-C10-C11-O11
6	T	5801	MD1	O3A-C10-C11-C12
6	T	5801	MD1	C5'-O5'-PA-O2A
6	T	5801	MD1	O4'-C4'-C5'-O5'
6	T	5801	MD1	C3'-C4'-C5'-O5'
6	W	5801	MD1	C10-O3A-PB-O3B
6	W	5801	MD1	O3A-C10-C11-O11
6	W	5801	MD1	O3A-C10-C11-C12
6	W	5801	MD1	C5'-O5'-PA-O2A
6	W	5801	MD1	O4'-C4'-C5'-O5'
6	W	5801	MD1	C3'-C4'-C5'-O5'
6	W	5802	MD1	O3A-C10-C11-O11
6	W	5802	MD1	O3A-C10-C11-C12
8	F	401	HEM	C3A-C2A-CAA-CBA
8	I	401	HEM	C1A-C2A-CAA-CBA
8	I	401	HEM	C3A-C2A-CAA-CBA
8	I	401	HEM	C2A-CAA-CBA-CGA
6	B	5801	MD1	O4'-C4'-C5'-O5'
6	E	5801	MD1	O4'-C4'-C5'-O5'
6	E	5801	MD1	C3'-C4'-C5'-O5'
6	H	5801	MD1	O4'-C4'-C5'-O5'
6	H	5801	MD1	C3'-C4'-C5'-O5'
6	K	5801	MD1	O4'-C4'-C5'-O5'
6	Q	5801	MD1	O4'-C4'-C5'-O5'
6	Q	5801	MD1	C3'-C4'-C5'-O5'
6	Q	5802	MD1	O4'-C4'-C5'-O5'
6	Q	5802	MD1	C3'-C4'-C5'-O5'
6	B	5801	MD1	PB-O3B-PA-O5'
6	E	5801	MD1	PB-O3B-PA-O5'
6	H	5801	MD1	PB-O3B-PA-O5'
6	K	5801	MD1	PB-O3B-PA-O5'
6	N	5801	MD1	PB-O3B-PA-O5'
6	T	5801	MD1	PB-O3B-PA-O5'
6	W	5801	MD1	PB-O3B-PA-O5'
6	B	5801	MD1	C4'-C5'-O5'-PA
6	K	5801	MD1	C4'-C5'-O5'-PA
6	Q	5801	MD1	C4'-C5'-O5'-PA
6	T	5801	MD1	C4'-C5'-O5'-PA
6	H	5801	MD1	C5'-O5'-PA-O3B
6	Q	5802	MD1	C5'-O5'-PA-O3B
6	Q	5802	MD1	O3A-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	E	5801	MD1	C4'-C5'-O5'-PA
6	H	5801	MD1	C4'-C5'-O5'-PA
6	N	5801	MD1	C4'-C5'-O5'-PA
6	W	5801	MD1	C4'-C5'-O5'-PA
6	B	5801	MD1	C10-O3A-PB-O1B
6	B	5801	MD1	C10-O3A-PB-O2B
6	E	5801	MD1	C5'-O5'-PA-O2A
6	H	5801	MD1	C10-O3A-PB-O1B
6	K	5801	MD1	C10-O3A-PB-O1B
6	K	5801	MD1	C10-O3A-PB-O2B
6	N	5801	MD1	C10-O3A-PB-O1B
6	N	5801	MD1	C10-O3A-PB-O2B
6	Q	5802	MD1	C5'-O5'-PA-O1A
6	T	5801	MD1	C10-O3A-PB-O1B
6	T	5801	MD1	C10-O3A-PB-O2B
6	W	5801	MD1	C10-O3A-PB-O1B
6	W	5801	MD1	C10-O3A-PB-O2B
6	W	5802	MD1	C10-O3A-PB-O1B
6	B	5802	MD1	O3A-C10-C11-O11
6	E	5802	MD1	O3A-C10-C11-O11
6	K	5802	MD1	O3A-C10-C11-O11
6	N	5802	MD1	O3A-C10-C11-O11
6	Q	5802	MD1	O3A-C10-C11-O11
6	T	5802	MD1	O3A-C10-C11-O11
8	F	401	HEM	C1A-C2A-CAA-CBA
6	B	5802	MD1	PA-O3B-PB-O1B
6	E	5802	MD1	PA-O3B-PB-O1B
6	H	5802	MD1	PA-O3B-PB-O1B
6	K	5802	MD1	PA-O3B-PB-O1B
6	N	5802	MD1	PA-O3B-PB-O1B
6	Q	5802	MD1	PA-O3B-PB-O1B
6	T	5802	MD1	PA-O3B-PB-O1B
6	W	5802	MD1	PA-O3B-PB-O1B
6	Q	5801	MD1	PB-O3B-PA-O5'
8	R	401	HEM	C2A-CAA-CBA-CGA
6	K	5801	MD1	C5'-O5'-PA-O3B
6	N	5801	MD1	C5'-O5'-PA-O3B
6	T	5801	MD1	C5'-O5'-PA-O3B
6	W	5802	MD1	C10-O3A-PB-O3B
6	B	5802	MD1	PA-O3B-PB-O2B
6	E	5802	MD1	PA-O3B-PB-O2B
6	H	5802	MD1	PA-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
6	K	5802	MD1	PA-O3B-PB-O2B
6	N	5802	MD1	PA-O3B-PB-O2B
6	Q	5802	MD1	PA-O3B-PB-O2B
6	T	5802	MD1	PA-O3B-PB-O2B
6	W	5802	MD1	PA-O3B-PB-O2B
8	C	401	HEM	C2A-CAA-CBA-CGA
8	U	401	HEM	C2A-CAA-CBA-CGA
6	B	5801	MD1	C5'-O5'-PA-O2A
6	E	5801	MD1	C10-O3A-PB-O2B
6	Q	5801	MD1	O3A-C10-C11-O11

There are no ring outliers.

48 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	5804	SF4	3	0
4	J	503	SF4	4	0
6	H	5802	MD1	7	0
6	T	5801	MD1	8	0
4	V	501	SF4	2	0
4	A	503	SF4	1	0
4	N	5804	SF4	3	0
8	R	401	HEM	5	0
8	L	401	HEM	6	0
8	I	401	HEM	29	0
4	W	5804	SF4	2	0
4	D	503	SF4	1	0
6	Q	5801	MD1	12	0
8	F	401	HEM	25	0
8	C	401	HEM	8	0
5	M	504	F3S	2	0
4	D	502	SF4	2	0
4	J	501	SF4	1	0
5	V	504	F3S	5	0
6	E	5801	MD1	14	0
6	K	5802	MD1	5	0
6	N	5801	MD1	10	0
4	M	503	SF4	2	0
4	G	501	SF4	1	0
6	T	5802	MD1	5	0
6	E	5802	MD1	5	0
6	W	5801	MD1	13	0

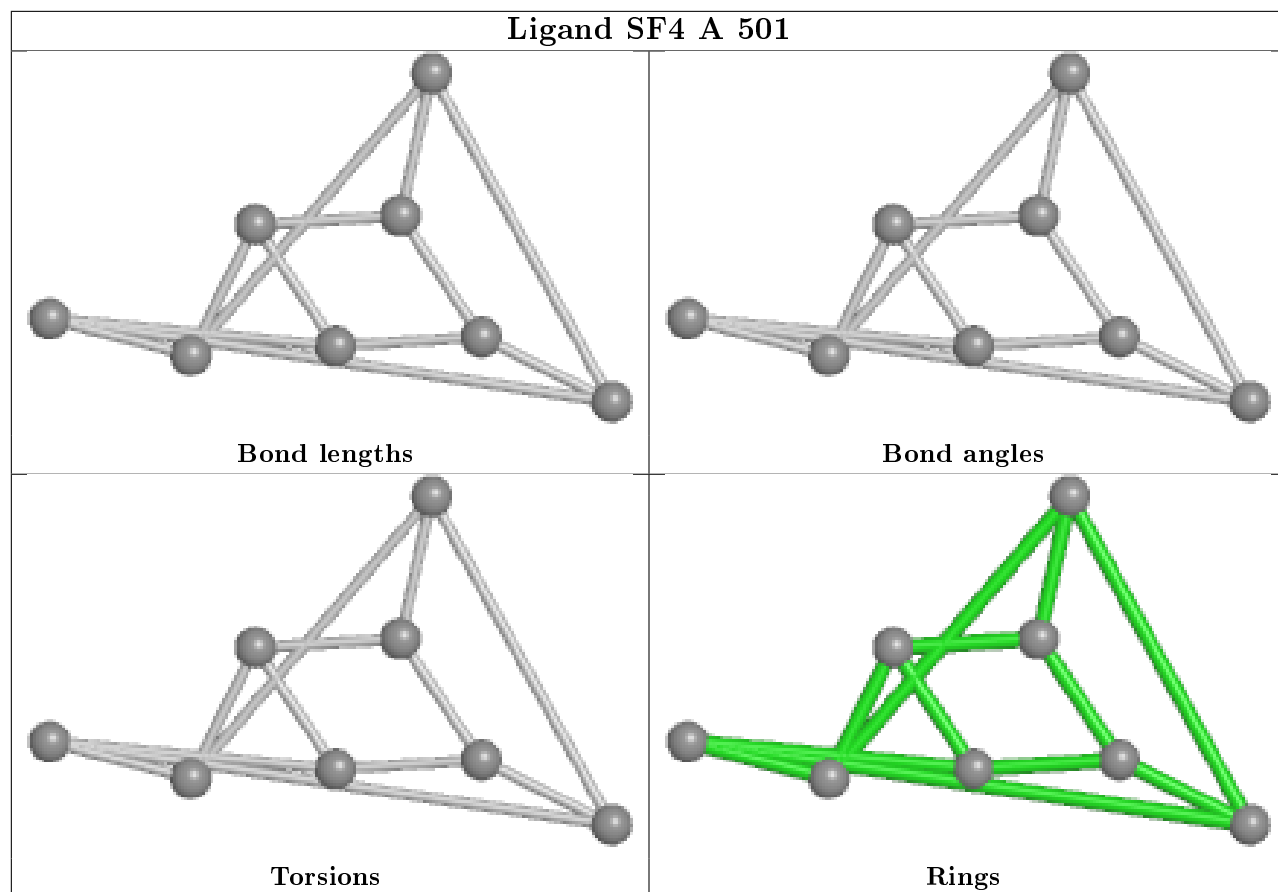
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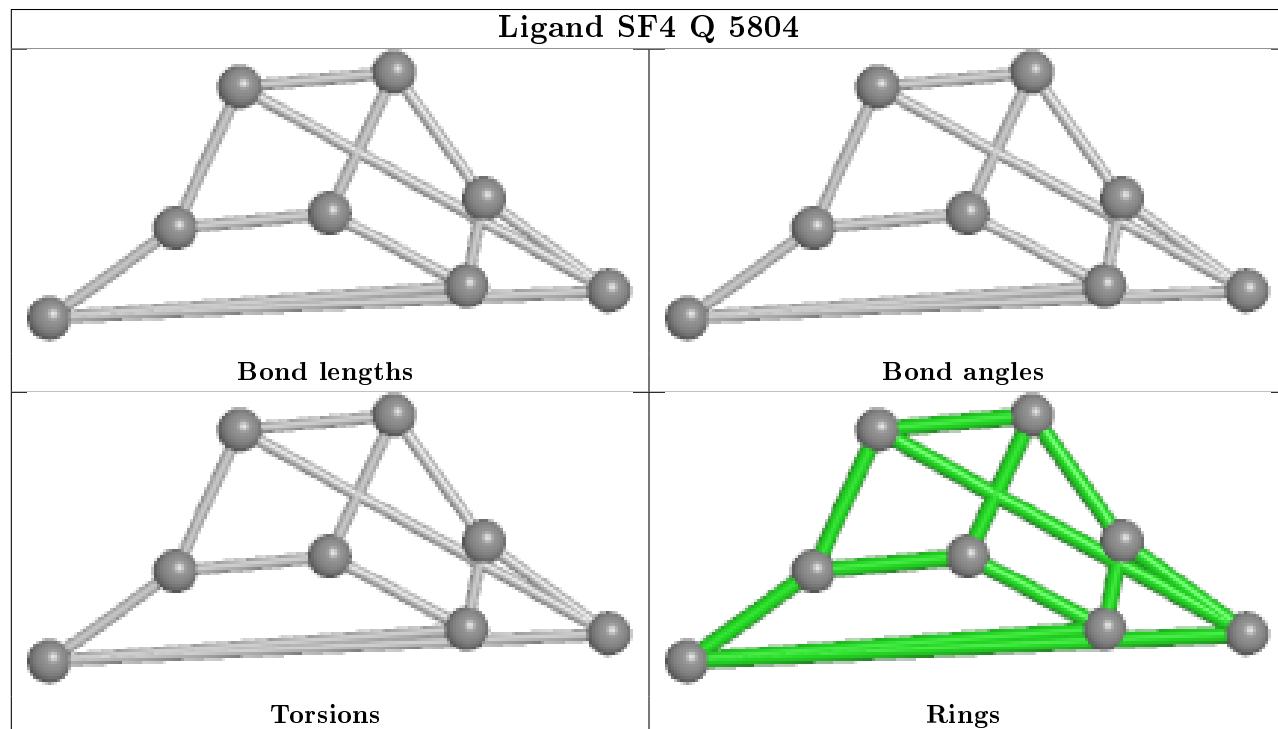
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	SF4	4	0
4	M	501	SF4	1	0
8	U	401	HEM	4	0
4	P	503	SF4	3	0
4	V	502	SF4	1	0
4	G	503	SF4	2	0
4	S	503	SF4	2	0
6	B	5801	MD1	6	0
8	O	401	HEM	11	0
6	Q	5802	MD1	7	0
4	S	501	SF4	1	0
6	N	5802	MD1	8	0
6	W	5802	MD1	8	0
6	H	5801	MD1	6	0
6	B	5802	MD1	6	0
5	D	504	F3S	3	0
4	T	5804	SF4	3	0
4	K	5804	SF4	1	0
4	V	503	SF4	3	0
6	K	5801	MD1	9	0
8	X	401	HEM	15	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.

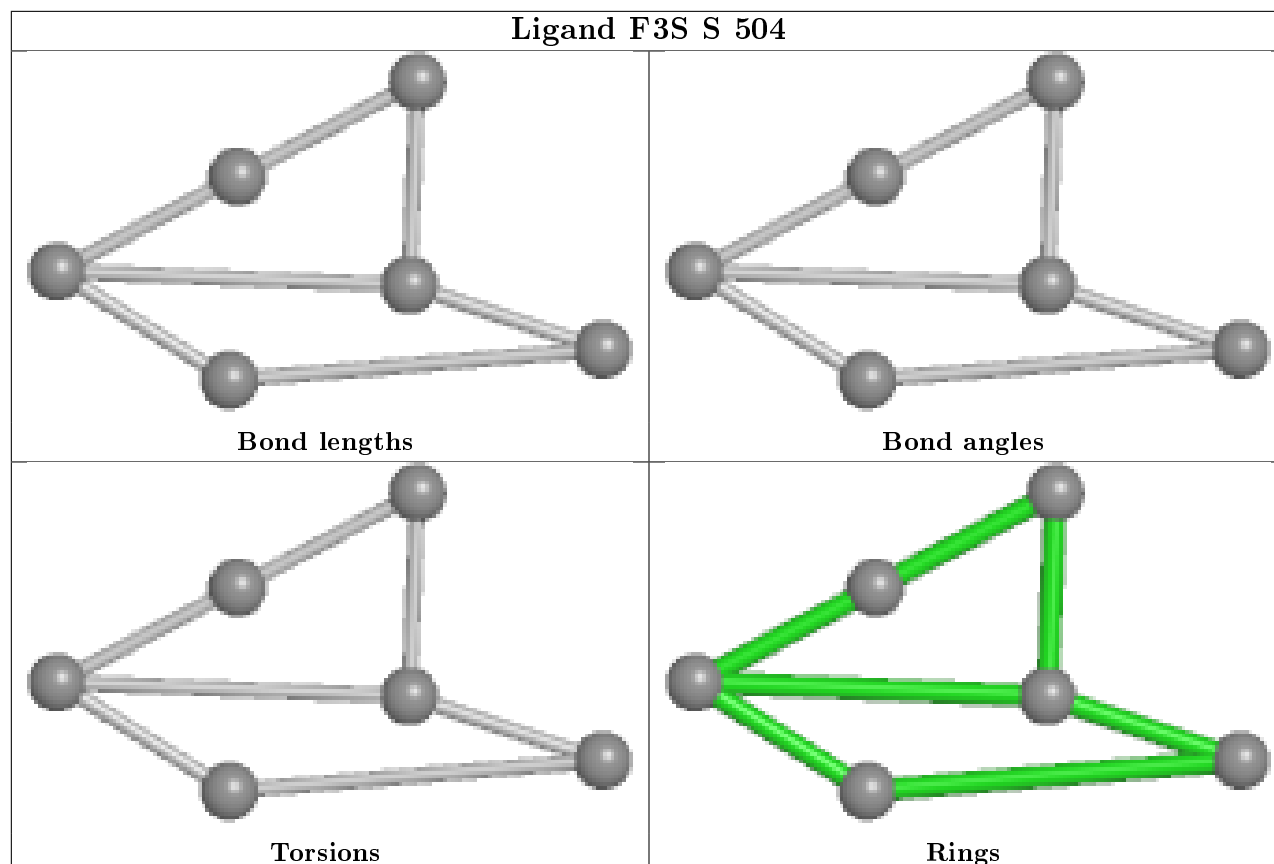
Ligand SF4 A 501



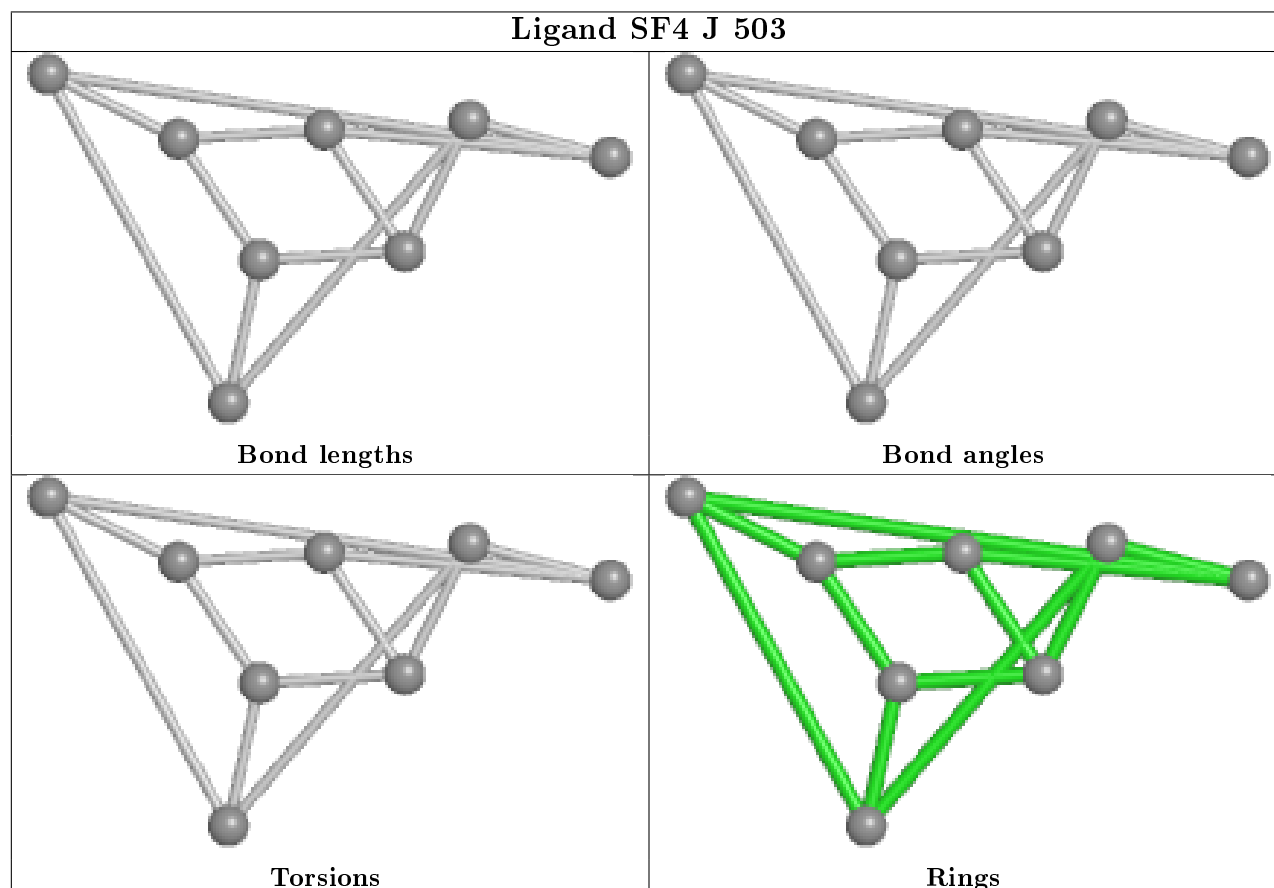
Ligand SF4 Q 5804



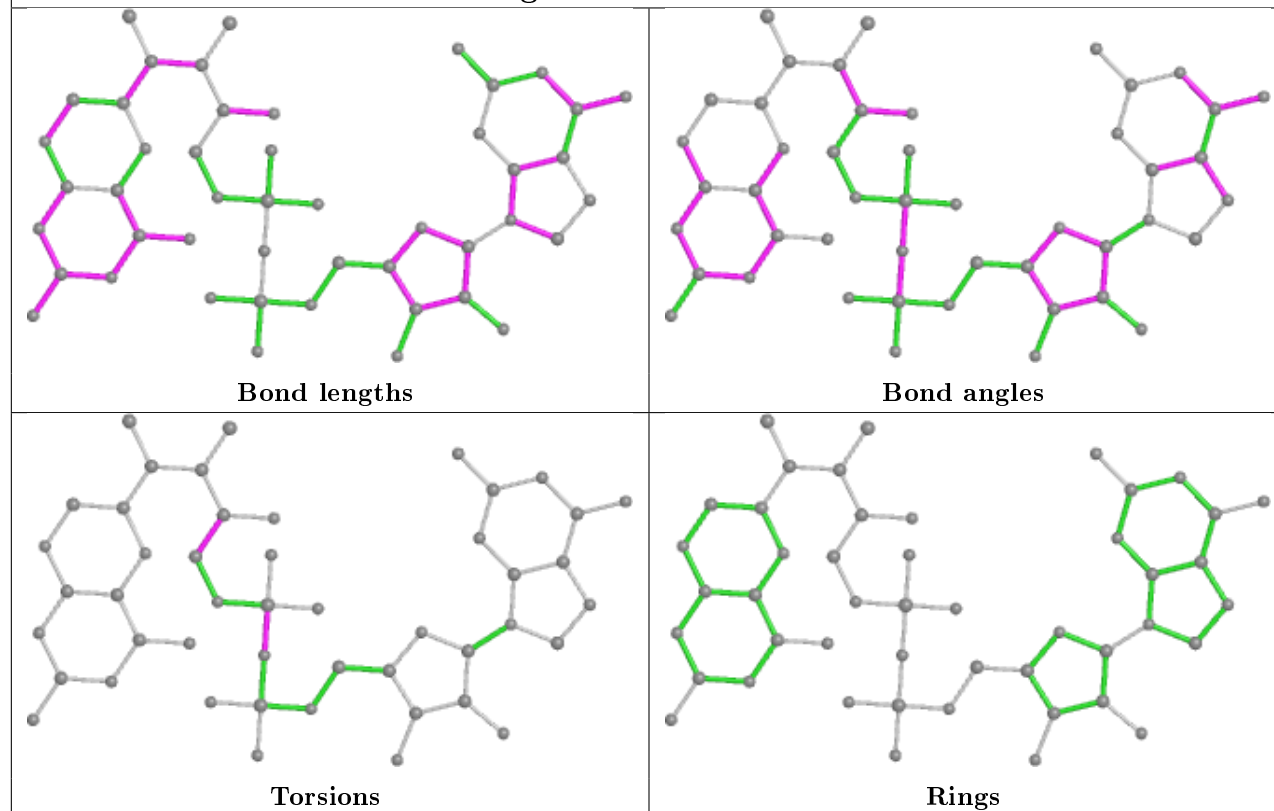
Ligand F3S S 504



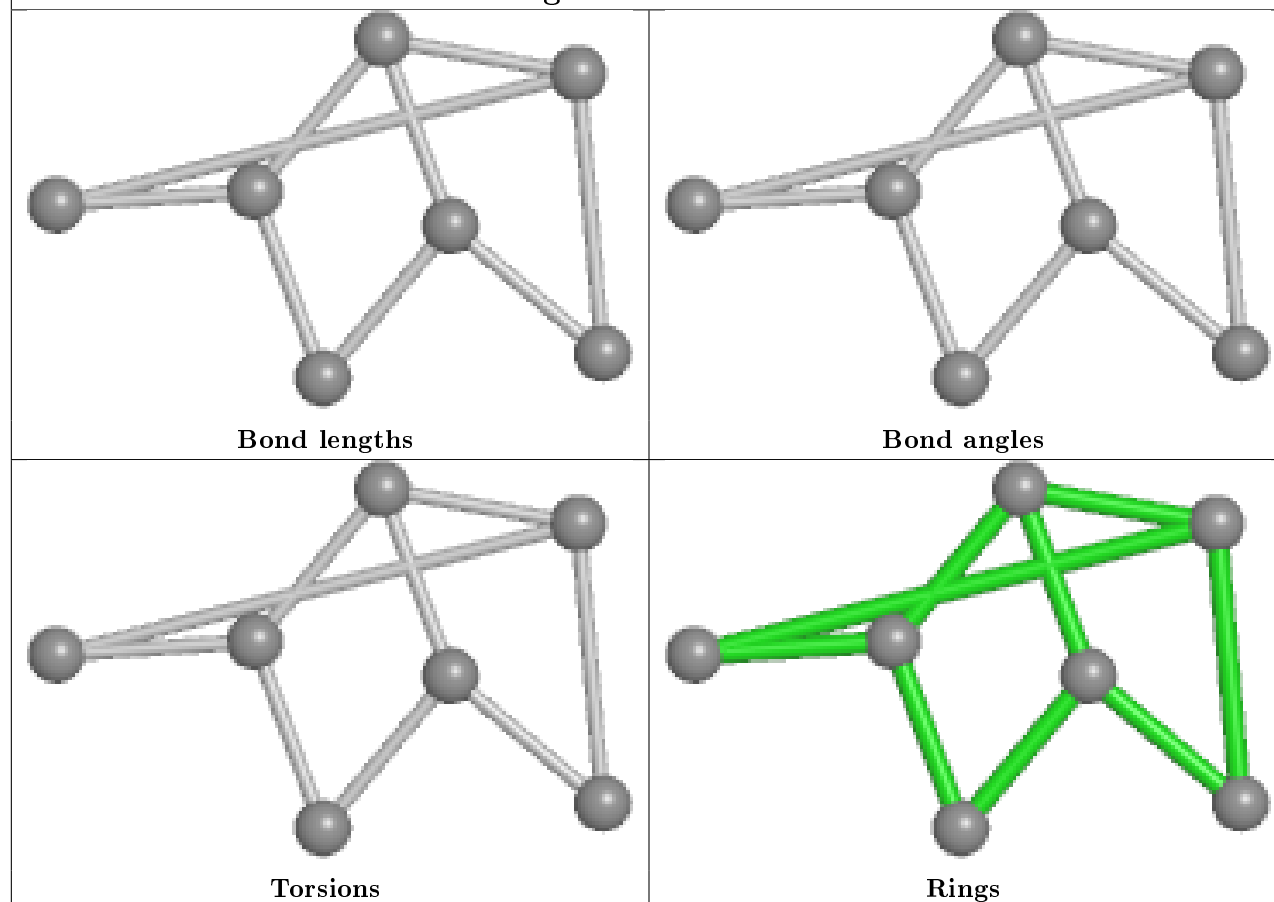
Ligand SF4 J 503



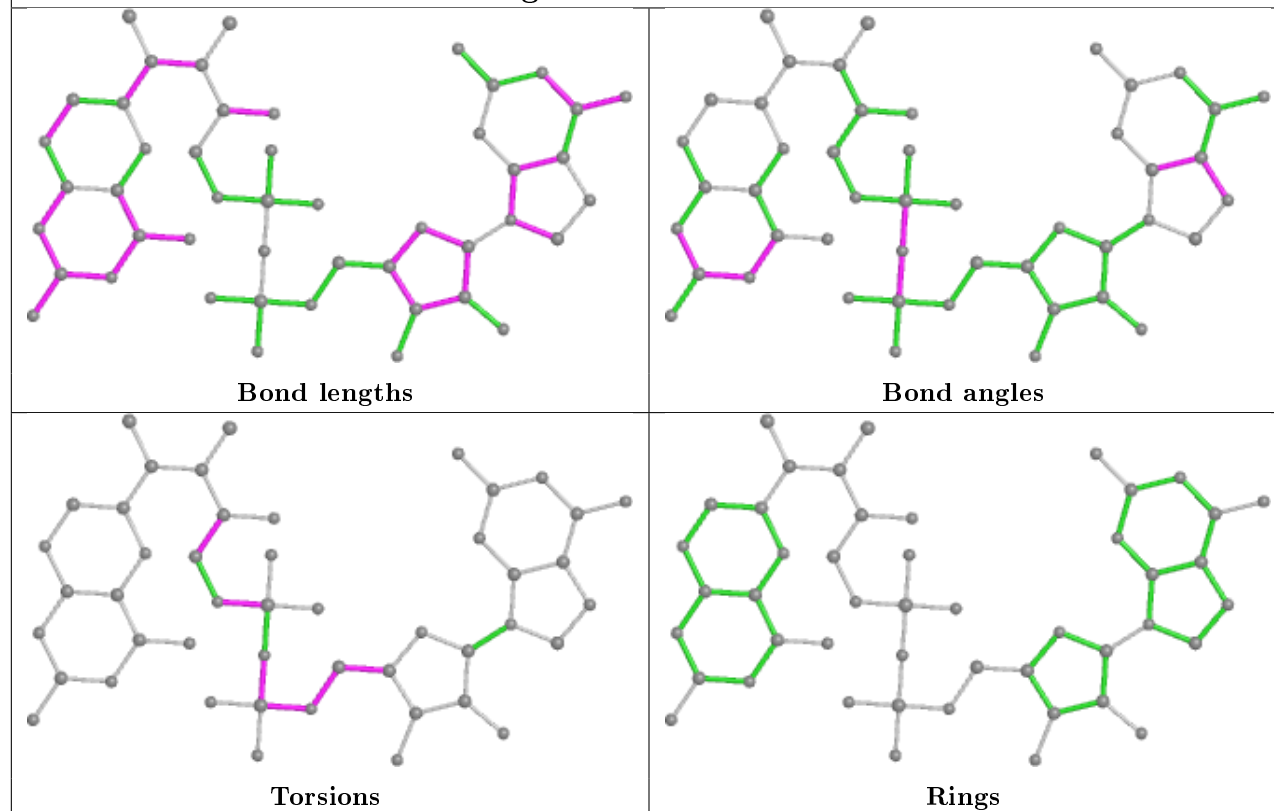
Ligand MD1 H 5802



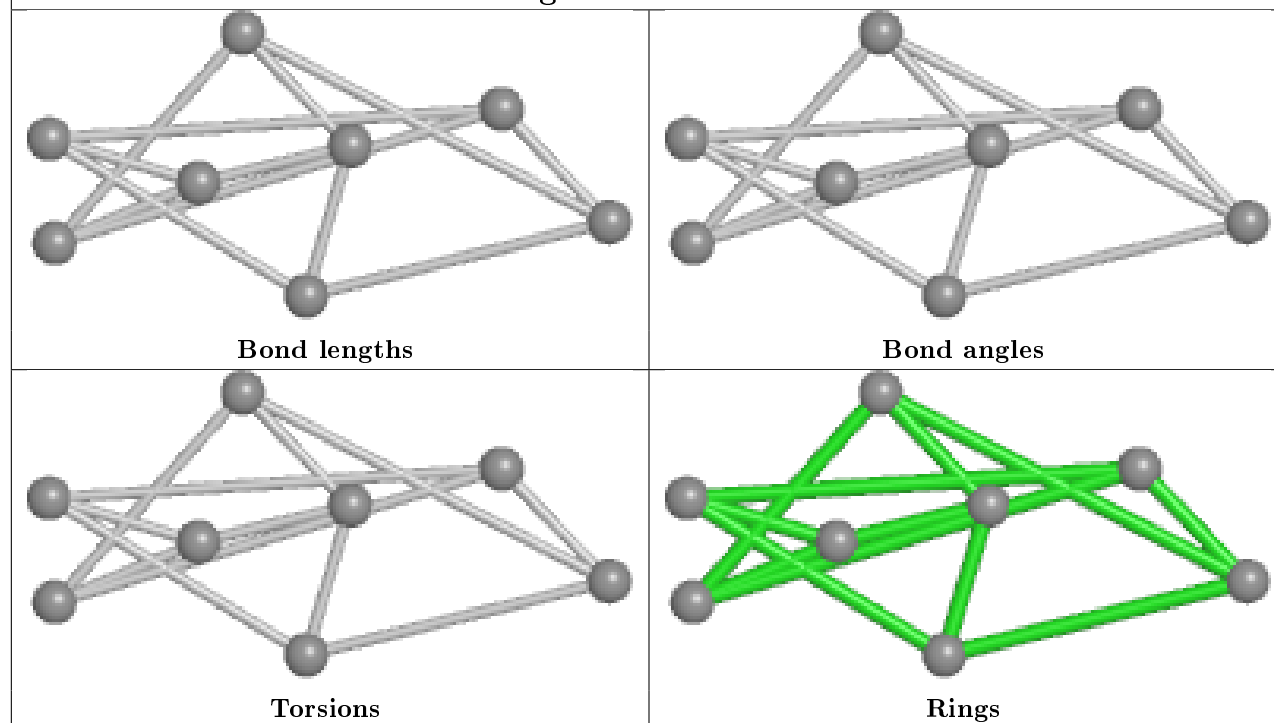
Ligand F3S J 504



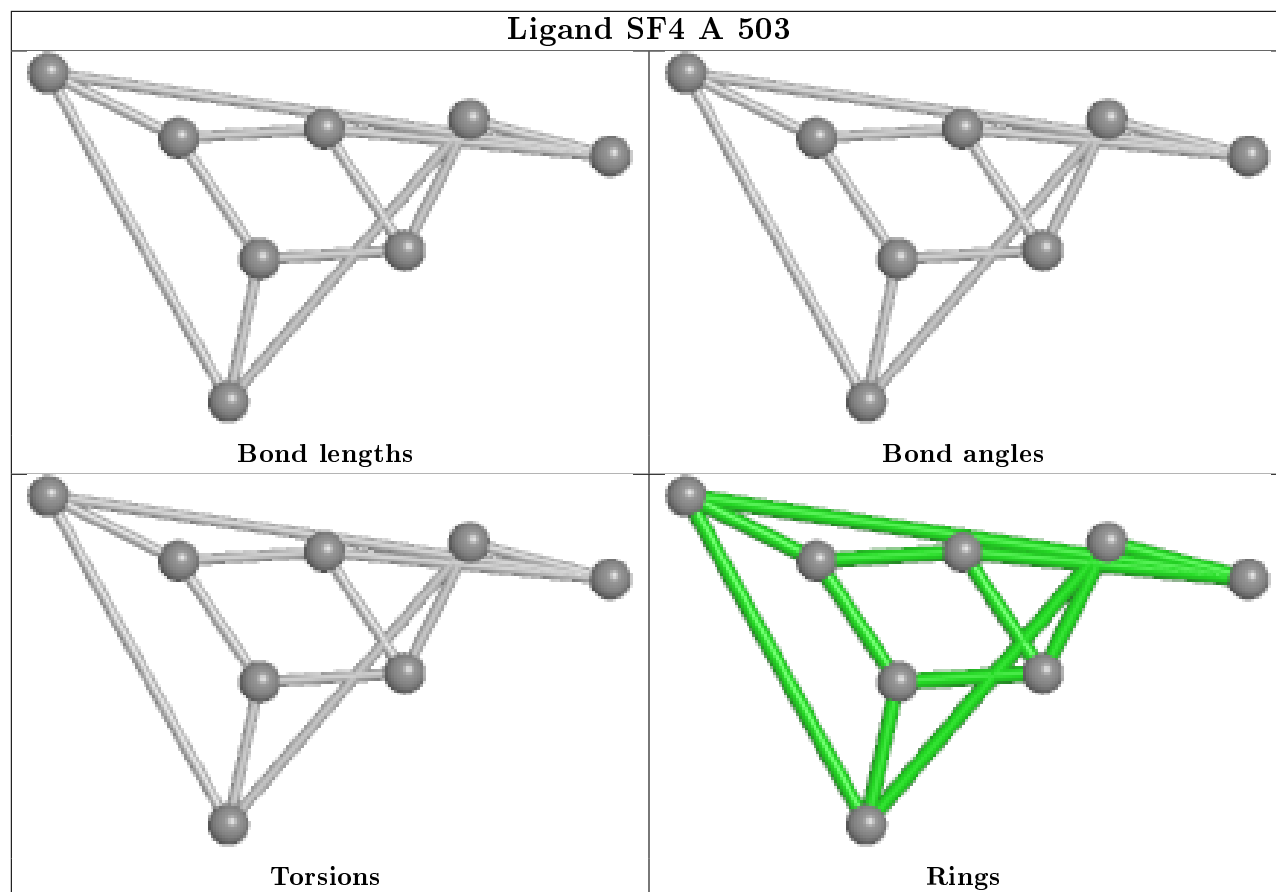
Ligand MD1 T 5801



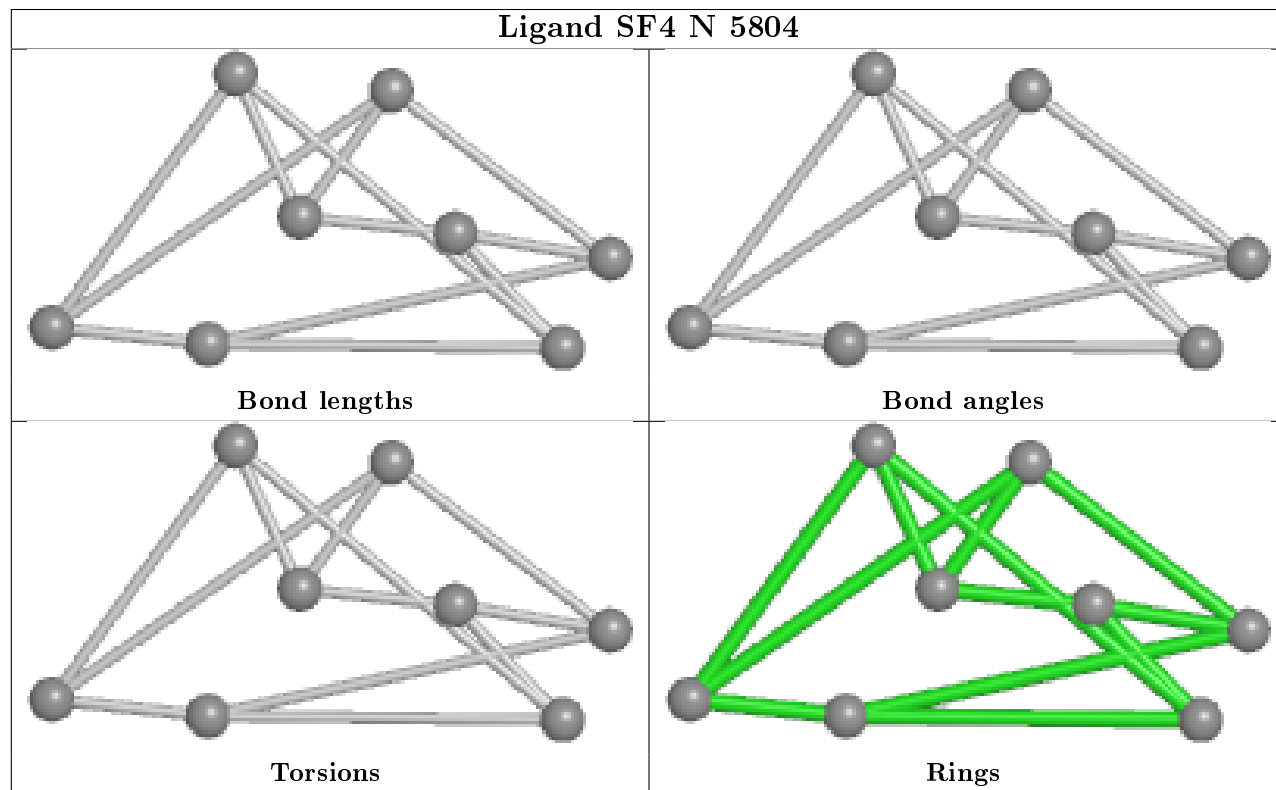
Ligand SF4 V 501

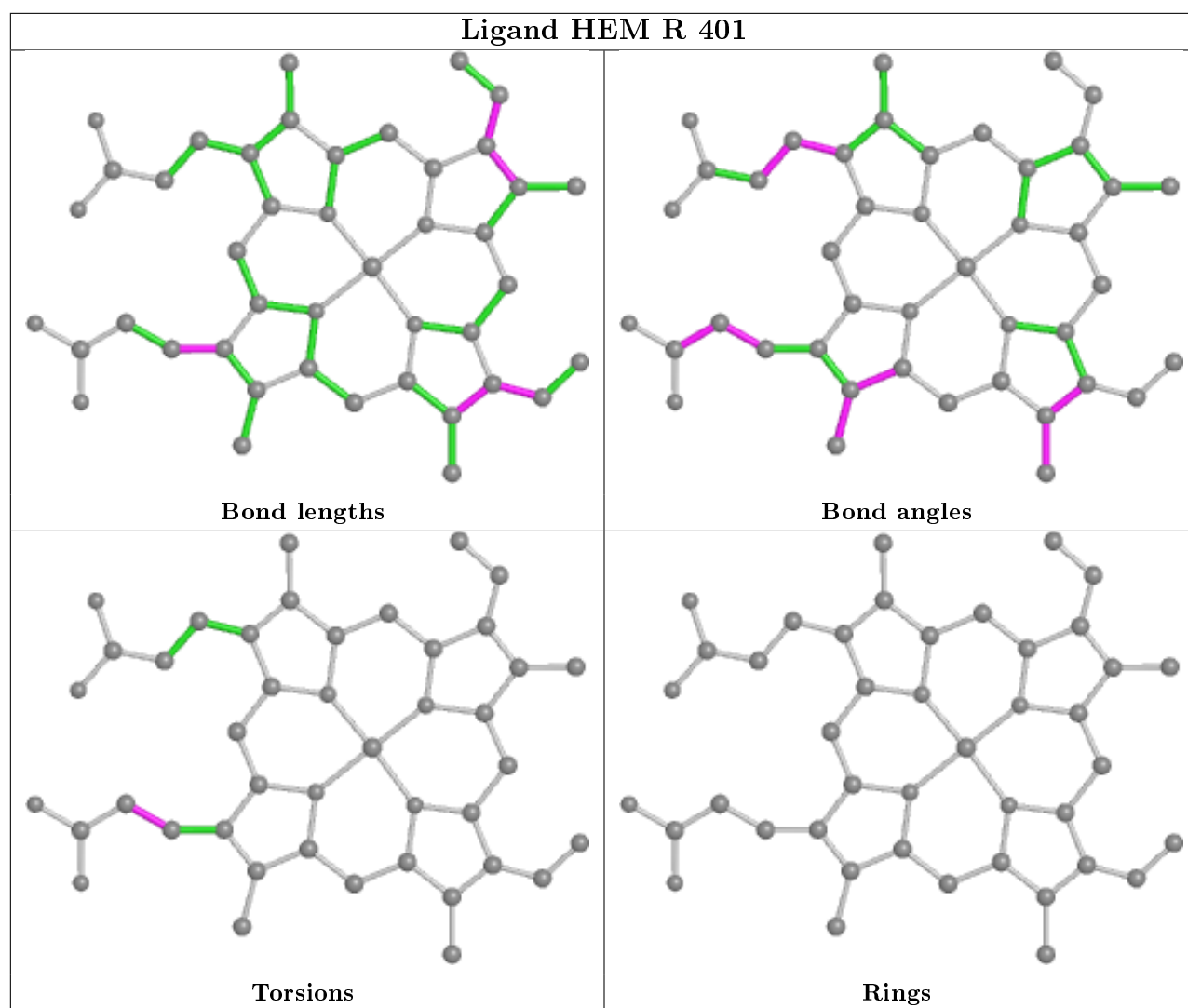


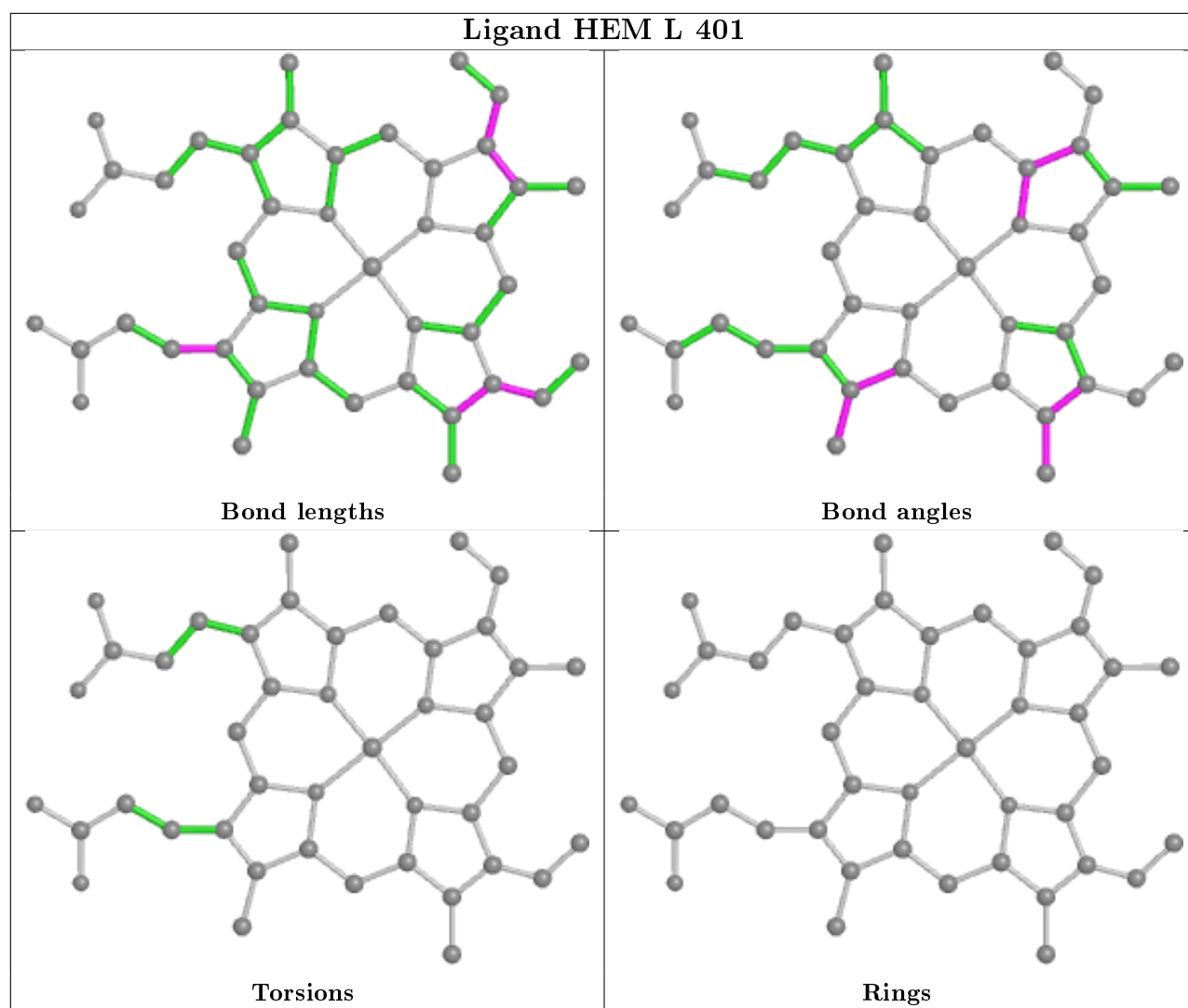
Ligand SF4 A 503



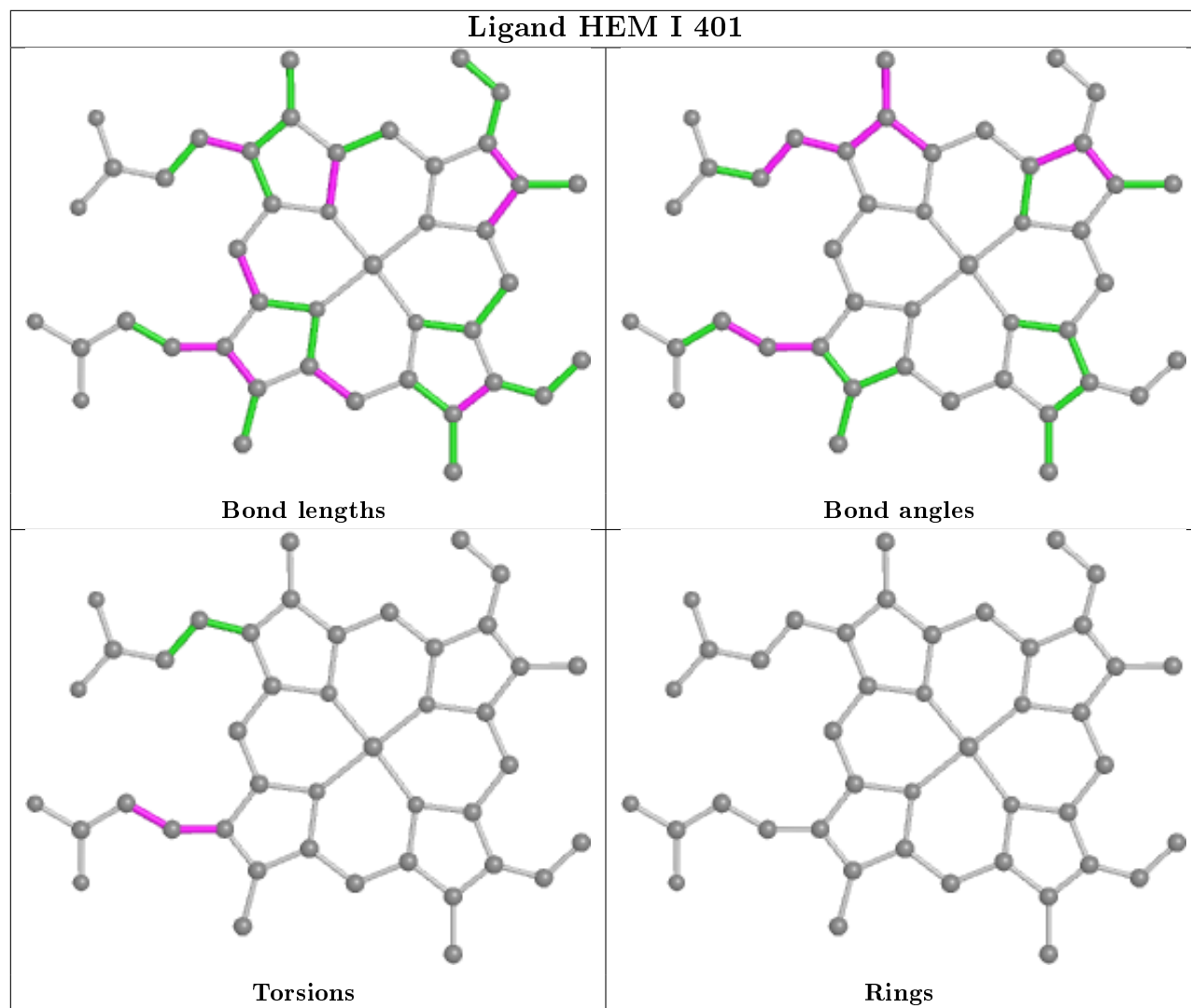
Ligand SF4 N 5804

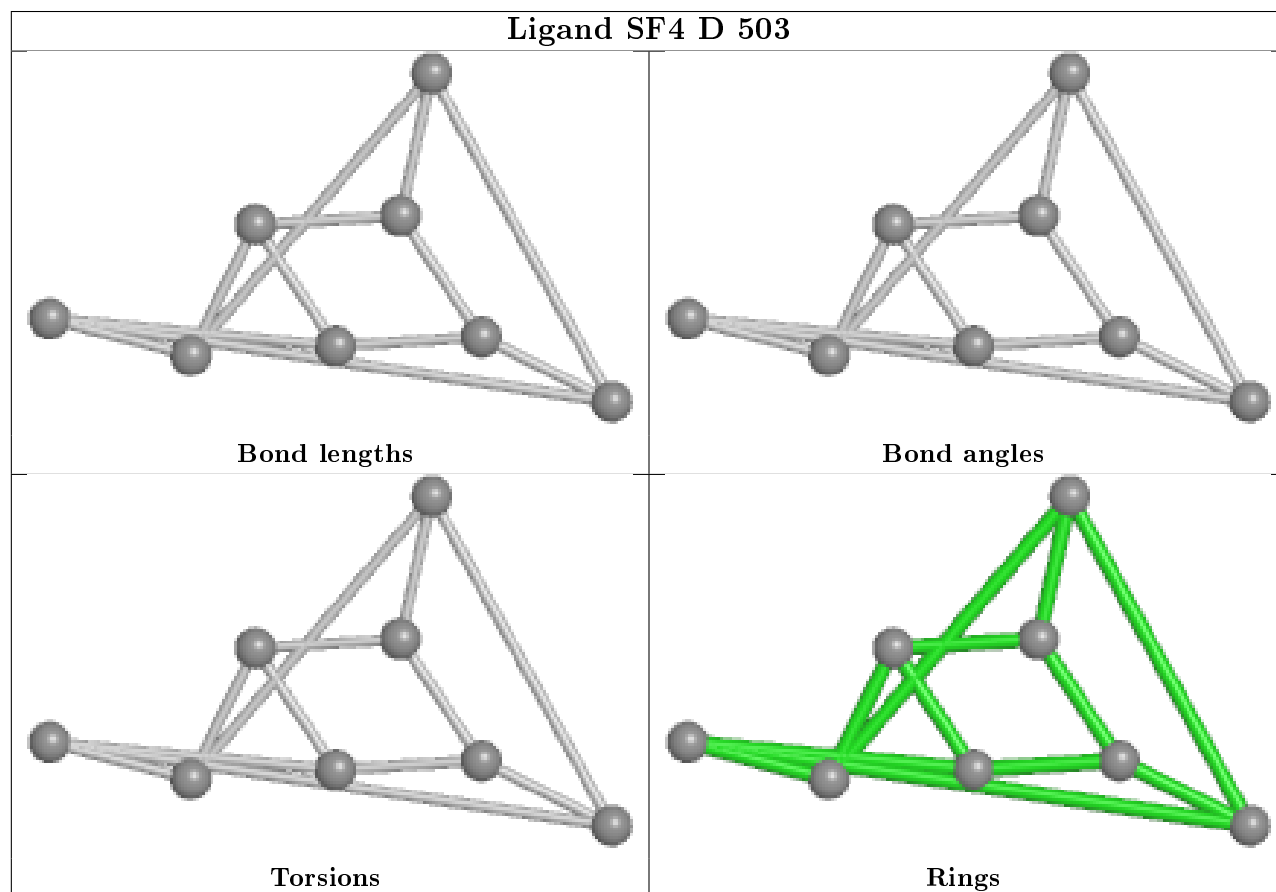
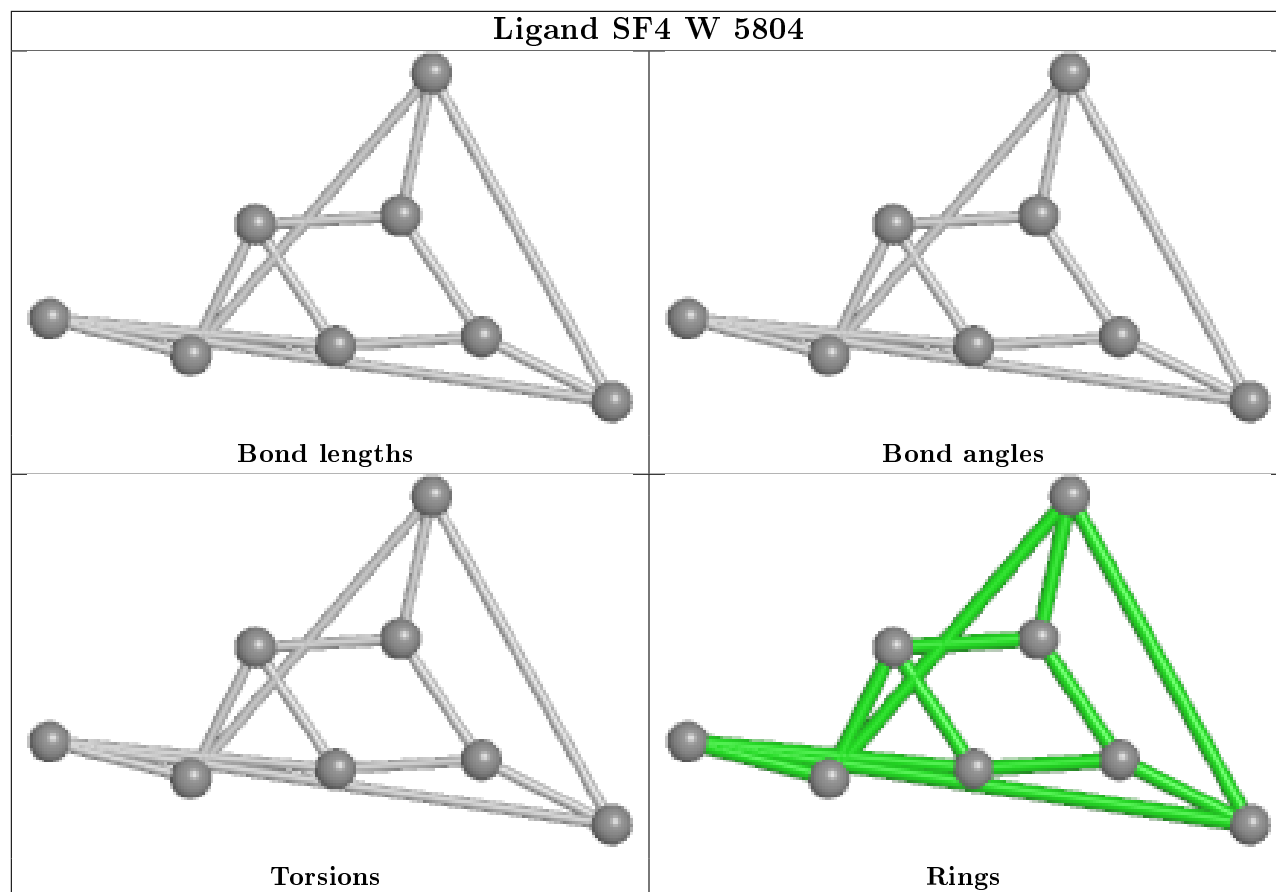




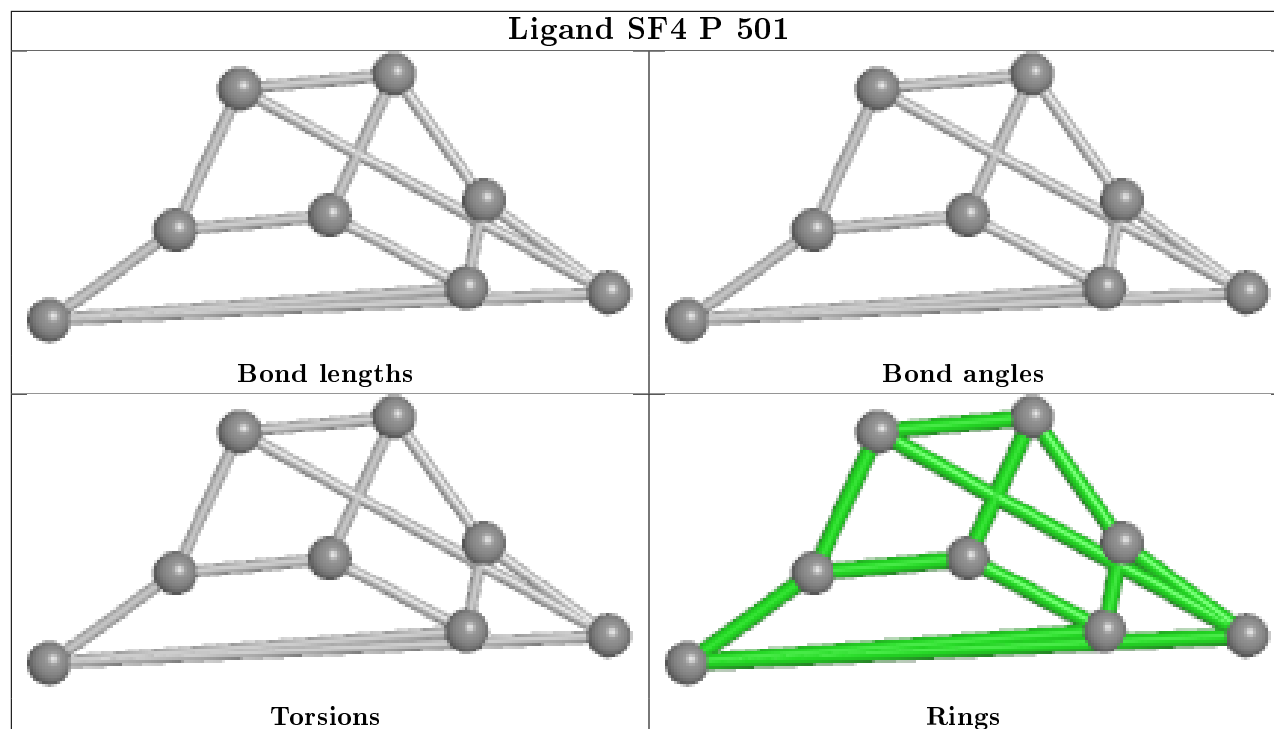


Ligand HEM I 401

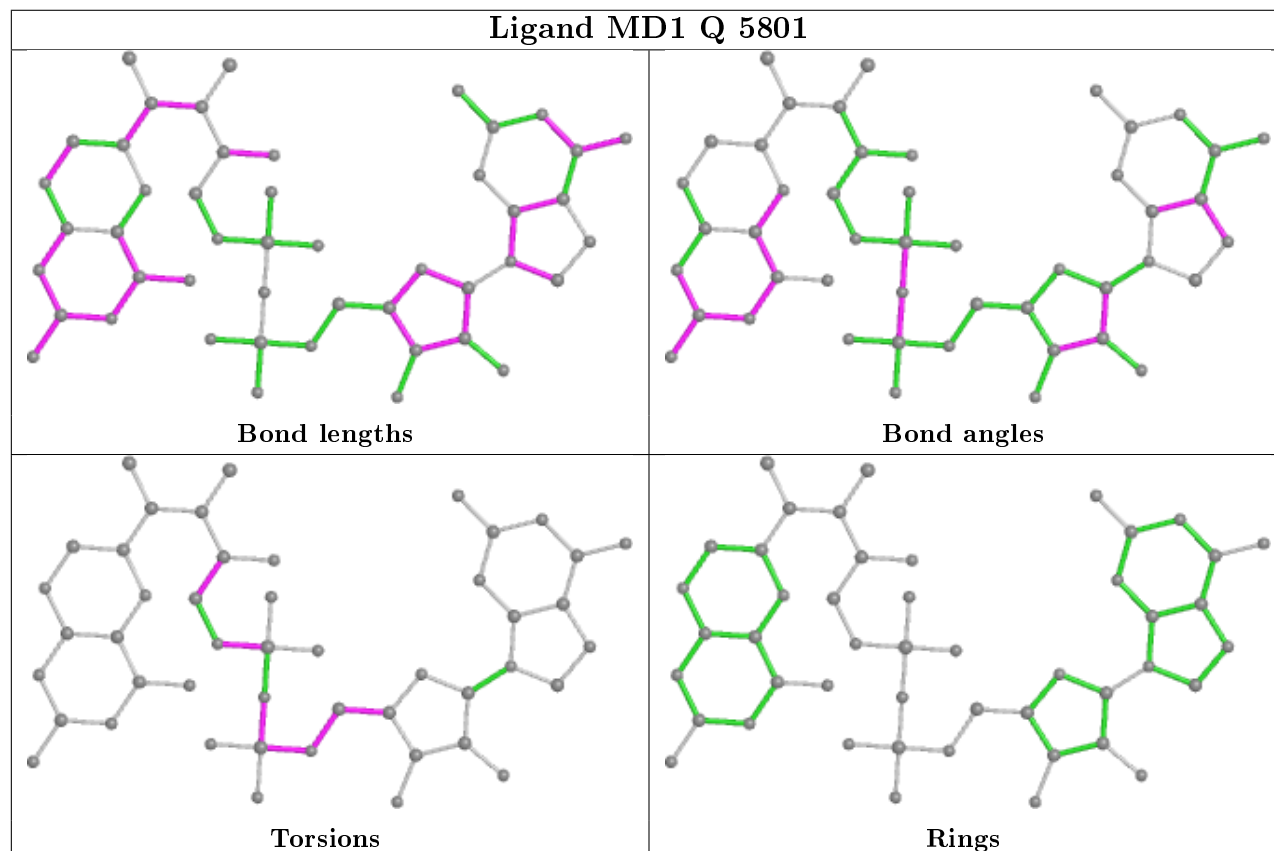


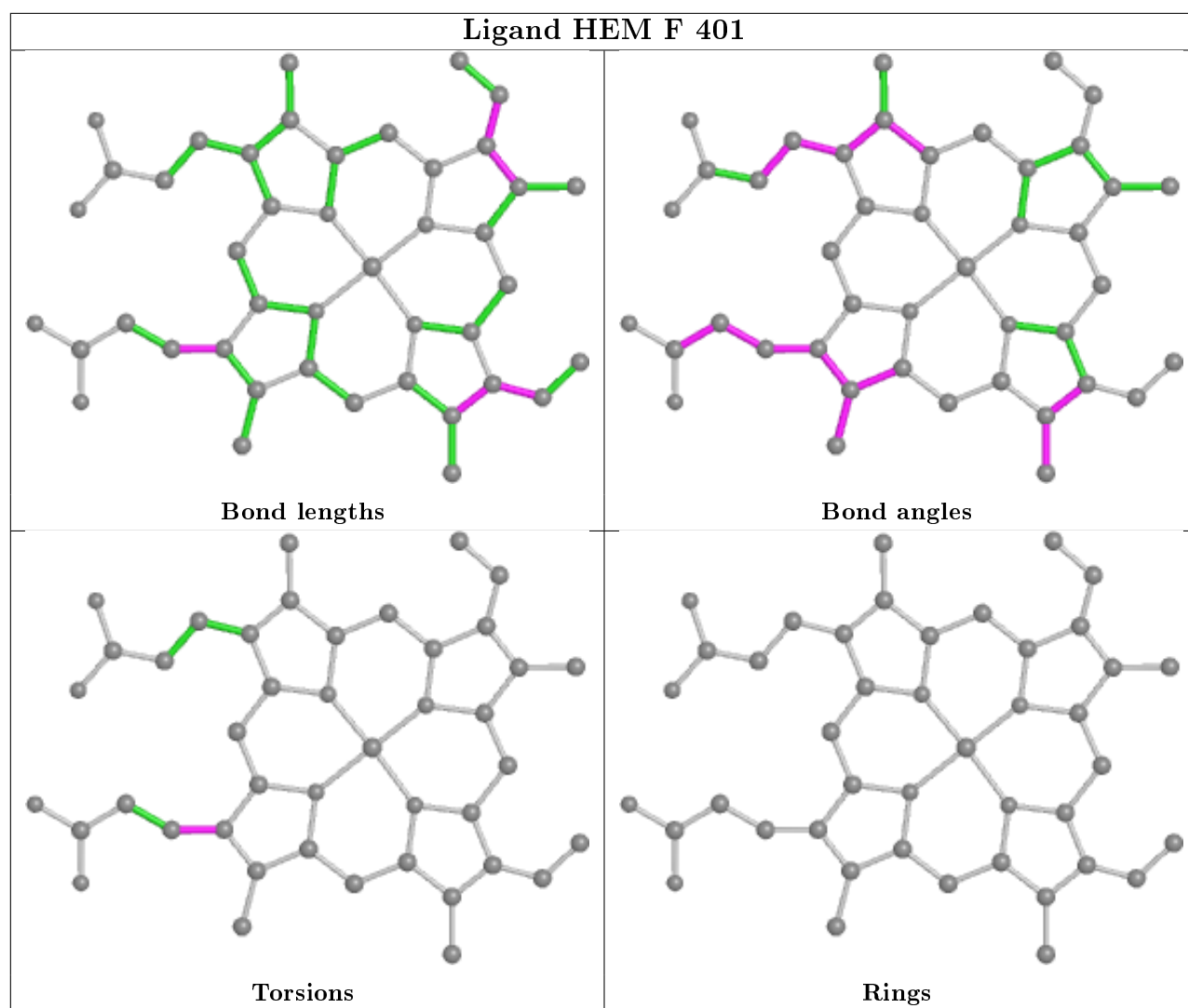


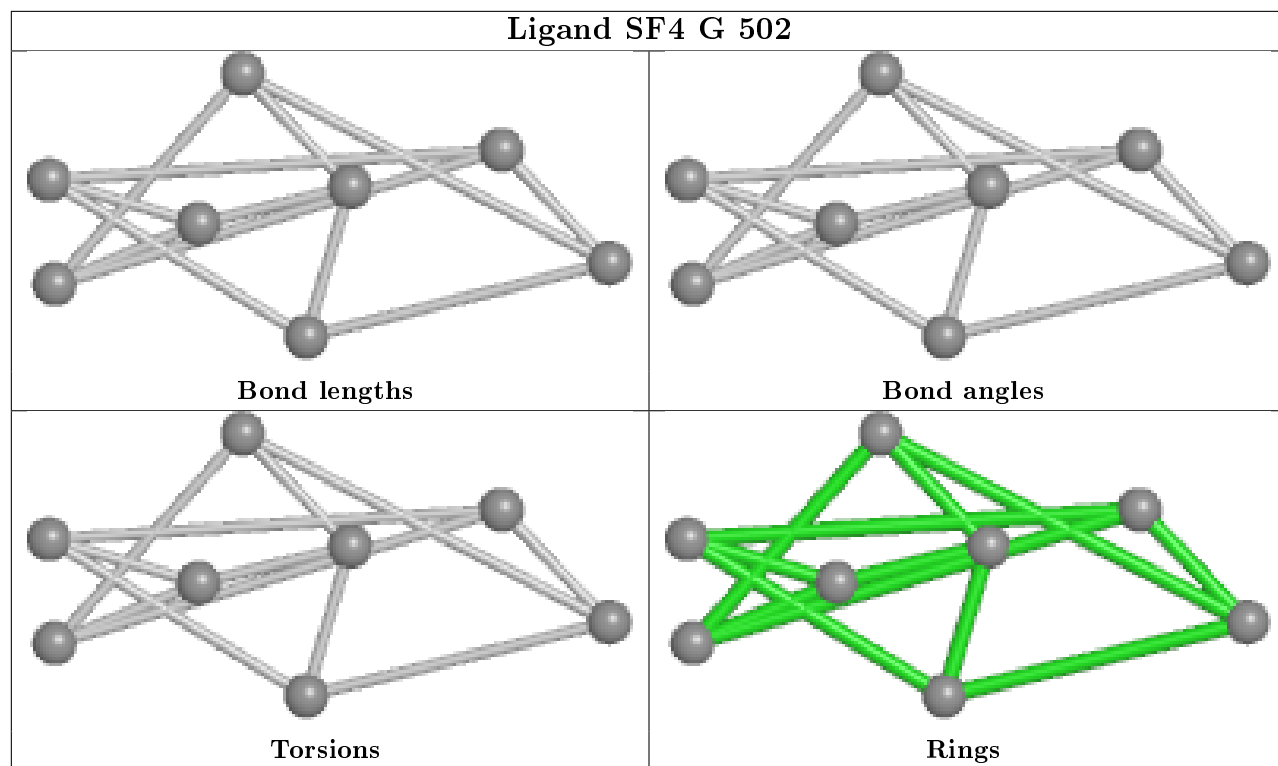
Ligand SF4 P 501

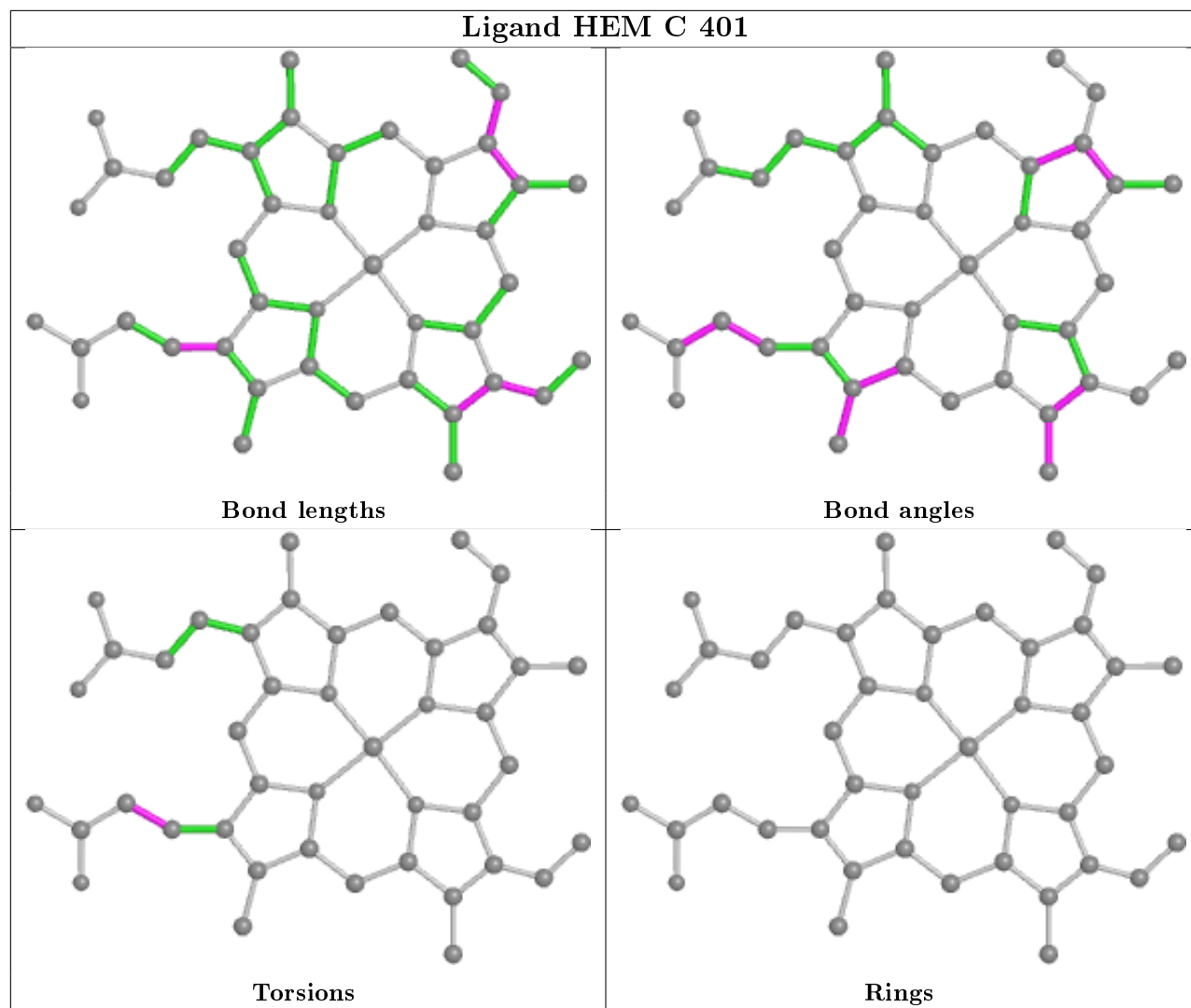


Ligand MD1 Q 5801

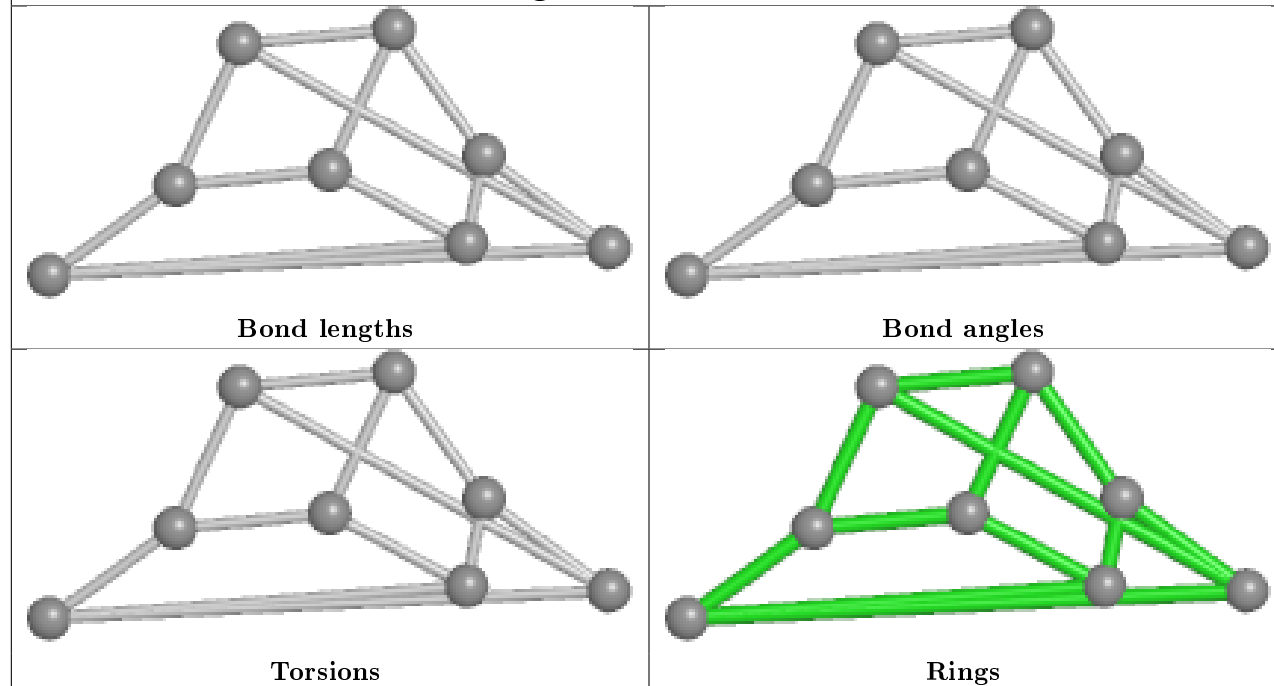




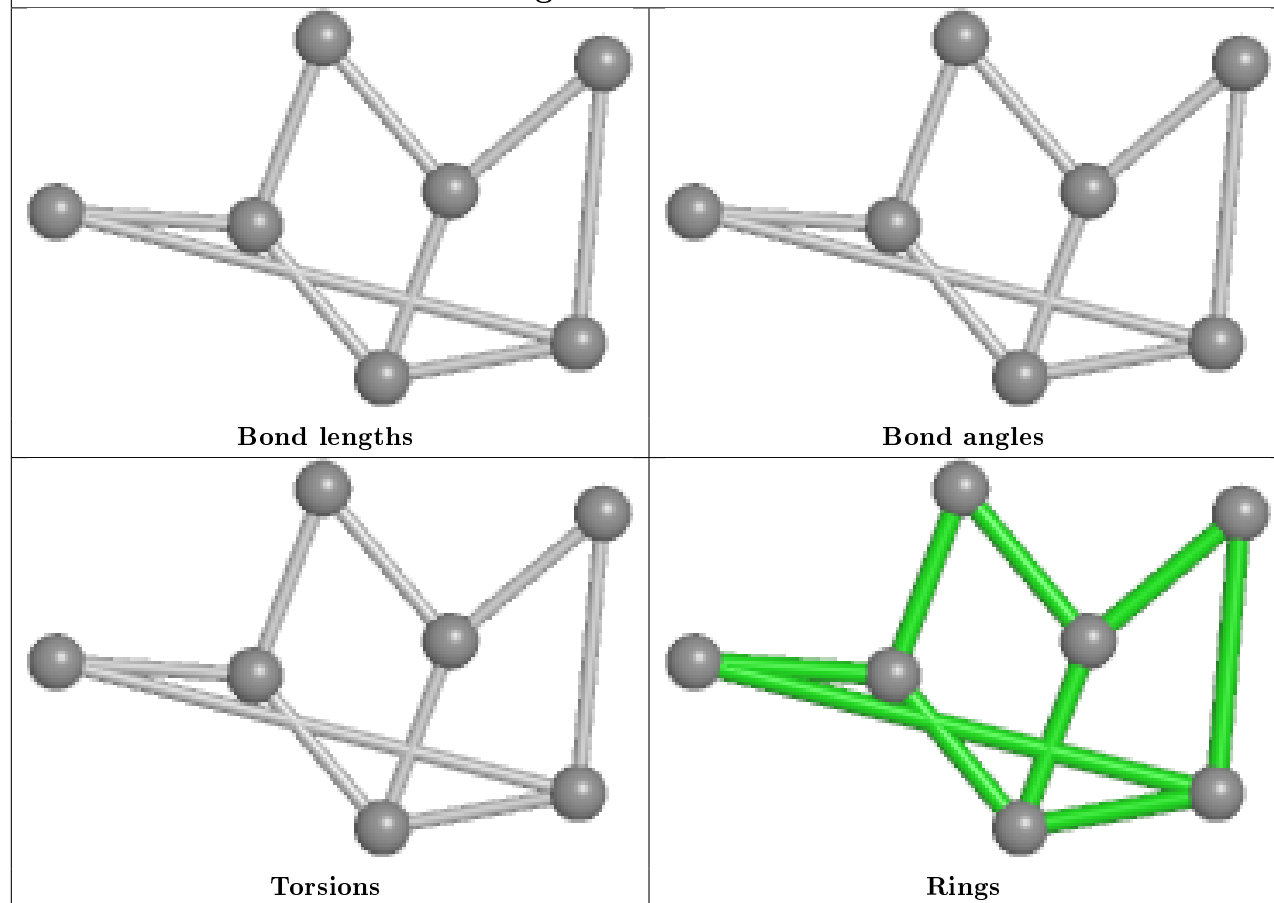


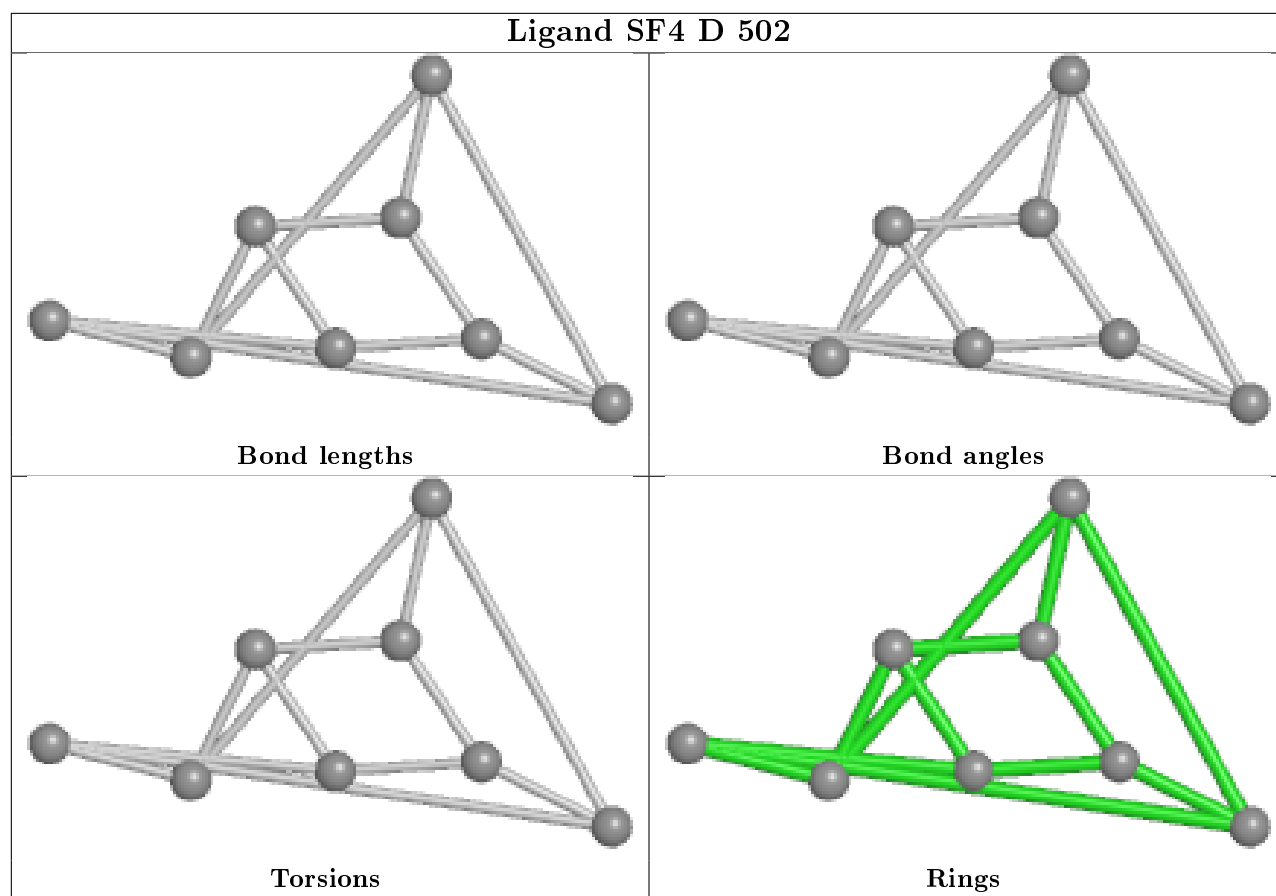
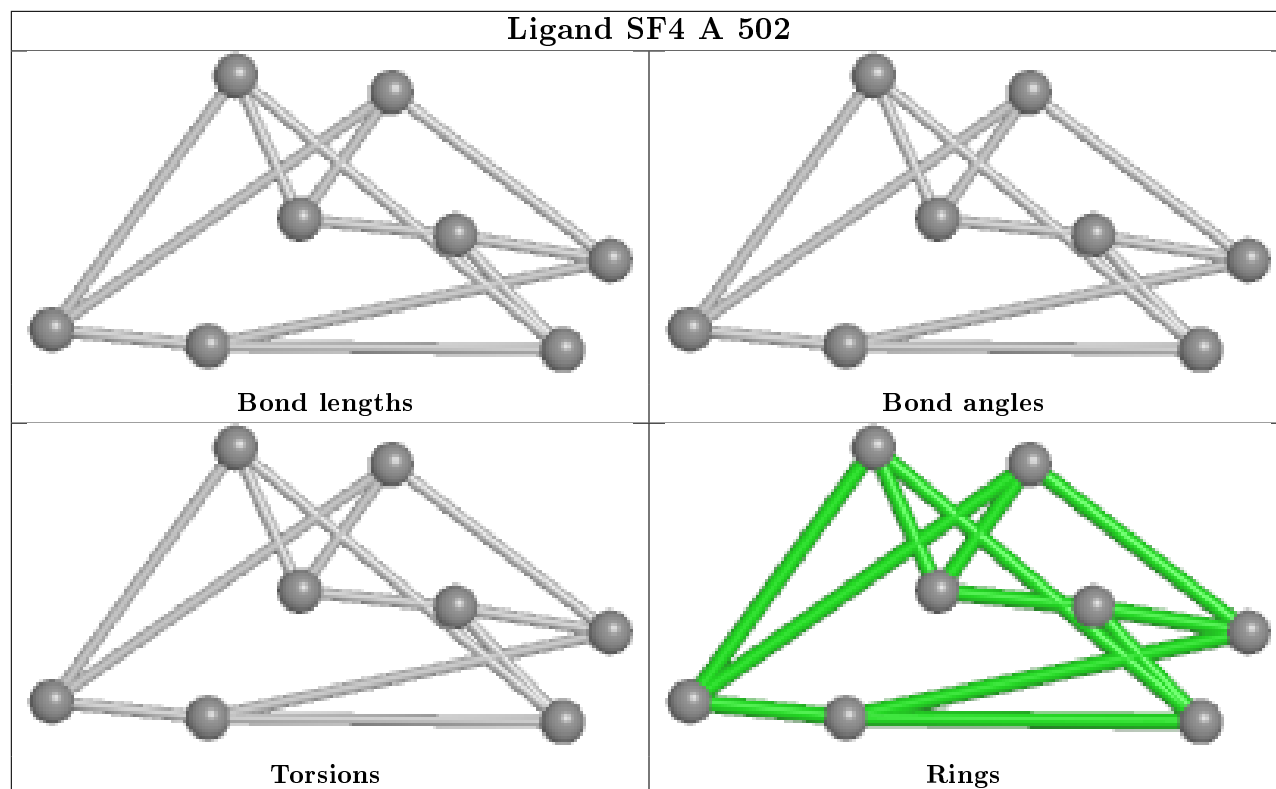


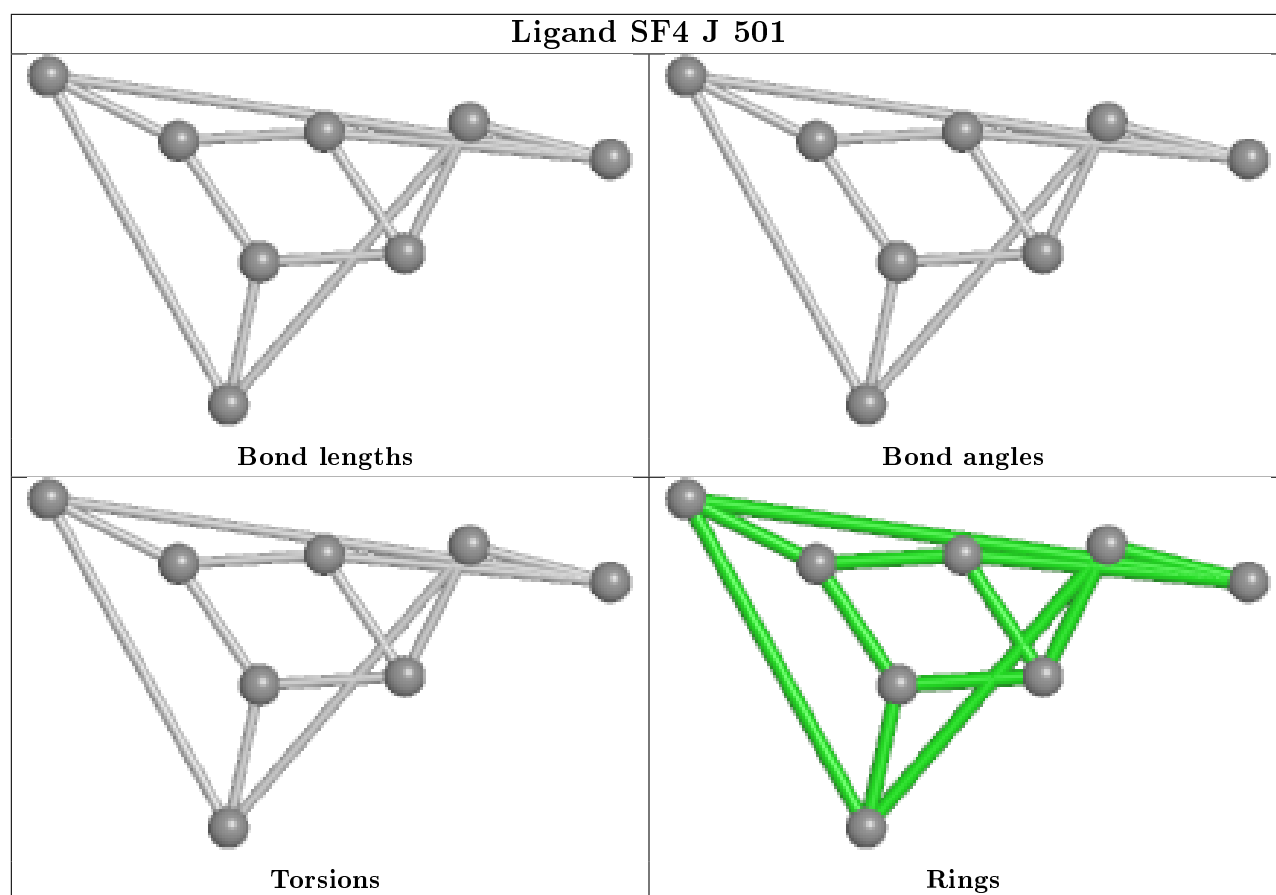
Ligand SF4 E 5804



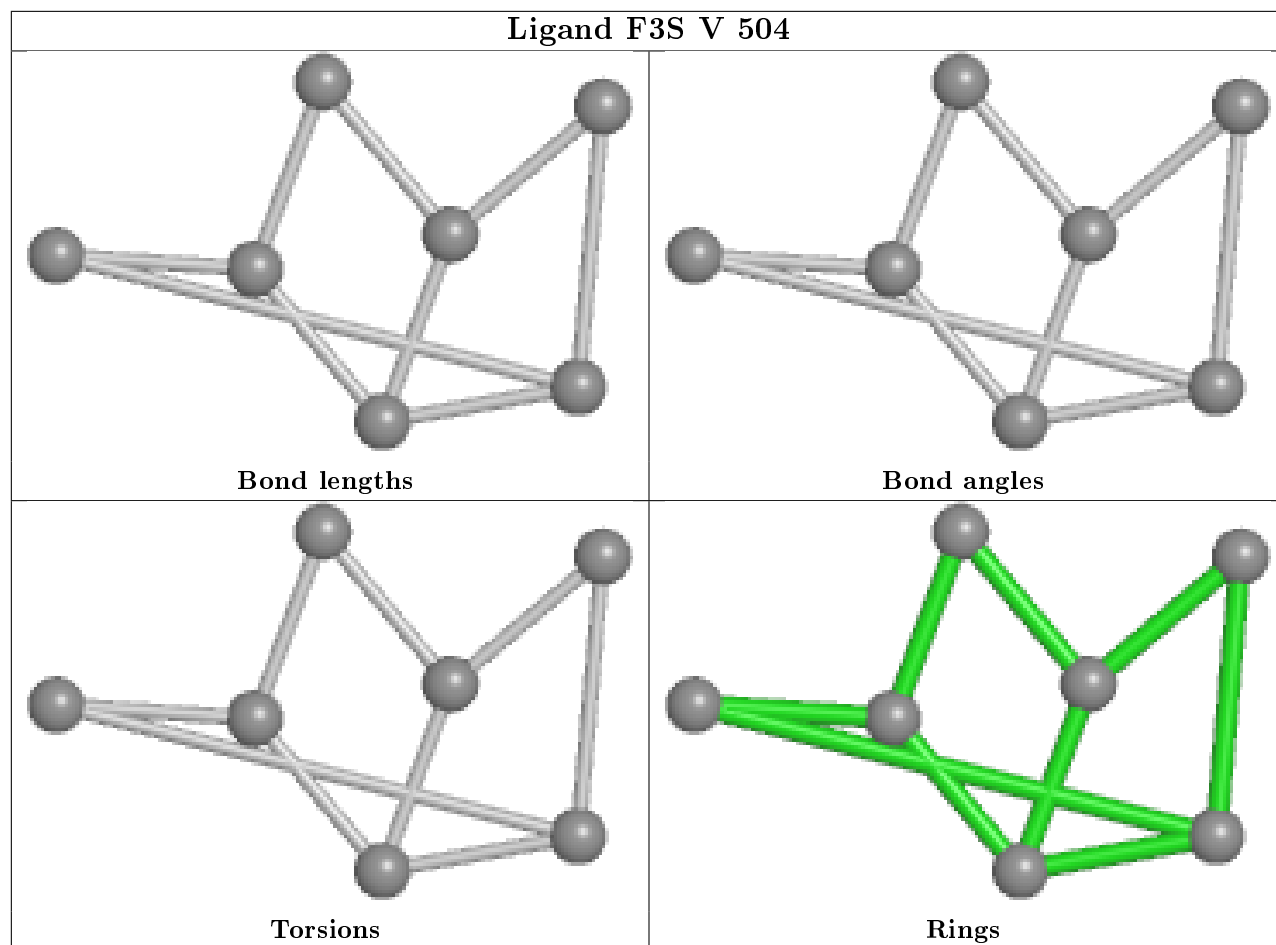
Ligand F3S M 504



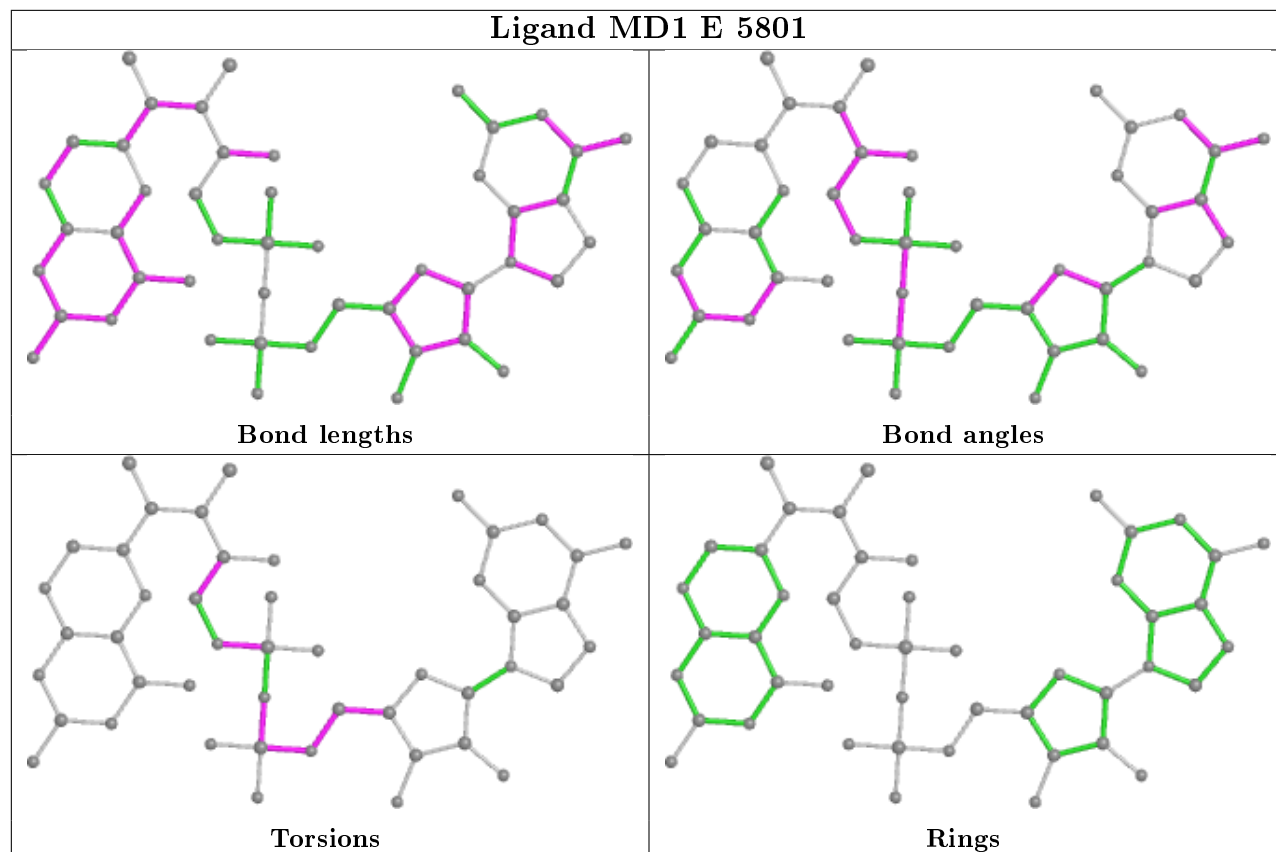




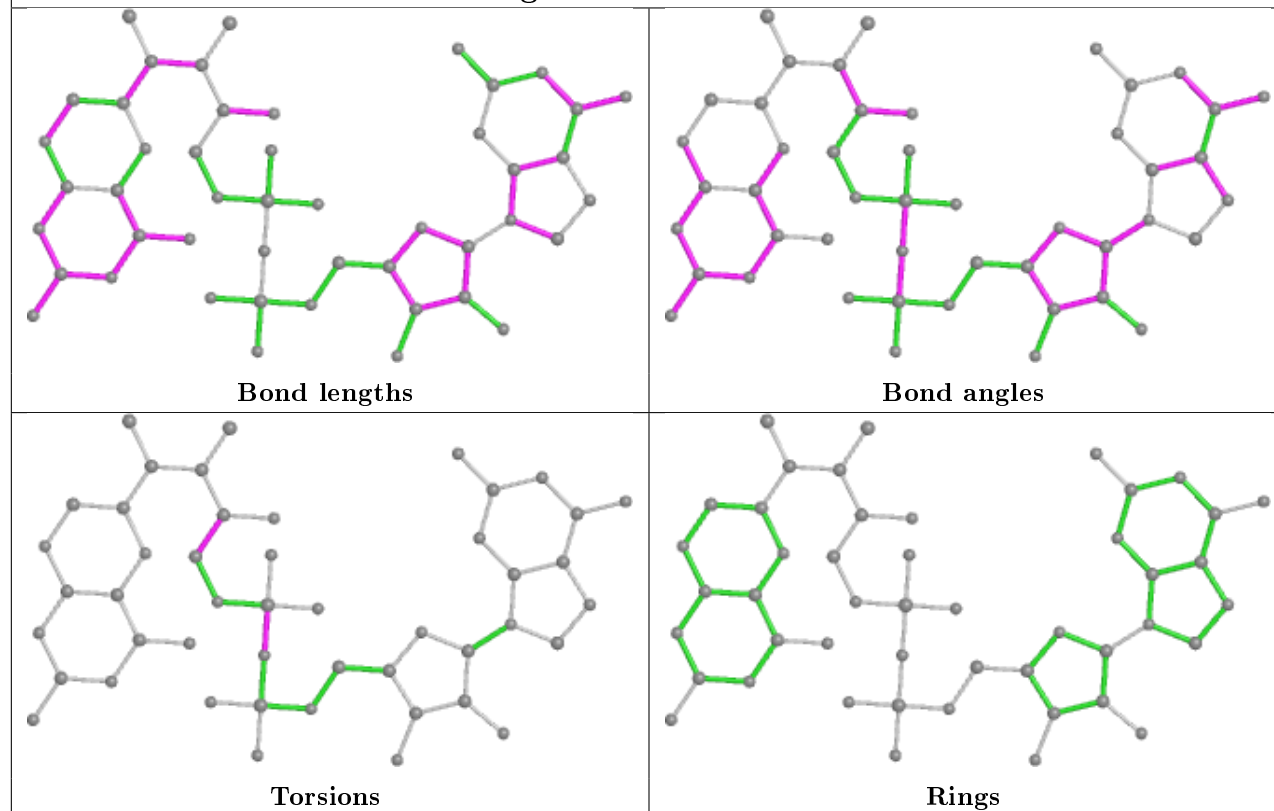
Ligand F3S V 504



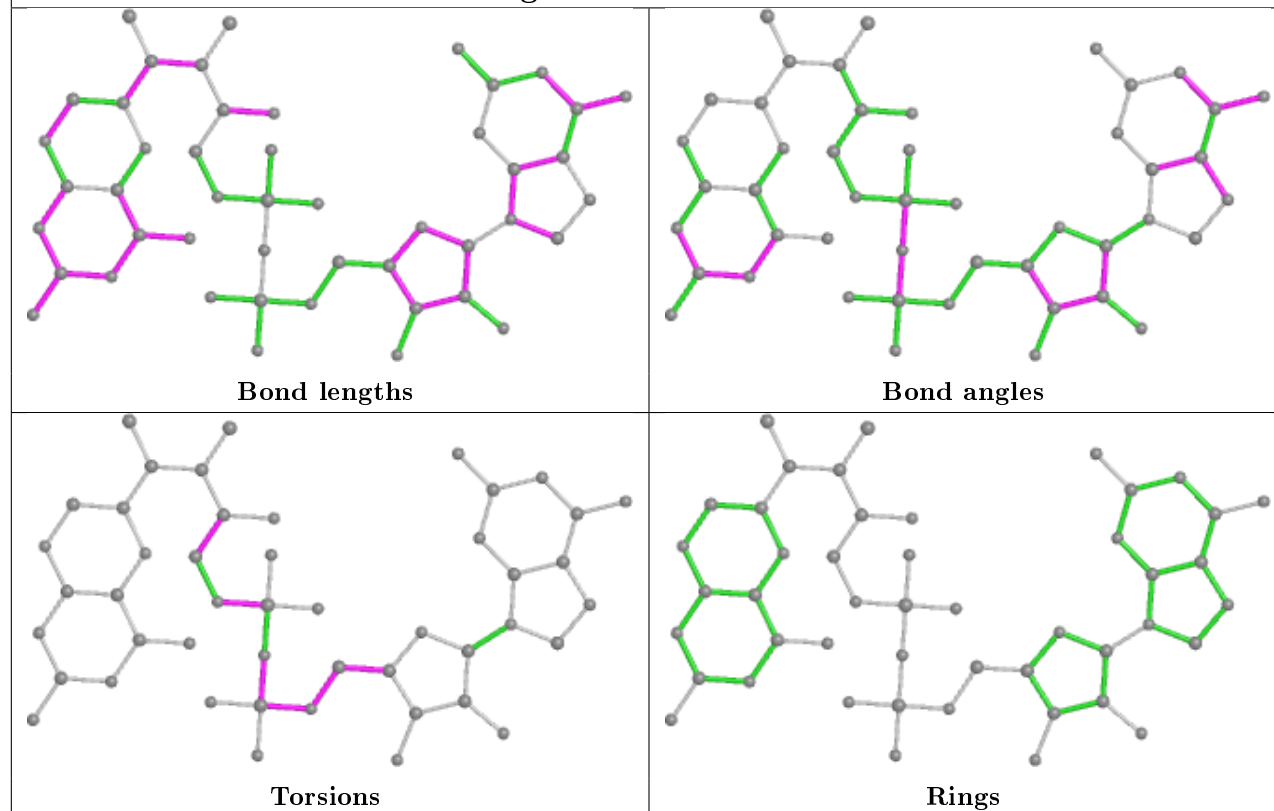
Ligand MD1 E 5801

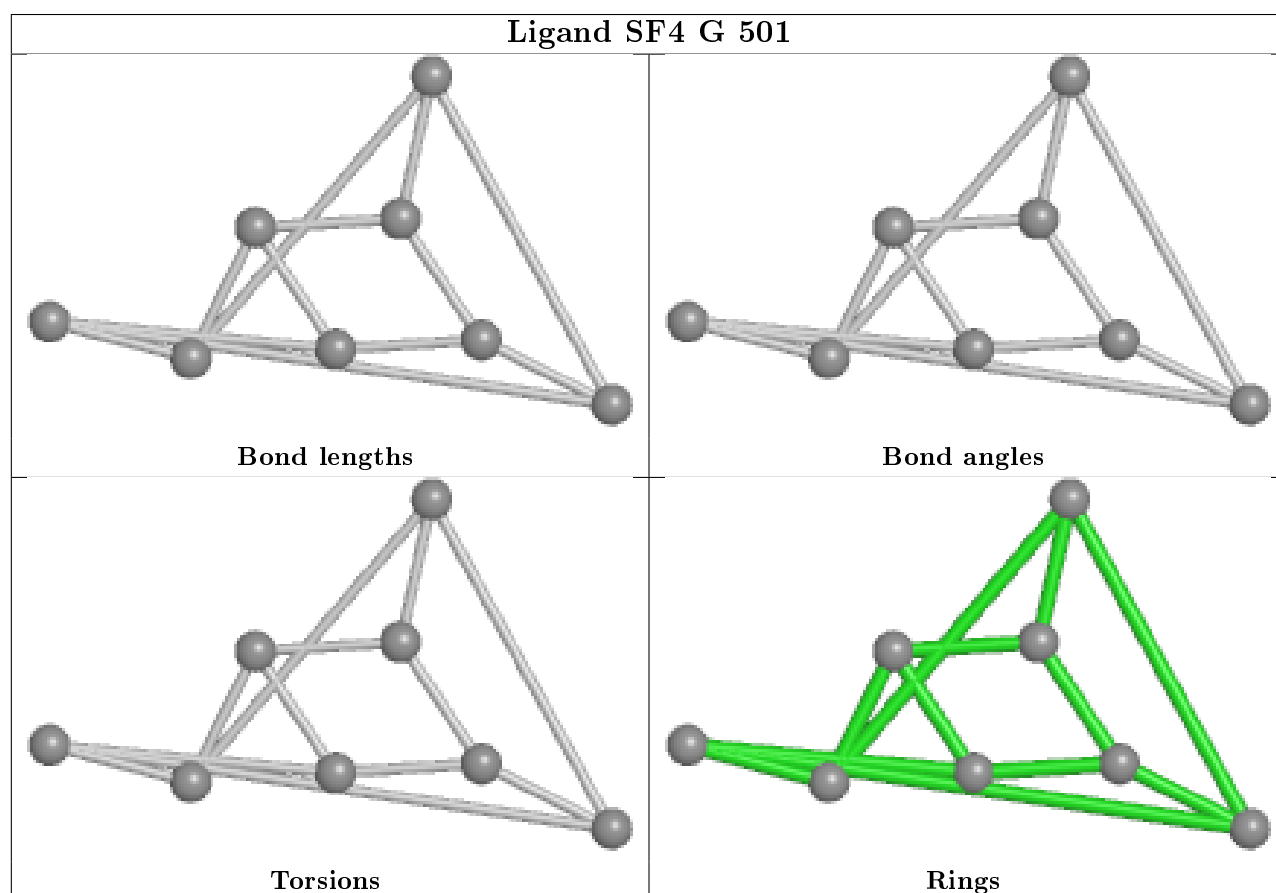
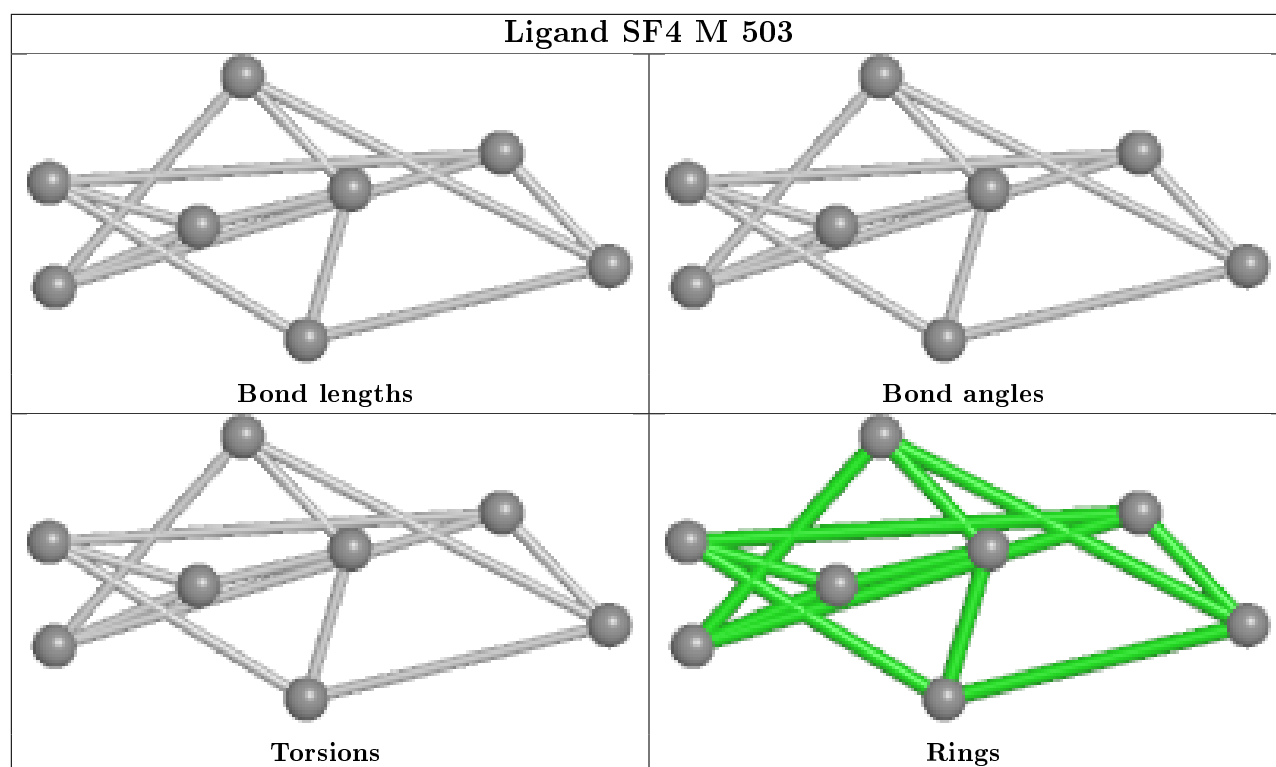


Ligand MD1 K 5802

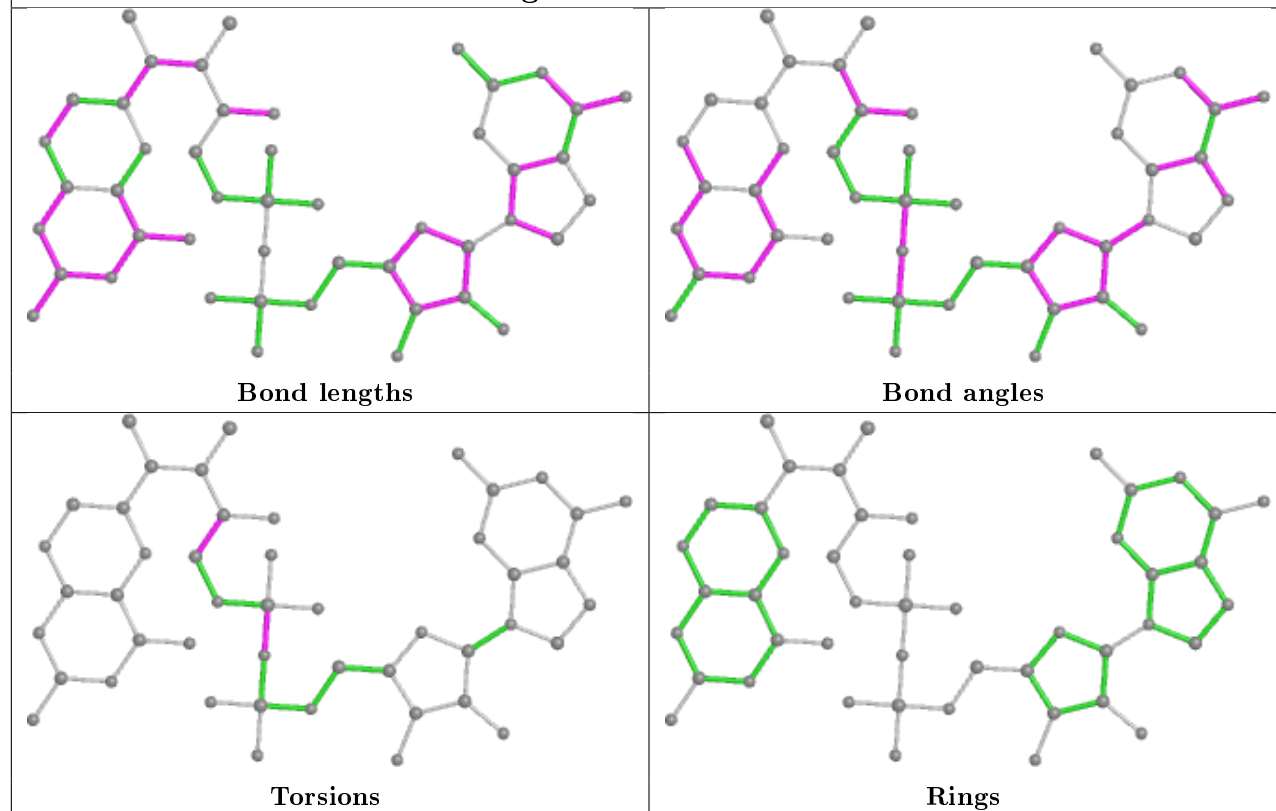


Ligand MD1 N 5801

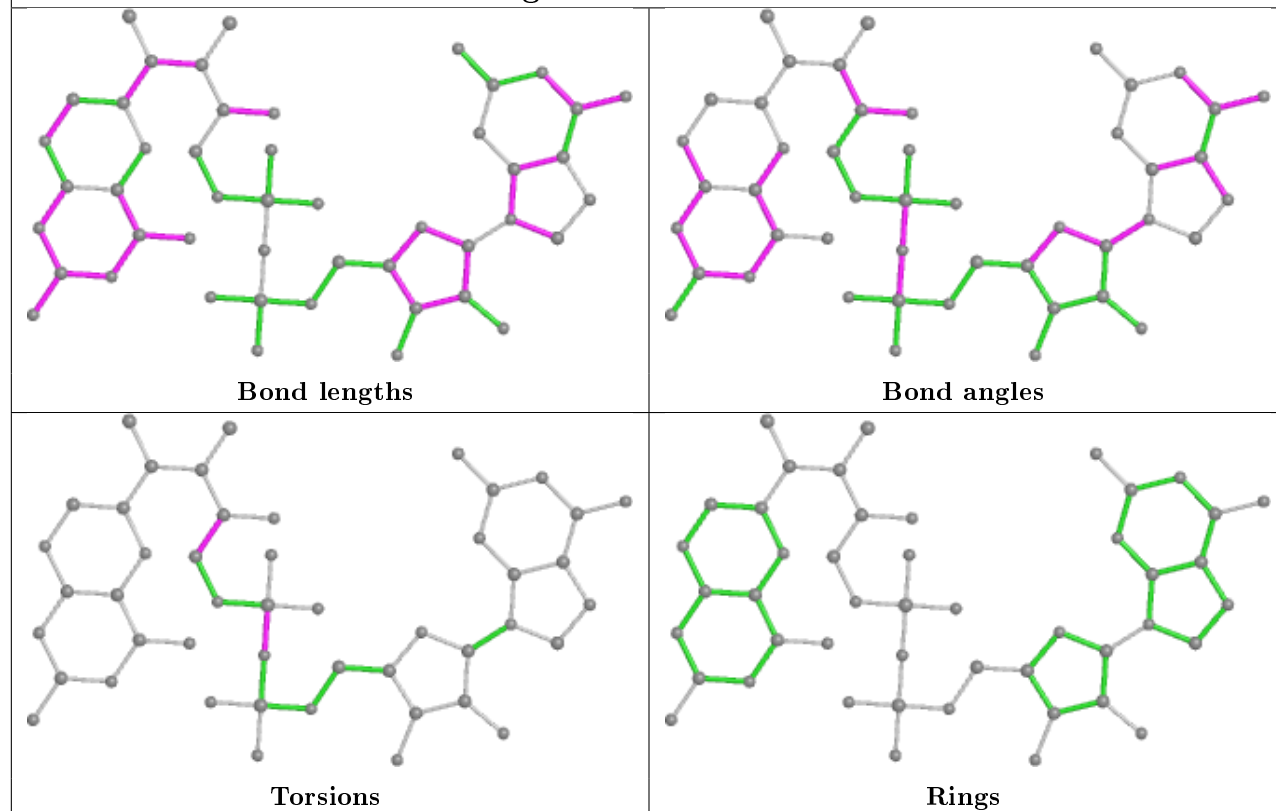




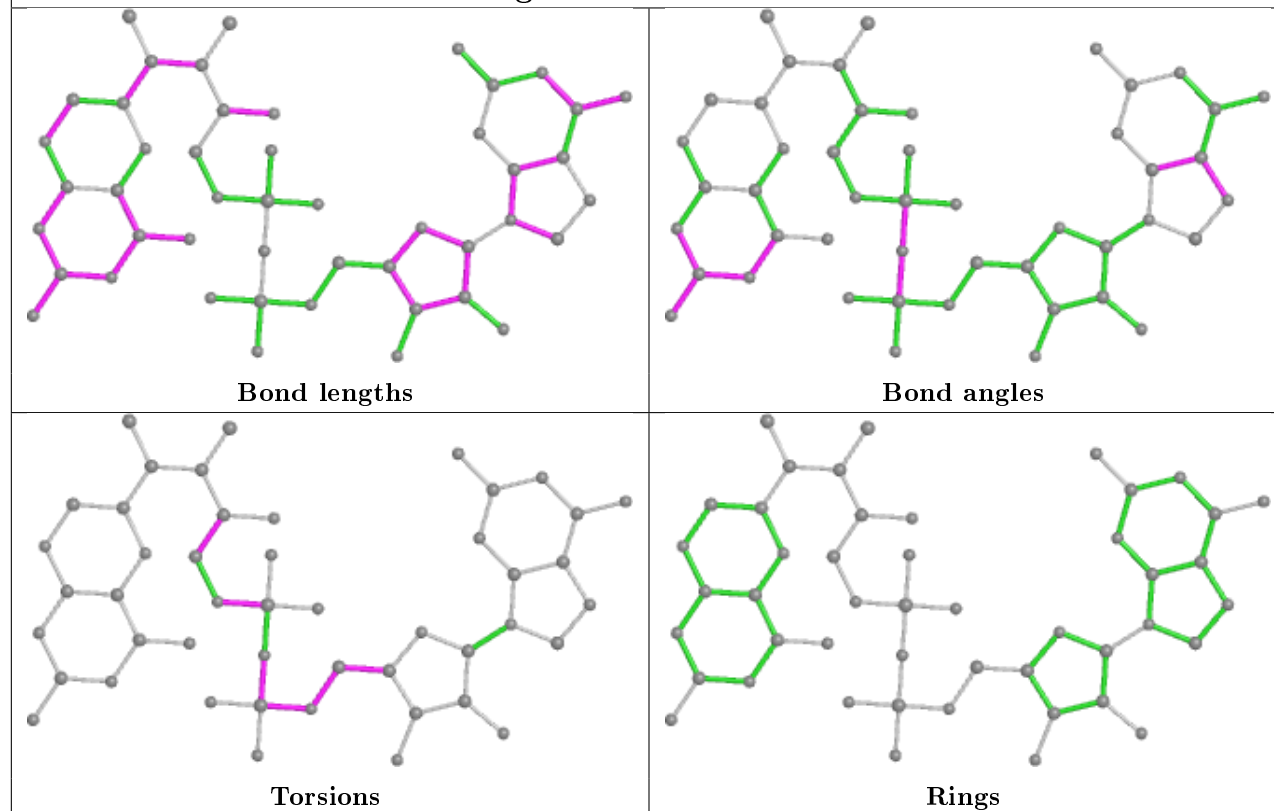
Ligand MD1 T 5802



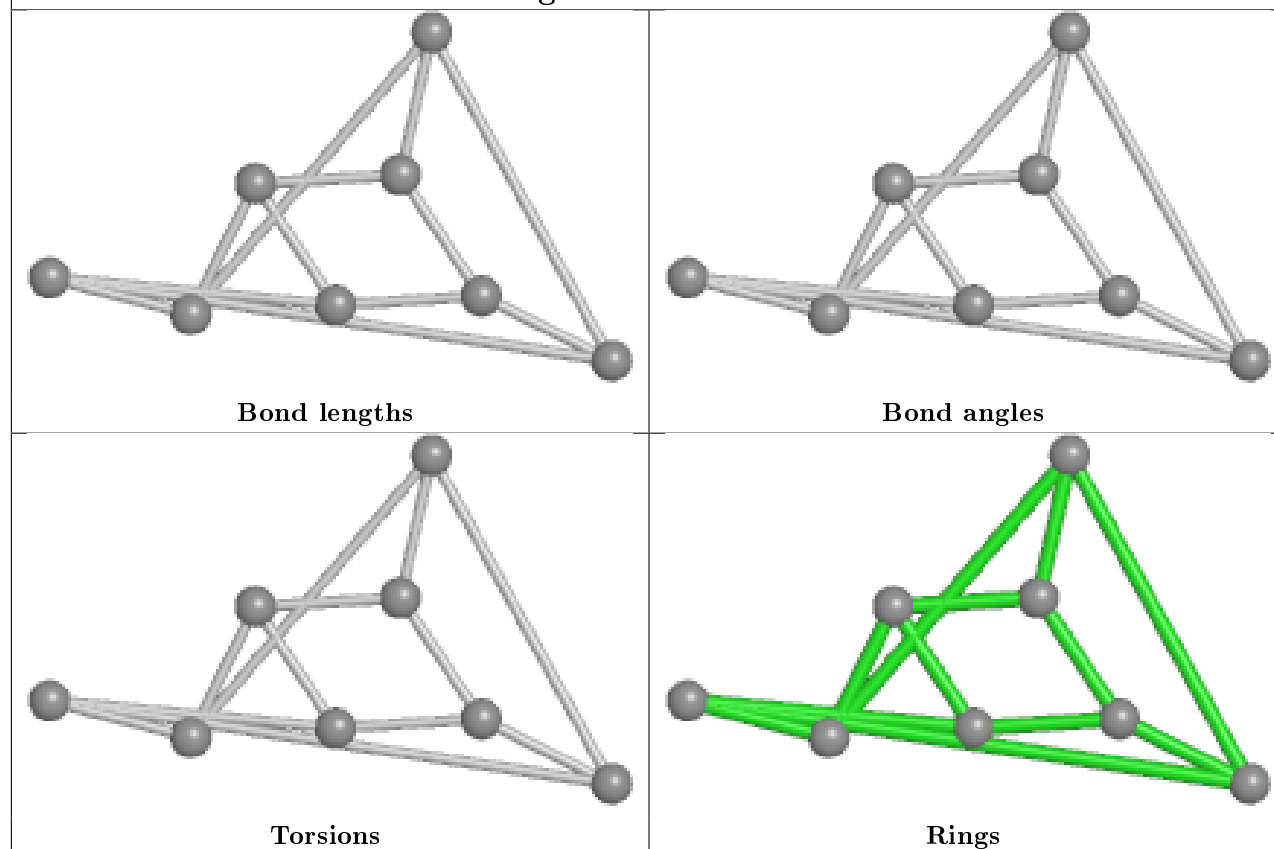
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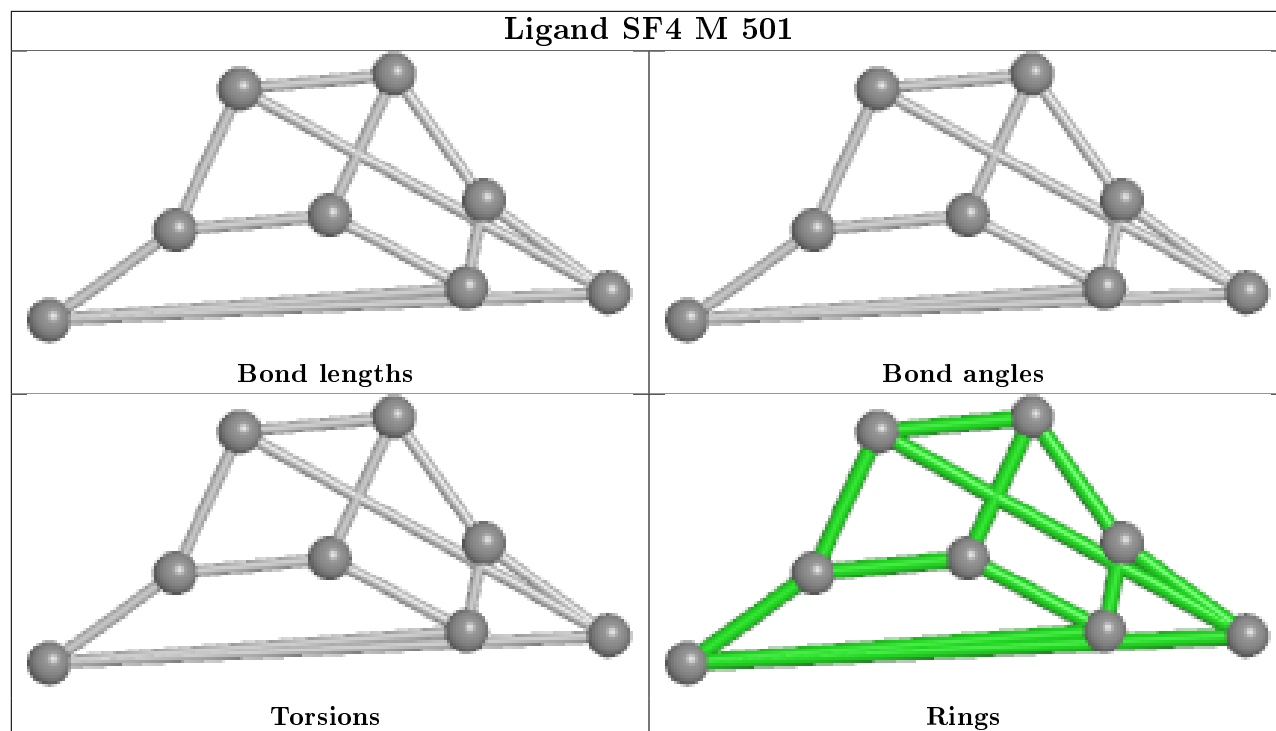


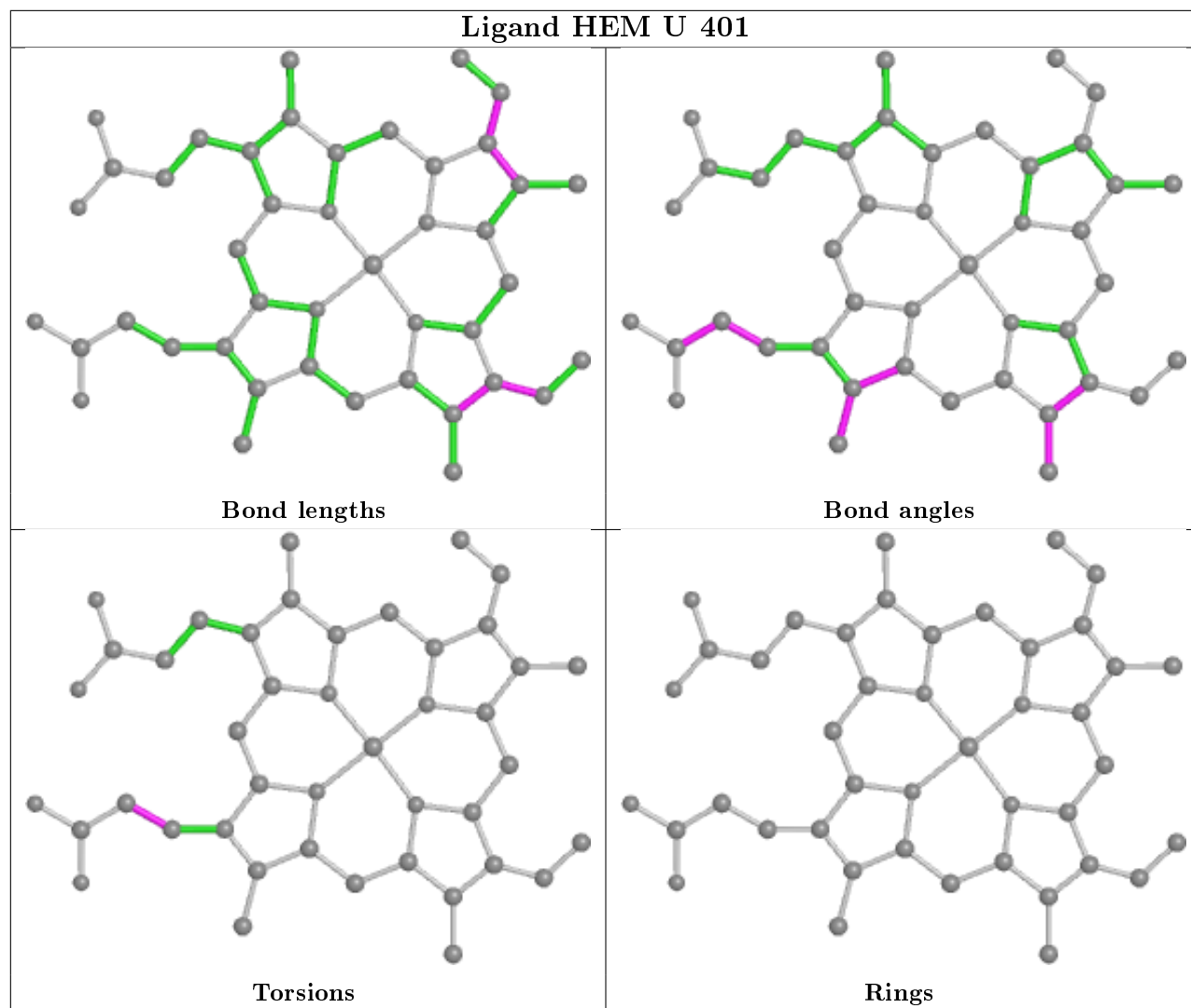
Ligand MD1 W 5801



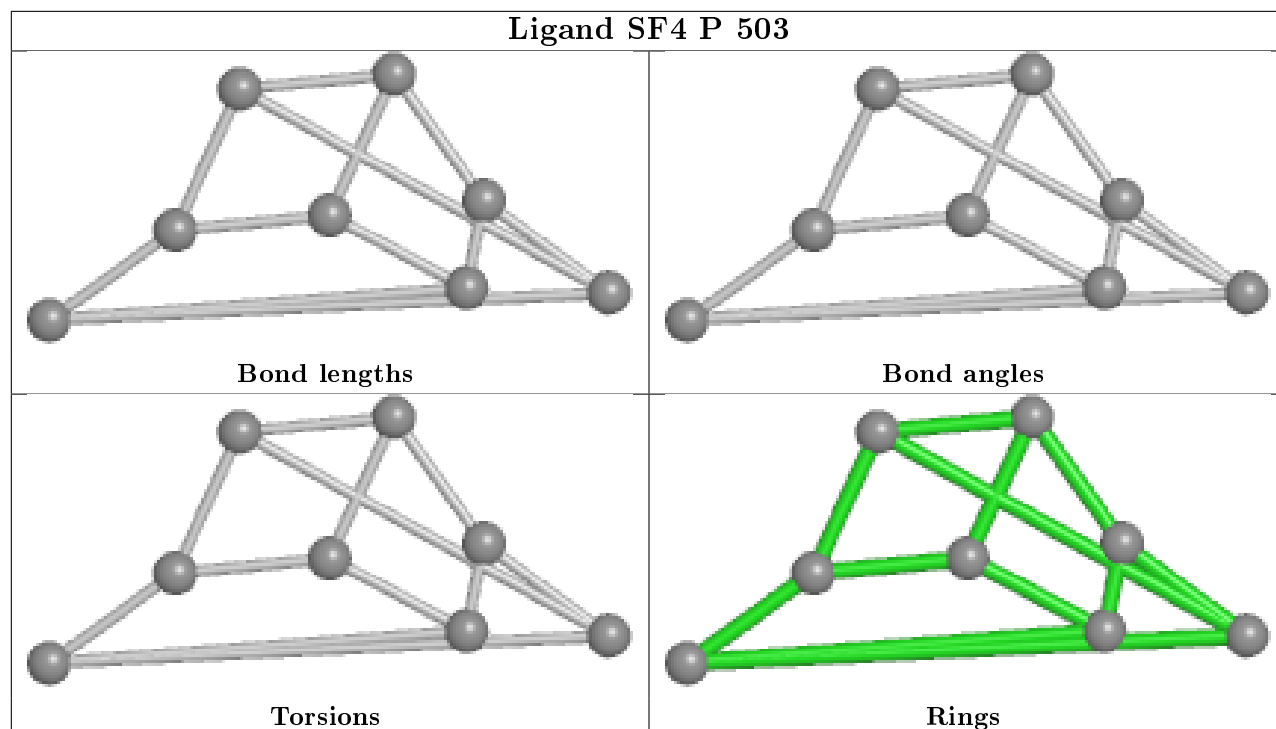
Ligand SF4 D 501



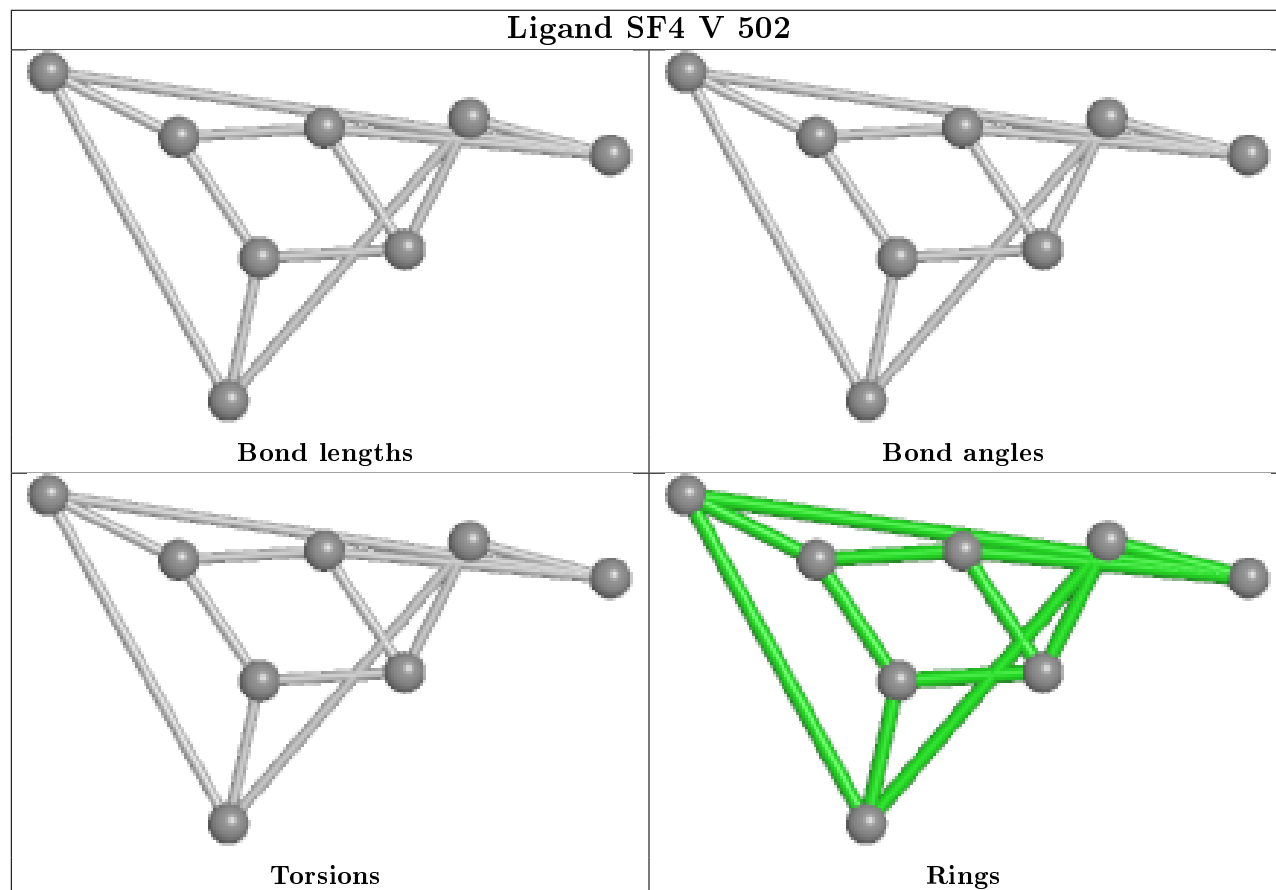




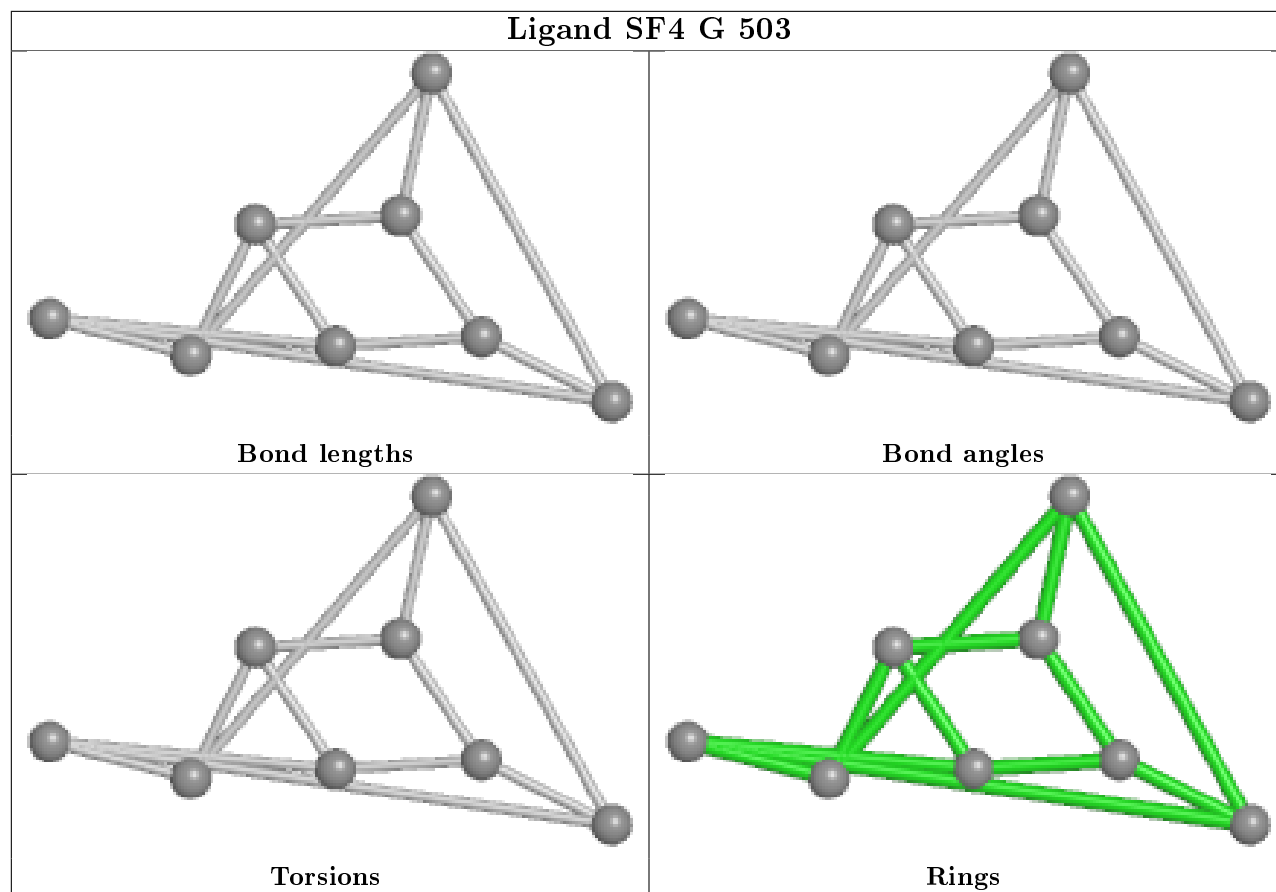
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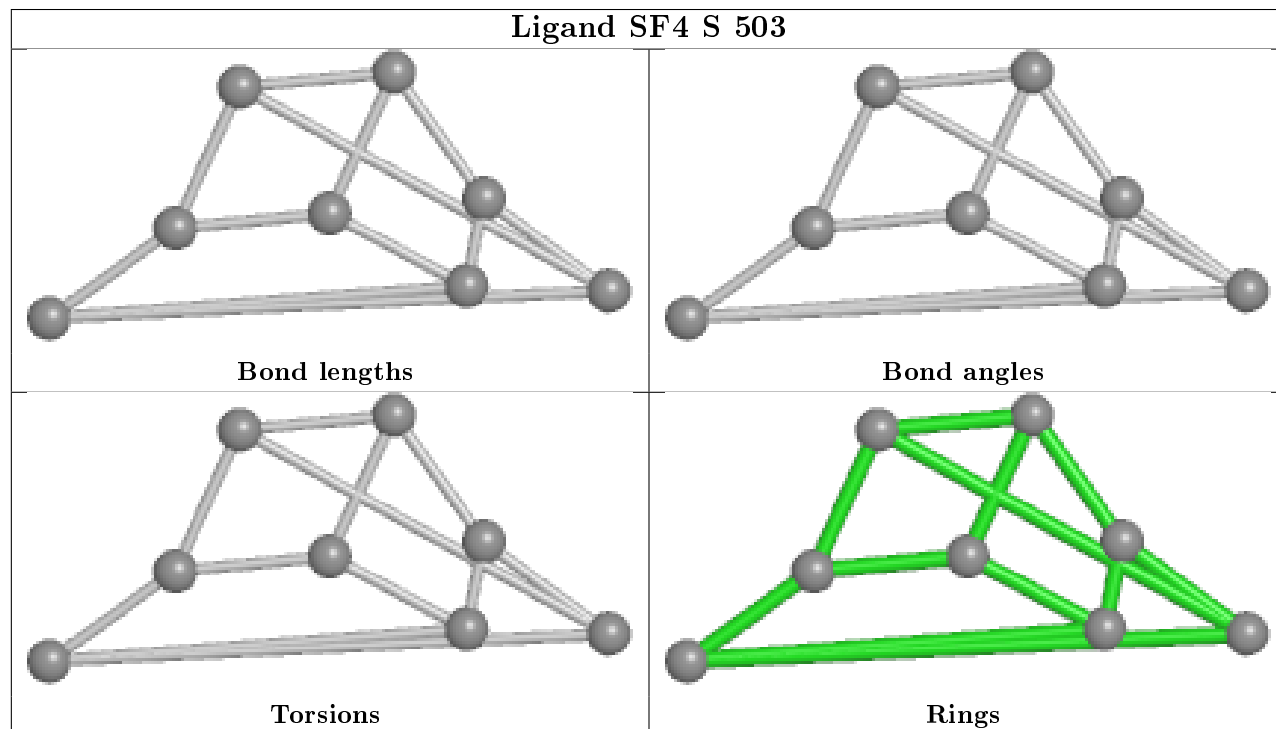
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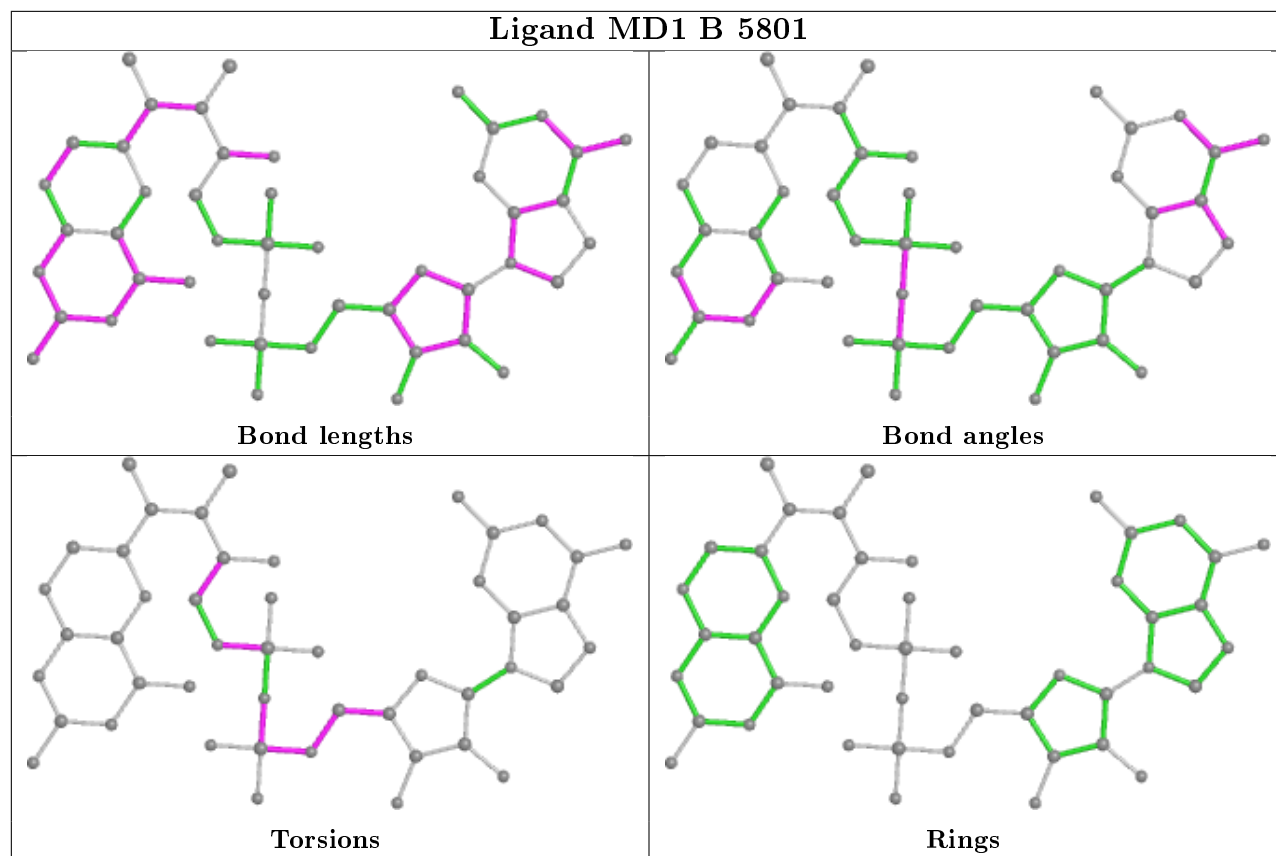


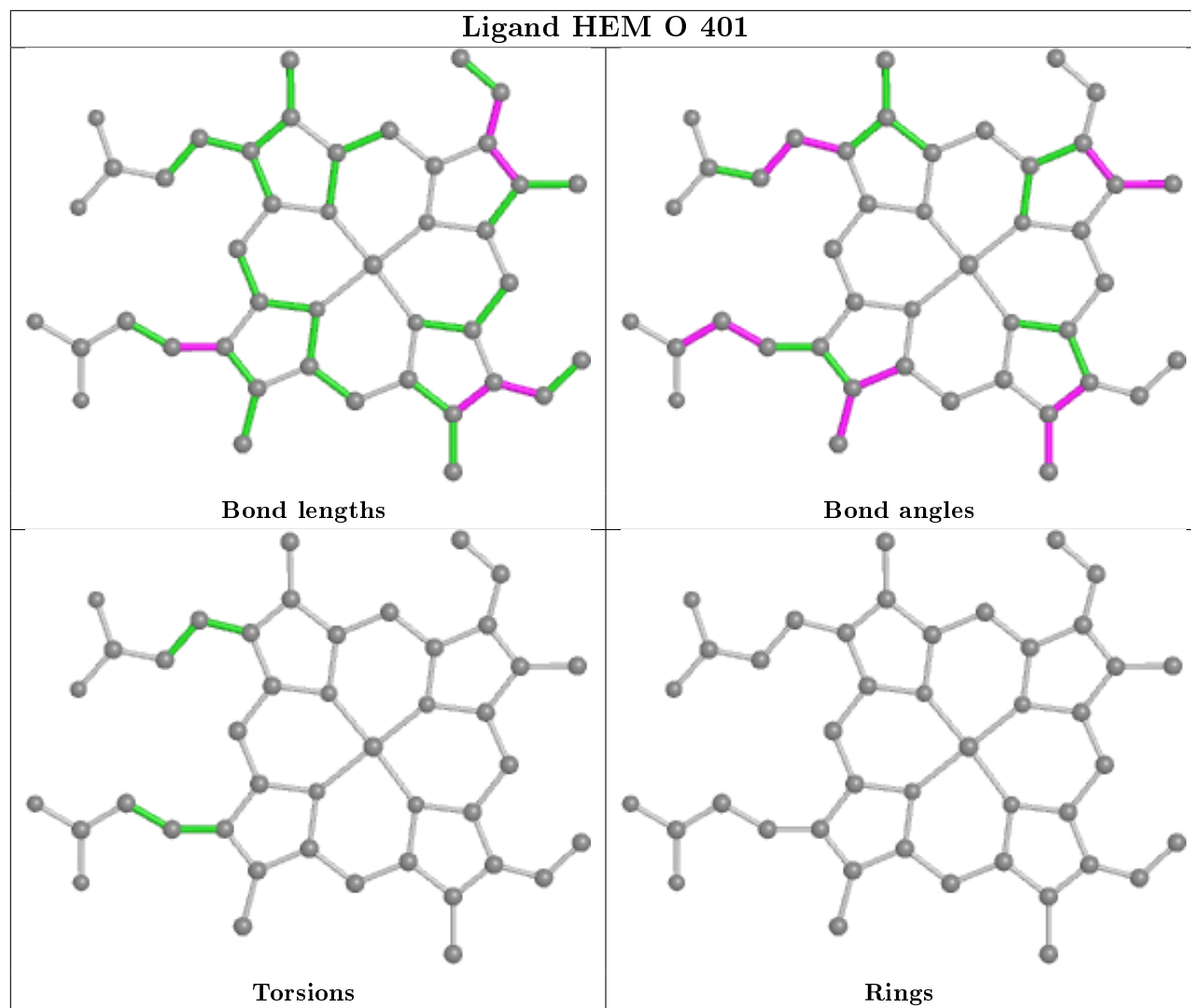
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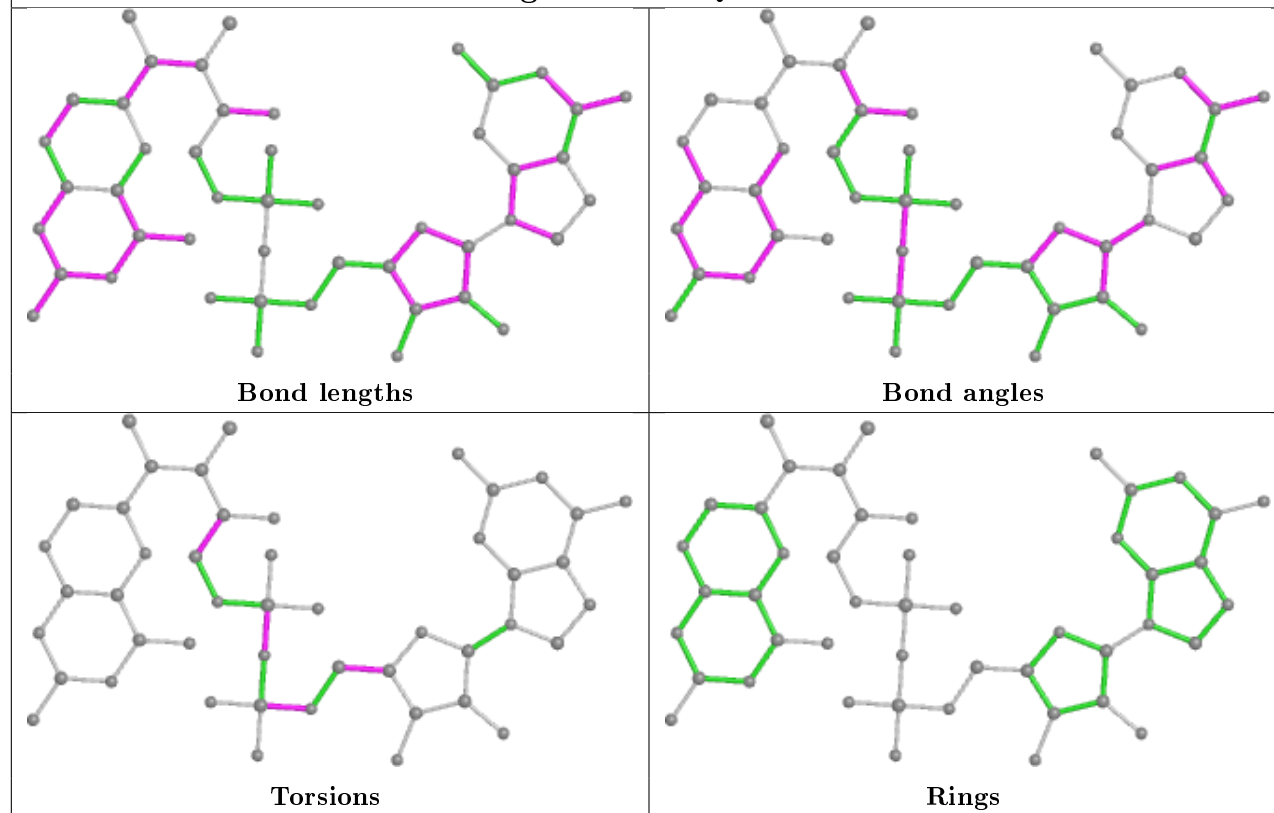
Ligand SF4 S 503



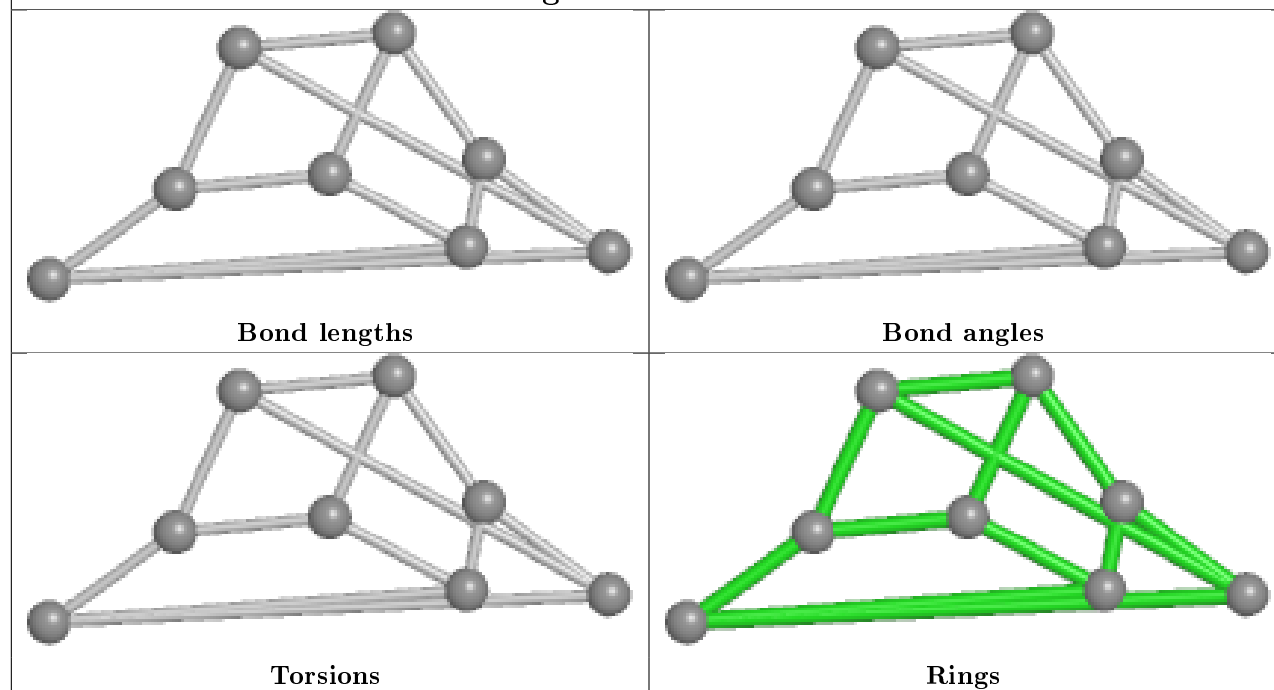


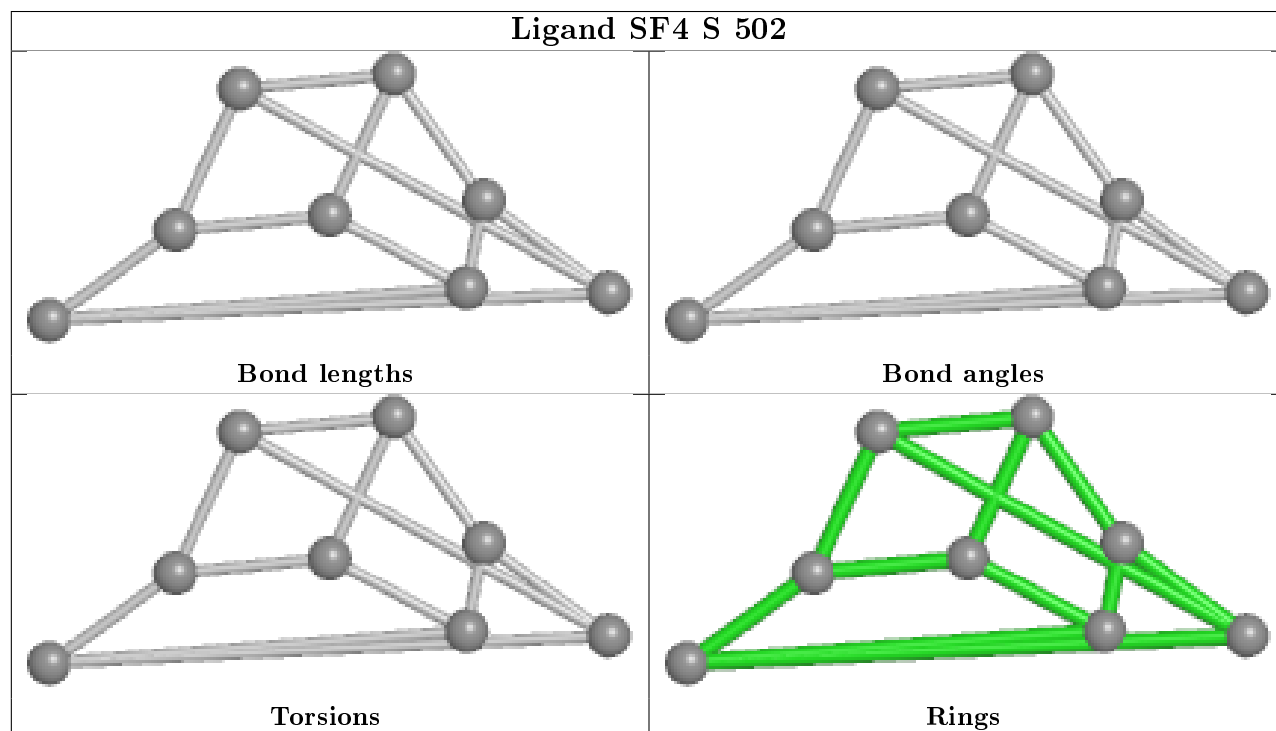
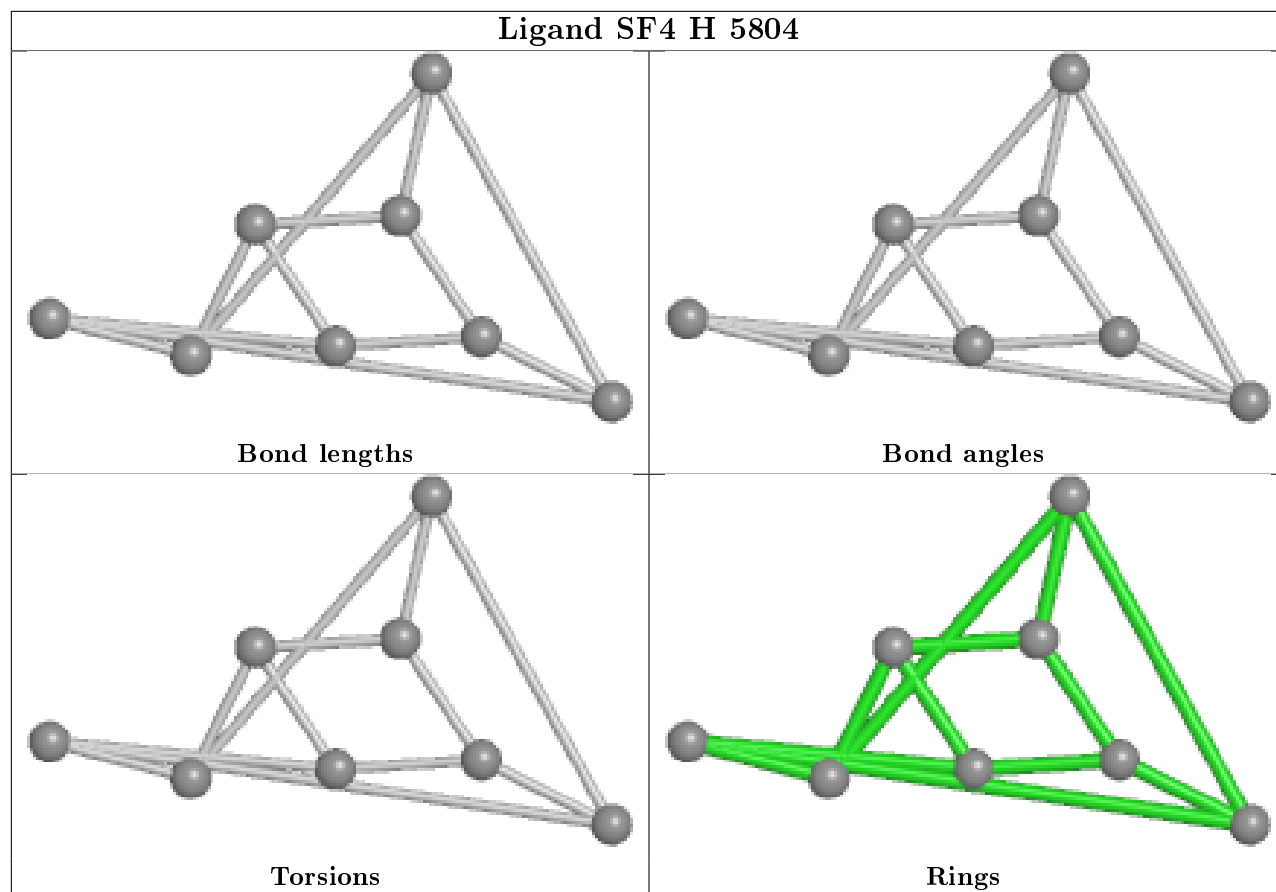


Ligand MD1 Q 5802

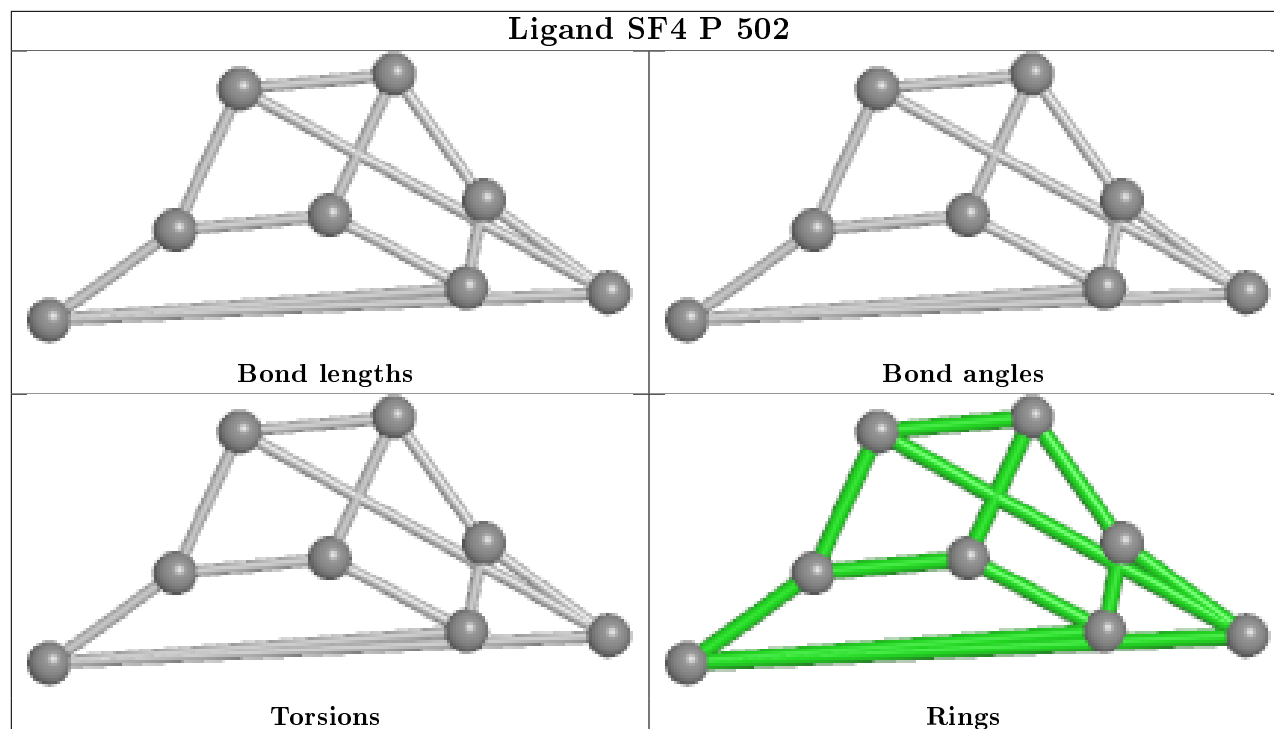


Ligand SF4 S 501

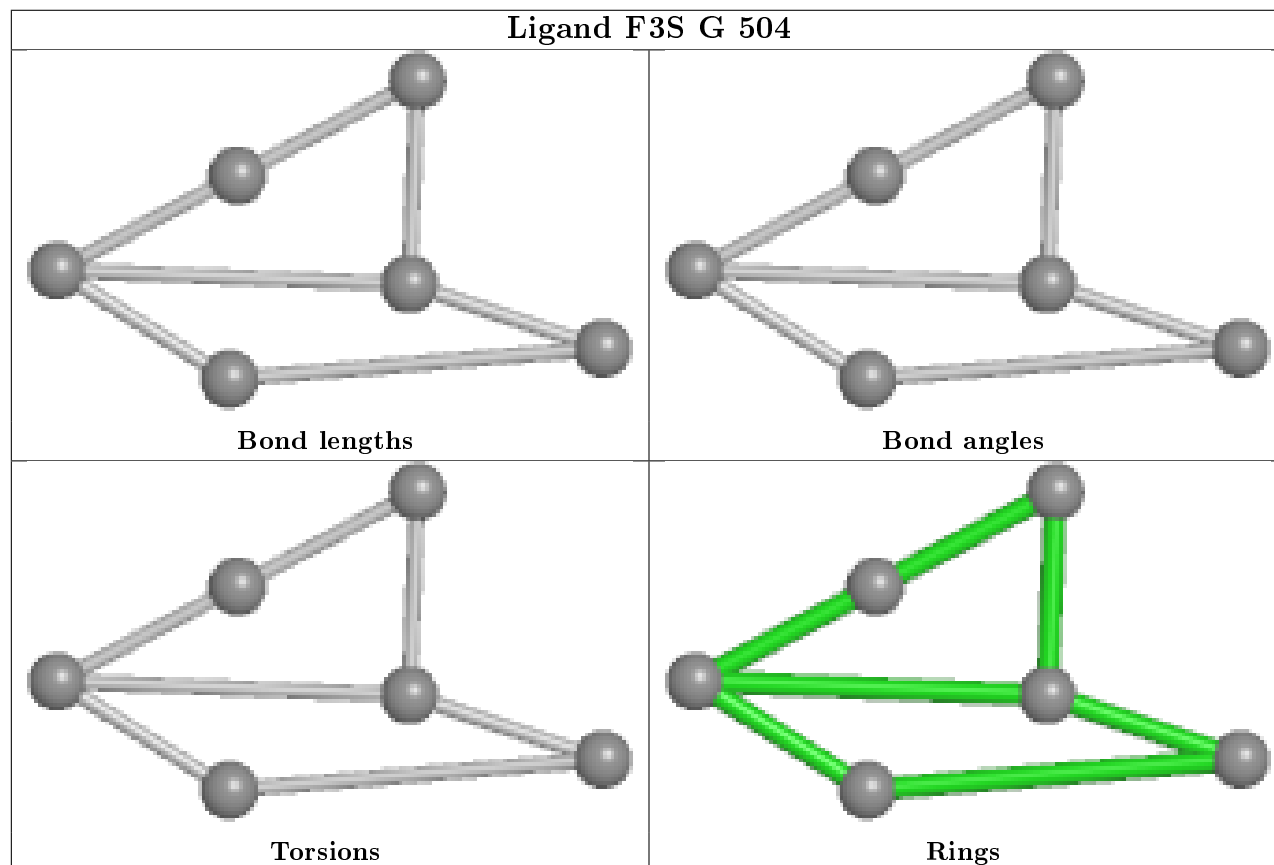




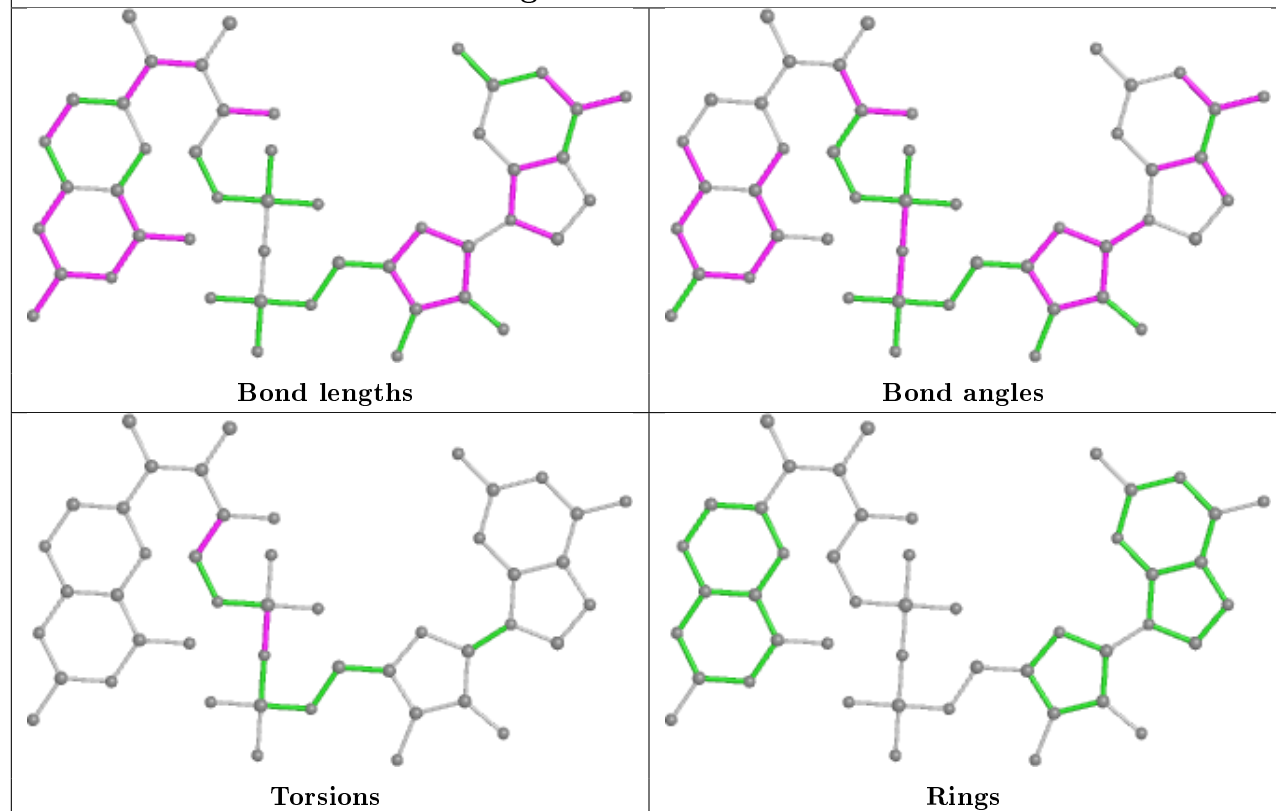
Ligand SF4 P 502



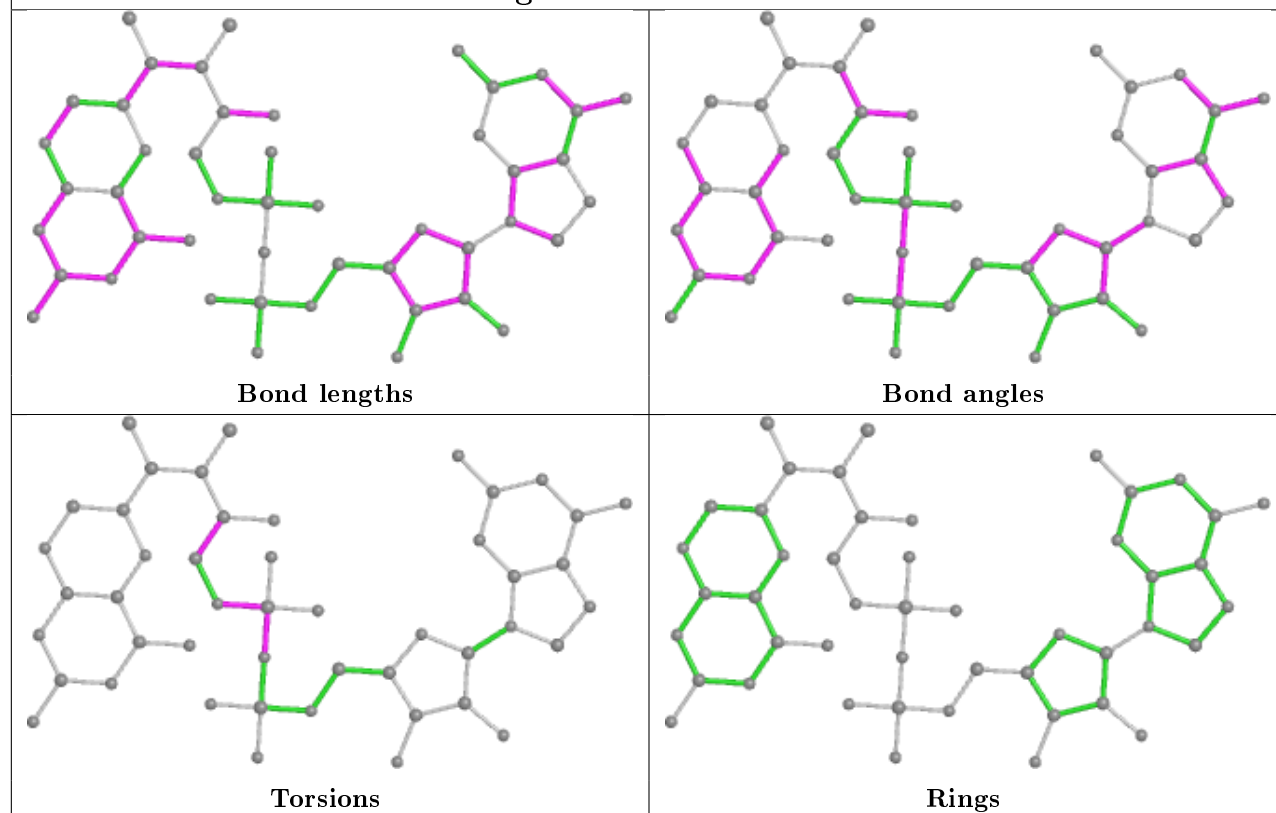
Ligand F3S G 504



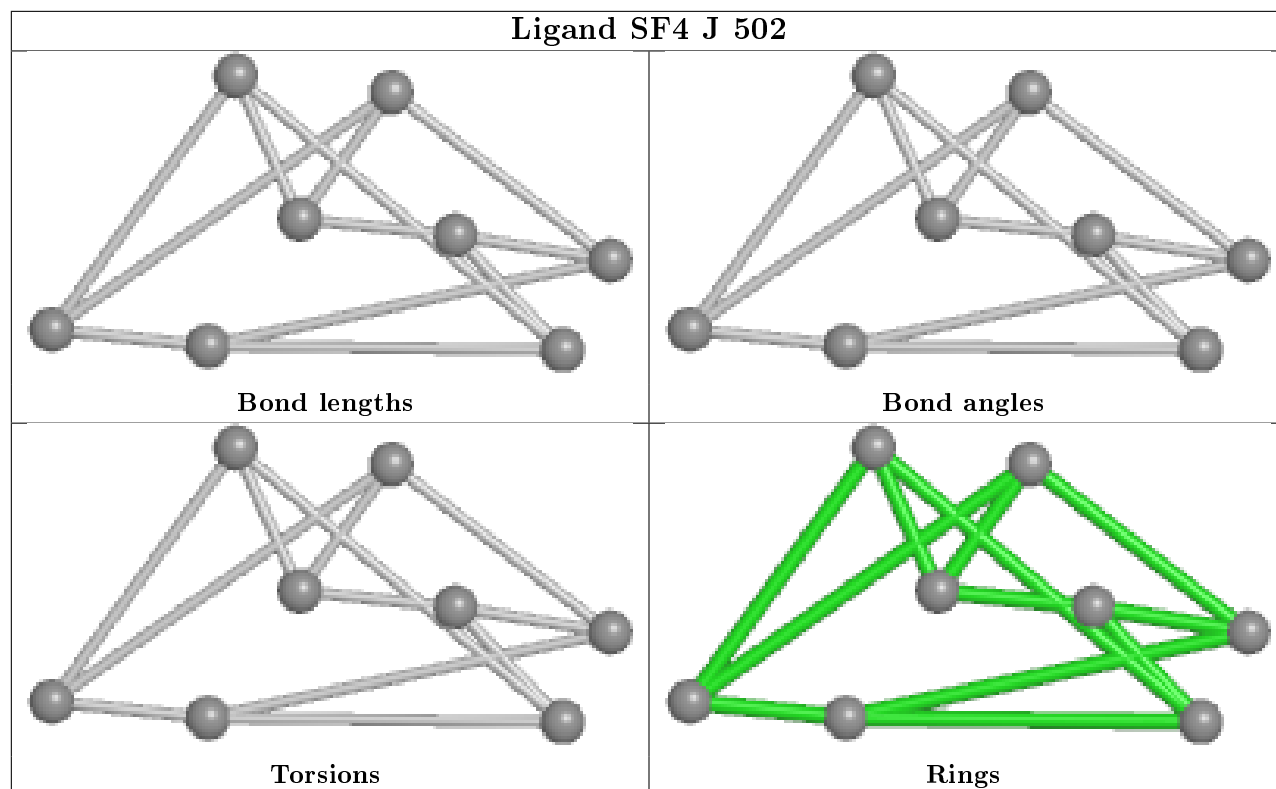
Ligand MD1 N 5802



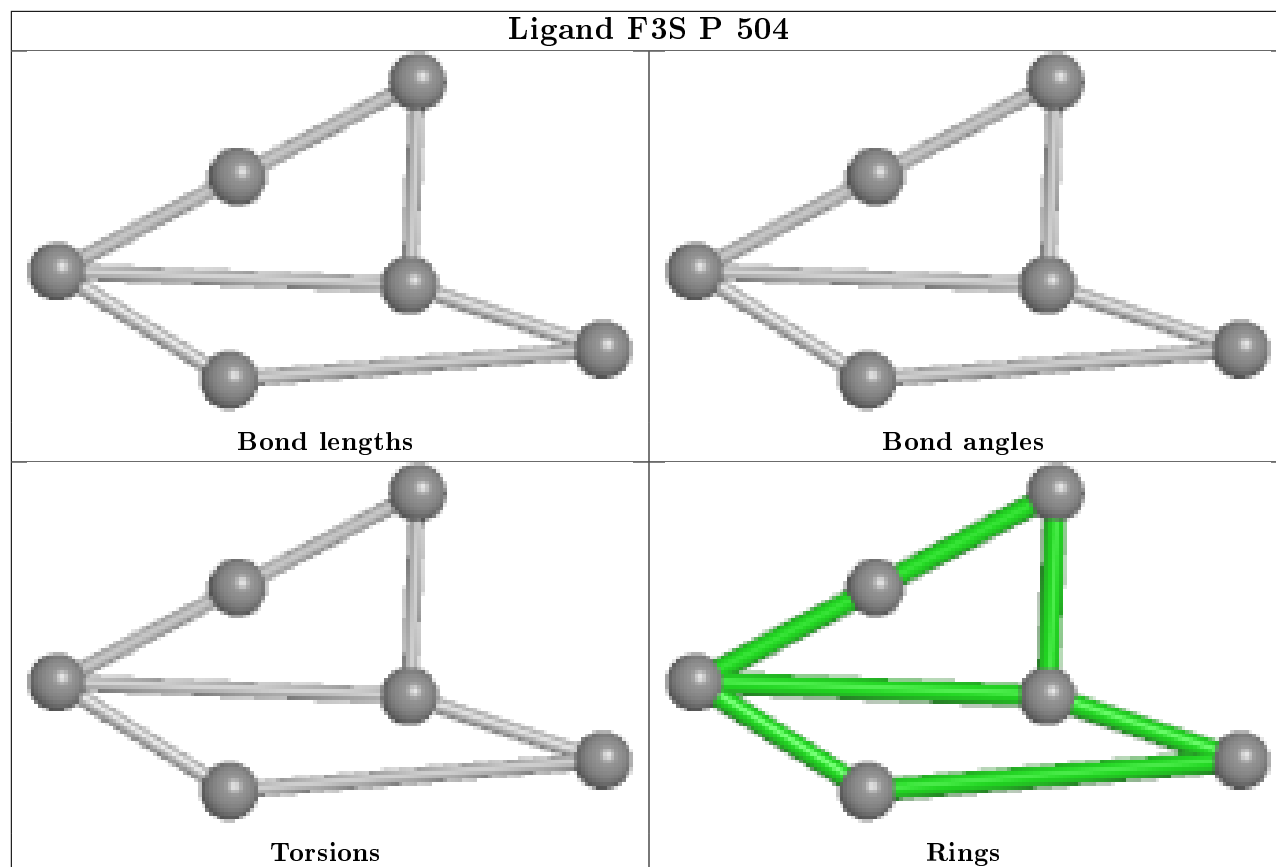
Ligand MD1 W 5802



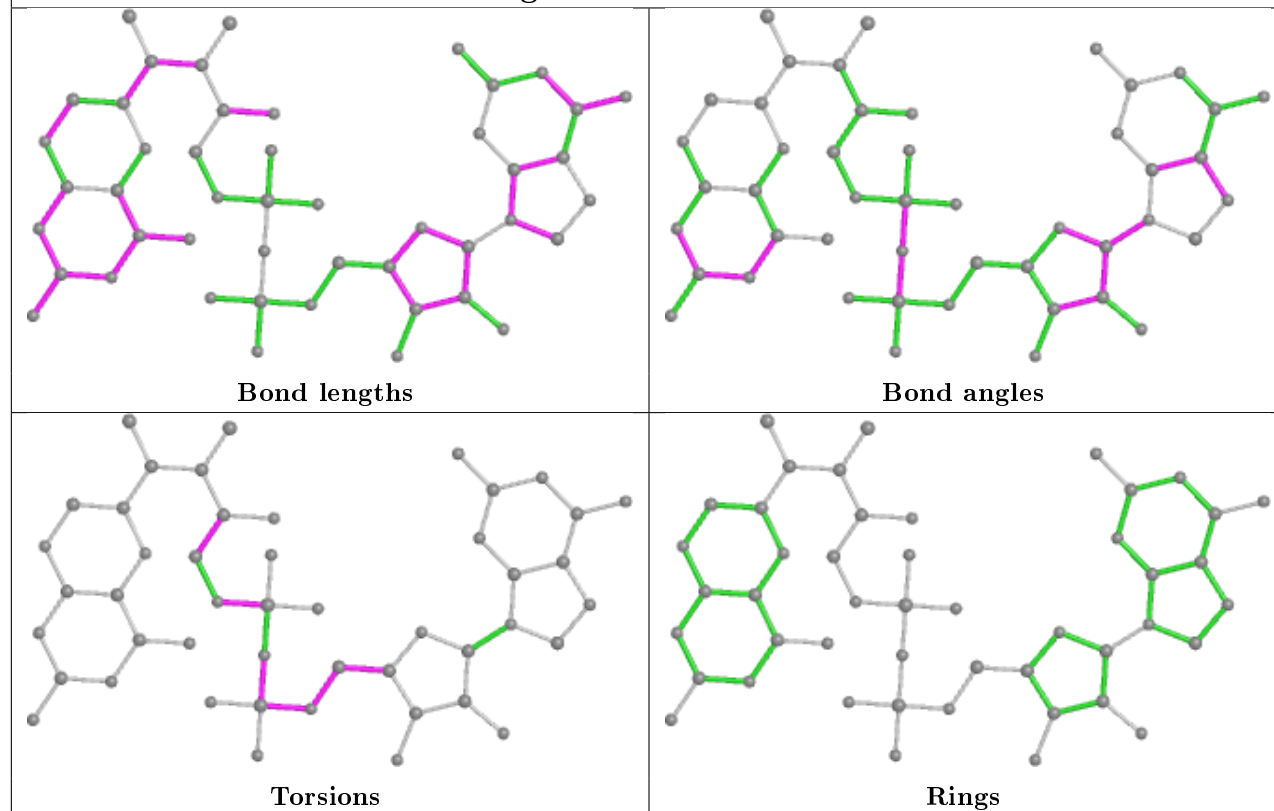
Ligand SF4 J 502



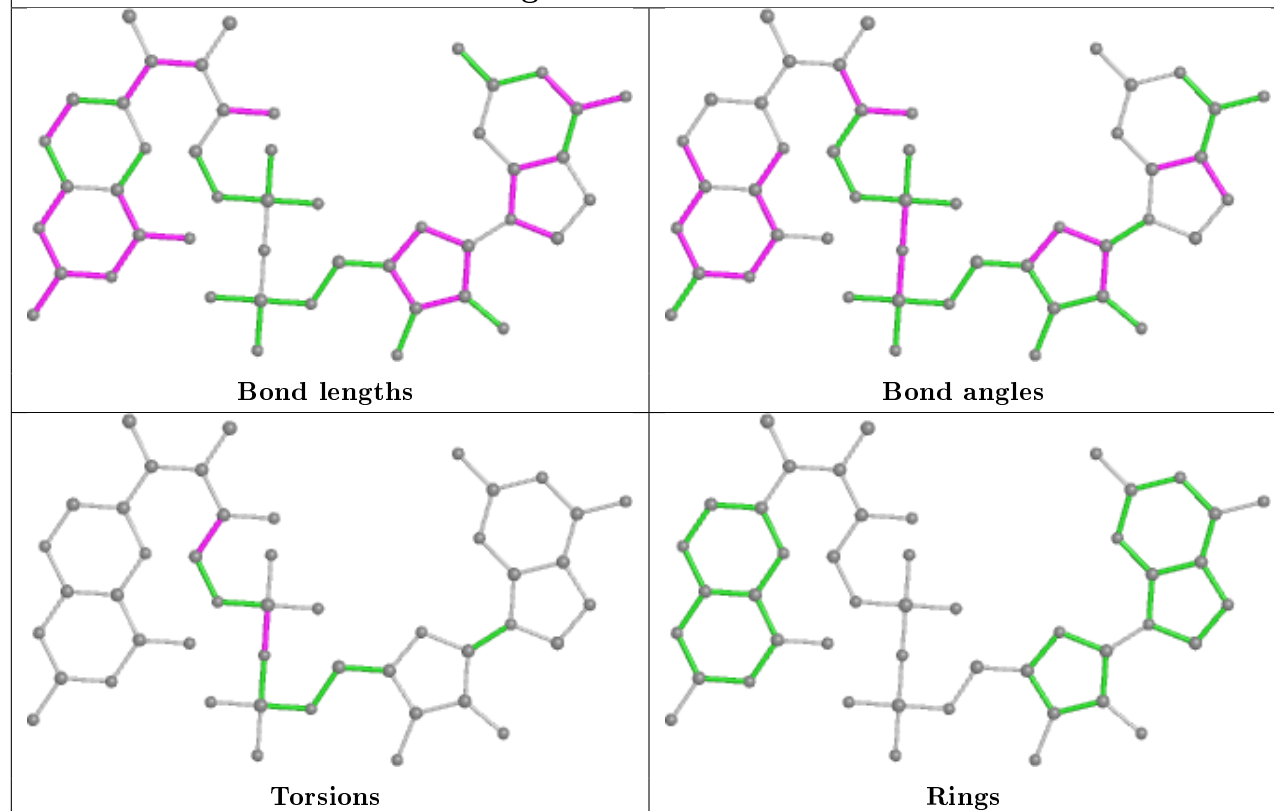
Ligand F3S P 504

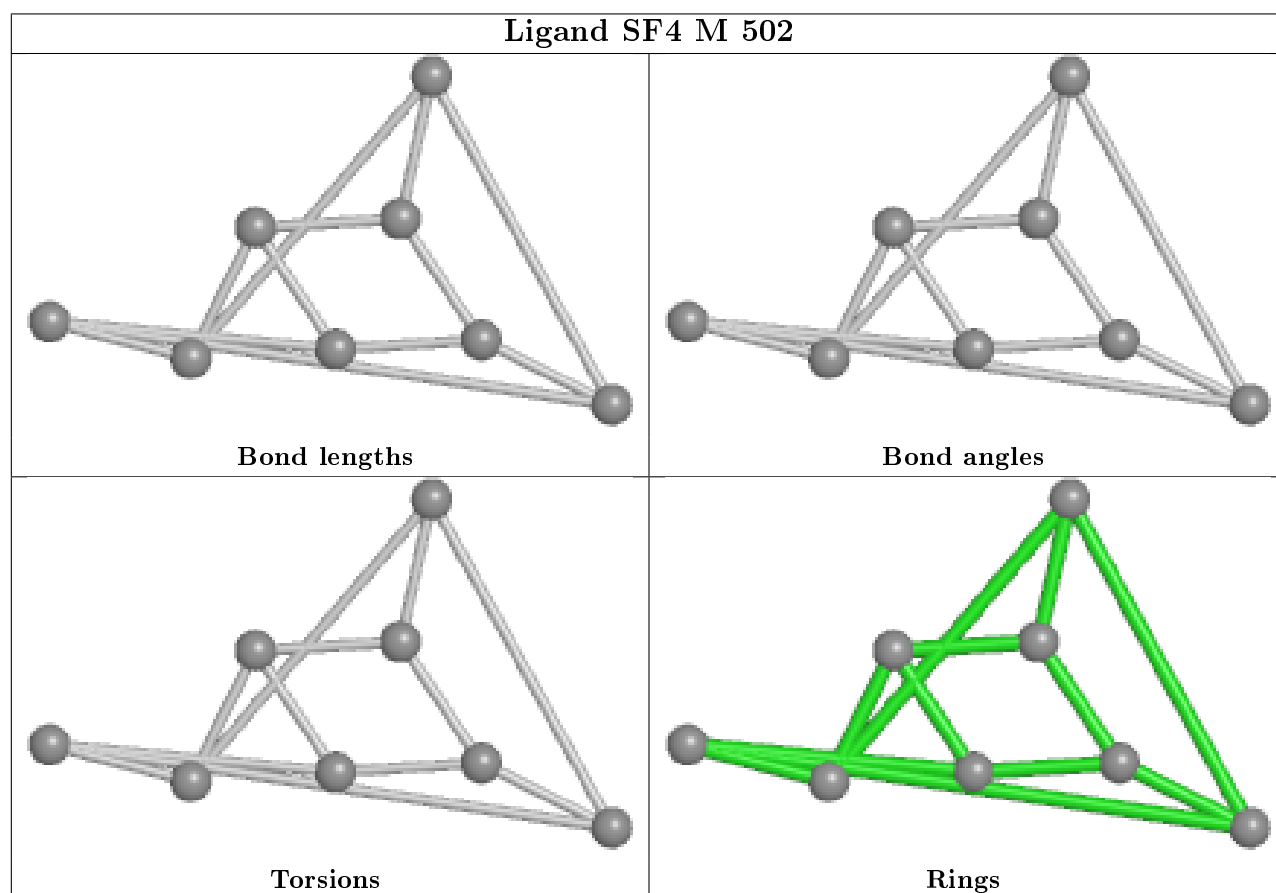
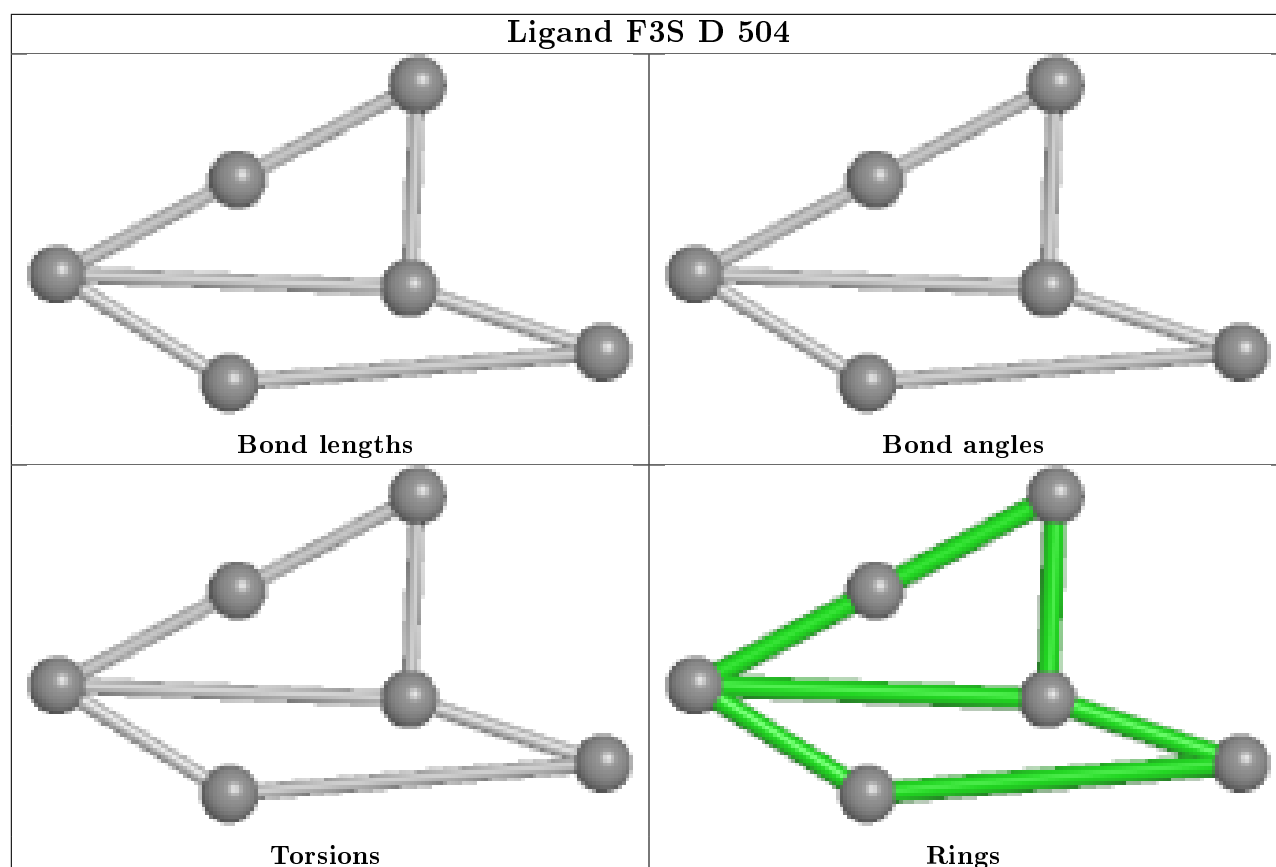


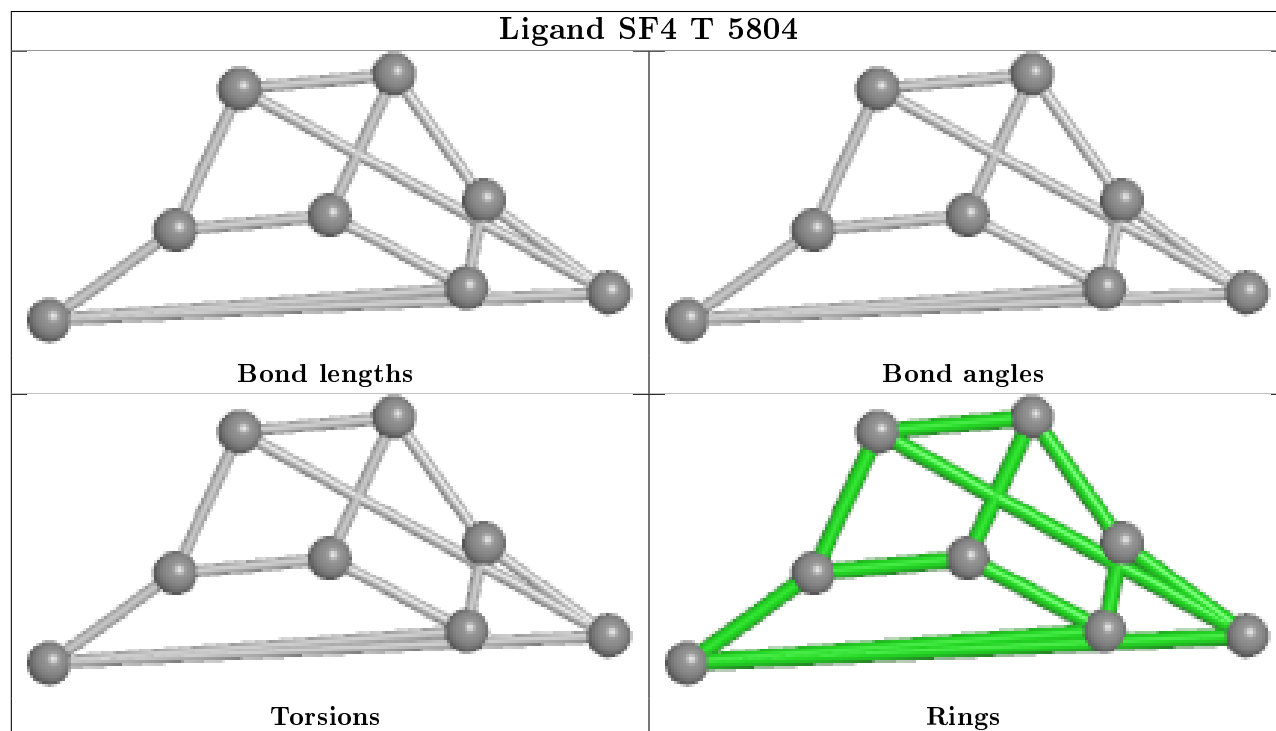
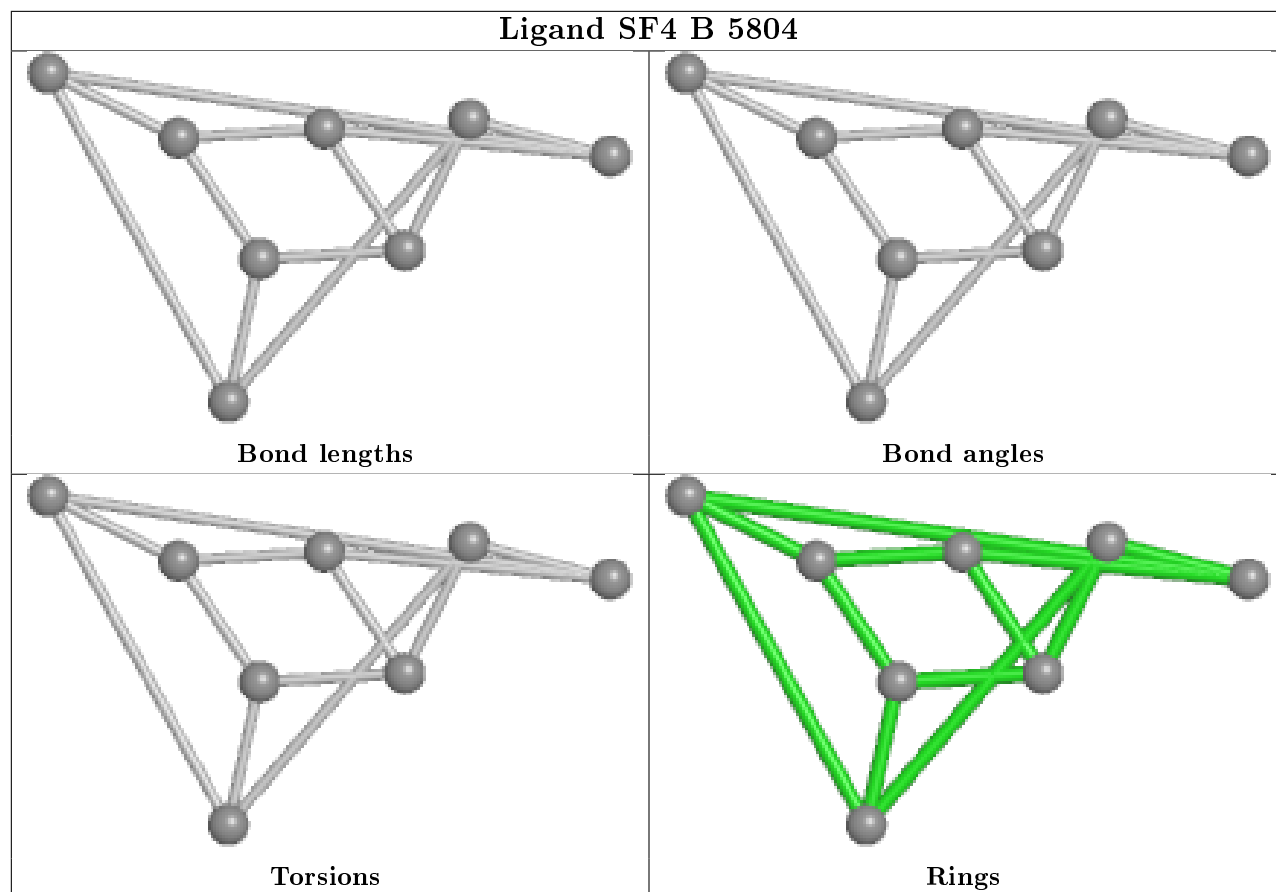
Ligand MD1 H 5801

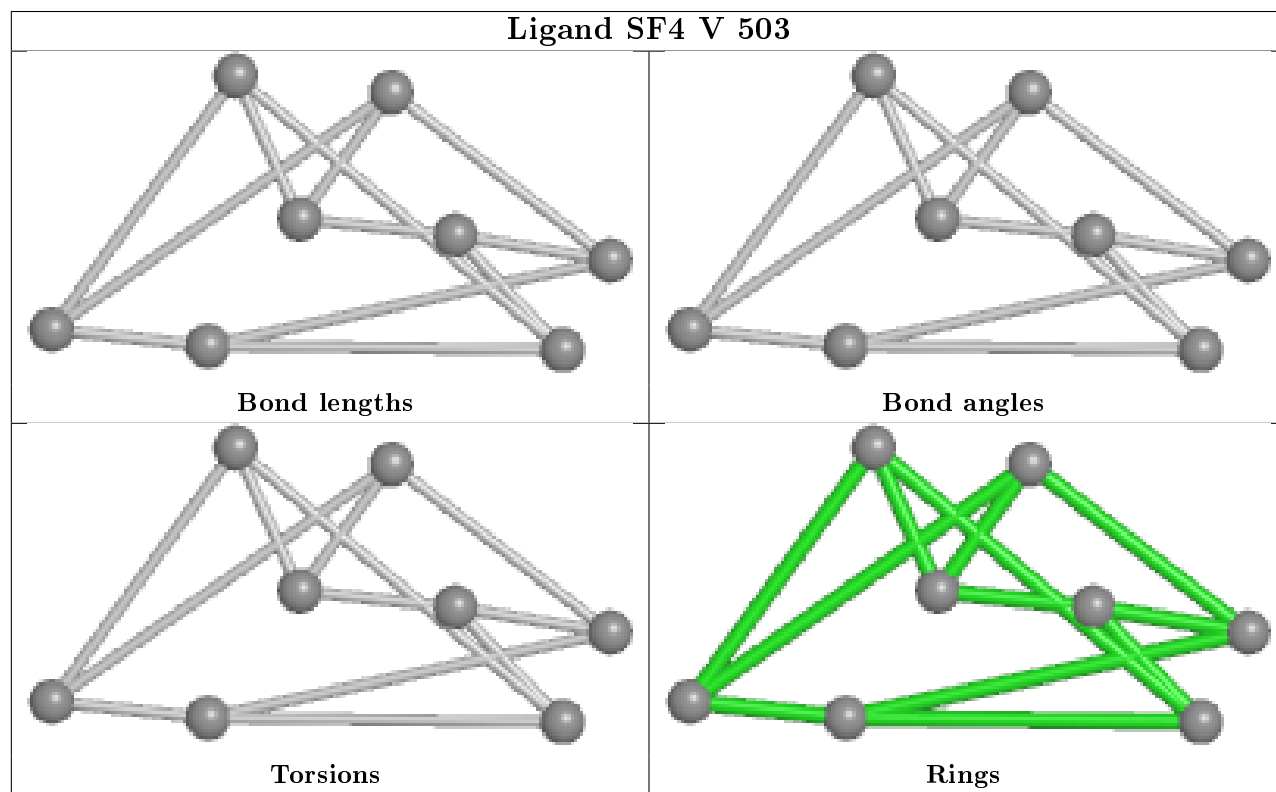
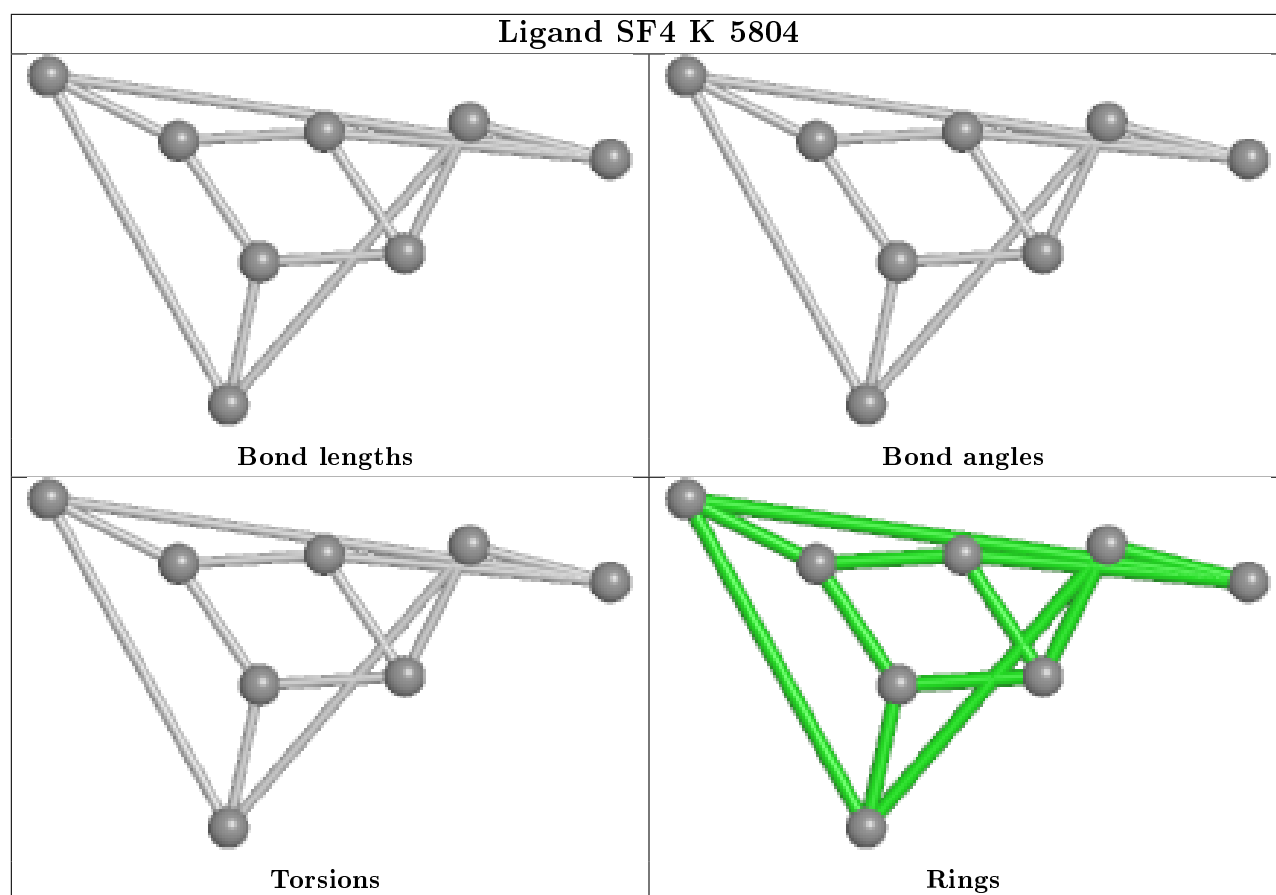


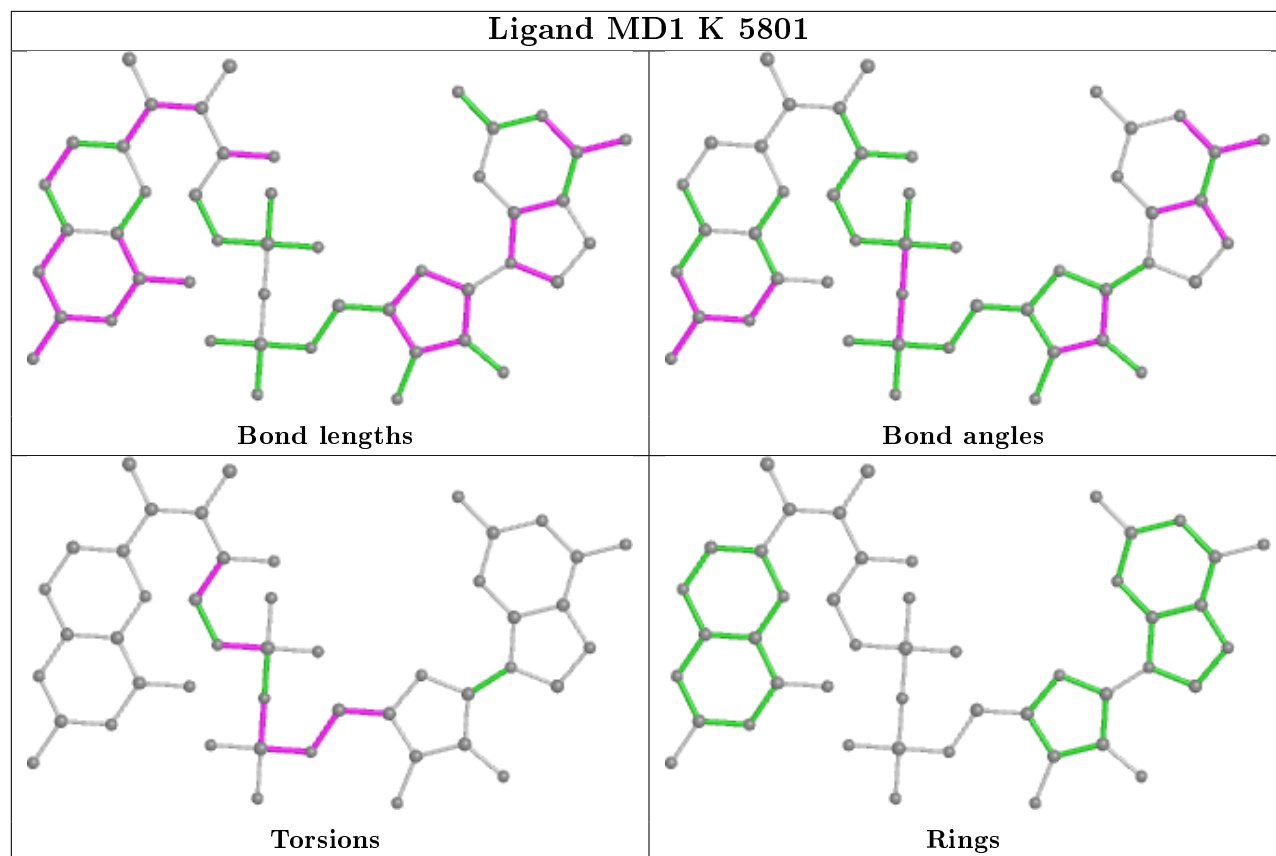
Ligand MD1 B 5802

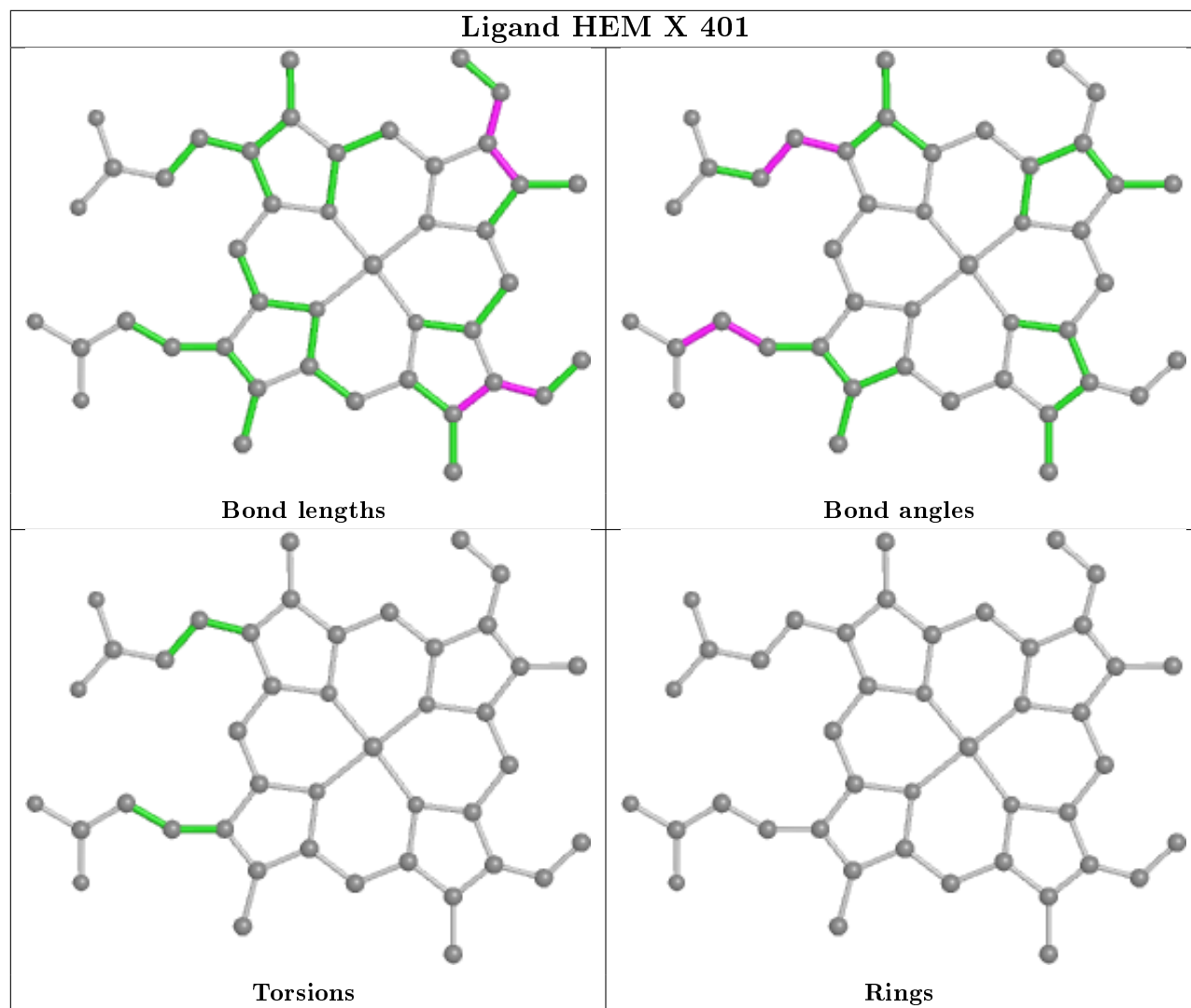


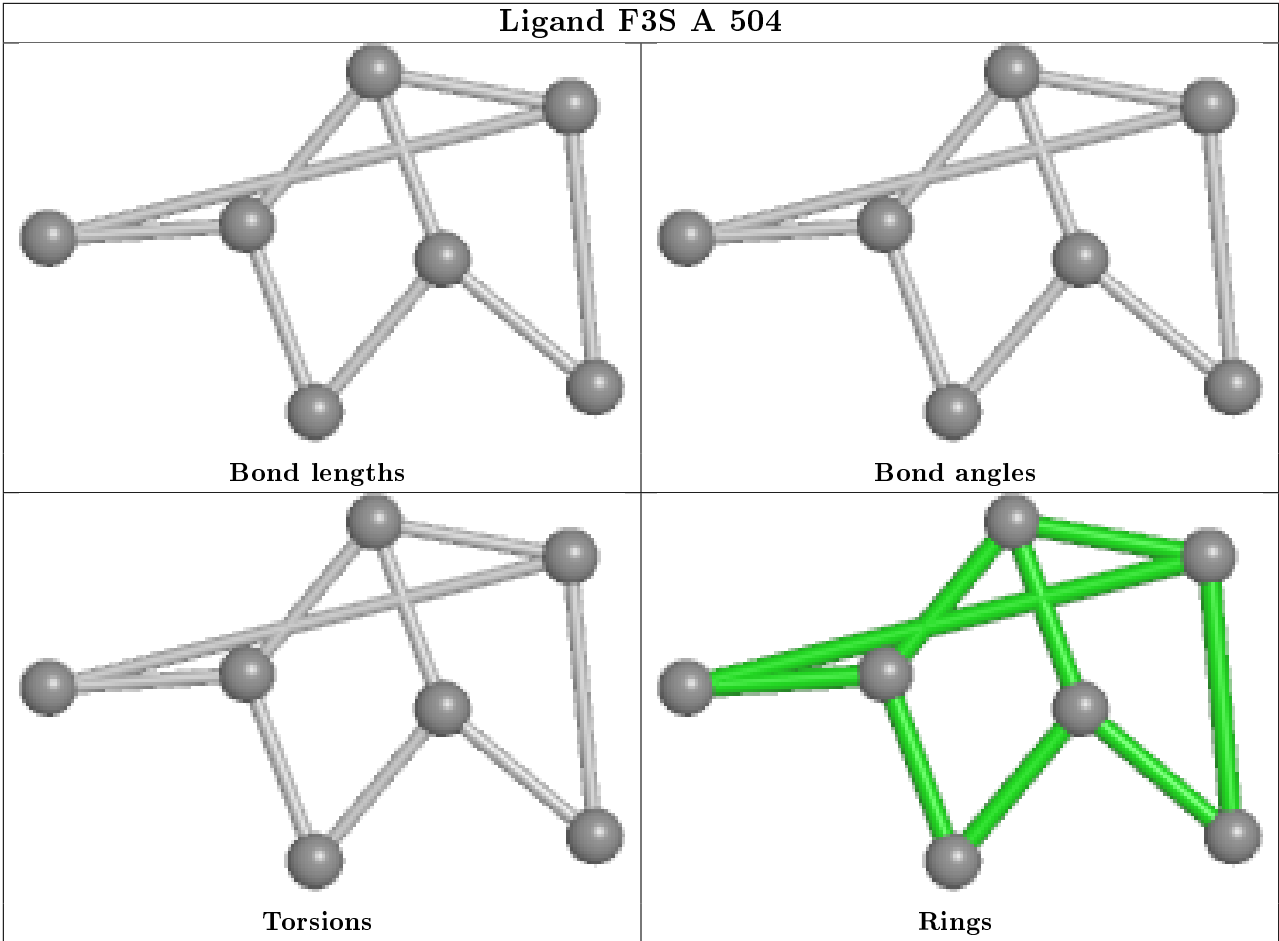












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	663:VAL	C	664:TYR	N	1.68

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	409/410 (99%)	0.15	3 (0%) 87 74	22, 37, 53, 68	2 (0%)
1	D	408/410 (99%)	1.29	106 (25%) 0 0	66, 97, 117, 133	0
1	G	409/410 (99%)	-0.09	1 (0%) 95 89	21, 32, 45, 93	0
1	J	409/410 (99%)	-0.01	0 100 100	18, 25, 37, 58	0
1	M	409/410 (99%)	0.25	1 (0%) 95 89	27, 48, 65, 79	0
1	P	409/410 (99%)	0.11	0 100 100	26, 46, 64, 77	3 (0%)
1	S	409/410 (99%)	-0.00	0 100 100	21, 33, 47, 61	1 (0%)
1	V	409/410 (99%)	0.28	9 (2%) 62 42	43, 61, 79, 86	1 (0%)
2	B	1120/1148 (97%)	0.10	3 (0%) 94 87	20, 41, 62, 92	1 (0%)
2	E	1111/1148 (96%)	1.57	384 (34%) 0 0	64, 117, 155, 175	0
2	H	1118/1148 (97%)	0.03	1 (0%) 95 91	16, 29, 45, 85	3 (0%)
2	K	1119/1148 (97%)	0.01	1 (0%) 95 91	17, 32, 47, 76	1 (0%)
2	N	1117/1148 (97%)	0.09	2 (0%) 95 89	18, 34, 54, 85	1 (0%)
2	Q	1116/1148 (97%)	0.42	17 (1%) 73 54	24, 47, 70, 92	6 (0%)
2	T	1119/1148 (97%)	0.00	3 (0%) 94 87	21, 37, 57, 88	3 (0%)
2	W	1118/1148 (97%)	0.12	6 (0%) 91 80	29, 49, 66, 95	4 (0%)
3	C	292/322 (90%)	0.21	4 (1%) 75 57	21, 31, 49, 72	0
3	F	292/322 (90%)	0.93	38 (13%) 3 1	57, 83, 104, 121	0
3	I	292/322 (90%)	0.19	1 (0%) 94 87	25, 51, 69, 83	0
3	L	292/322 (90%)	0.06	1 (0%) 94 87	19, 31, 47, 70	0
3	O	291/322 (90%)	1.00	45 (15%) 2 1	35, 69, 89, 102	0
3	R	291/322 (90%)	-0.02	0 100 100	23, 35, 51, 72	1 (0%)
3	U	292/322 (90%)	0.03	3 (1%) 82 66	23, 34, 51, 70	1 (0%)
3	X	292/322 (90%)	0.01	1 (0%) 94 87	30, 62, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	14543/15040 (96%)	0.28	630 (4%) 35 20	16, 41, 109, 175	28 (0%)

All (630) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	799	ALA	9.0
2	E	626	VAL	8.7
2	E	112	PRO	7.8
2	E	564	GLY	7.0
2	E	417	ILE	6.8
2	E	715	PRO	6.7
2	E	598	ALA	6.6
2	E	251	ALA	6.6
2	E	66	CYS	6.5
2	E	550	GLY	6.5
1	D	345	PHE	6.2
1	D	307	PRO	6.2
2	E	91	GLN	6.1
2	E	444	ILE	6.0
2	E	806	TYR	6.0
2	E	485	TYR	6.0
3	O	265	VAL	6.0
3	O	266	VAL	5.9
2	E	404	TYR	5.9
2	E	443	ALA	5.9
2	E	384	PRO	5.9
1	D	182	GLY	5.7
2	E	457	GLY	5.7
1	D	49	TRP	5.7
2	E	465	SER	5.7
2	E	283	SER	5.6
2	E	710	ASN	5.6
2	E	408	ASP	5.6
2	E	780	MET	5.5
2	E	694	ALA	5.5
2	E	563	ALA	5.4
2	E	783	TYR	5.4
2	E	74	ALA	5.4
2	E	344	ALA	5.3
2	E	774	LEU	5.3
2	E	429	GLY	5.3
2	E	625	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
3	O	141	GLY	5.2
2	E	597	TYR	5.2
1	D	253	PRO	5.2
2	E	266	ASN	5.1
2	E	359	PHE	5.1
2	E	358	LEU	5.1
1	D	290	ALA	5.1
2	E	571	PHE	5.0
2	E	637	THR	5.0
2	E	596	PRO	5.0
1	D	394	THR	5.0
1	D	311	ALA	5.0
2	E	798	VAL	4.9
1	D	352	VAL	4.9
2	E	623	PRO	4.9
2	E	782	GLY	4.9
2	E	102	TYR	4.9
2	E	452	THR	4.8
2	E	298	PHE	4.8
2	E	801	LEU	4.8
2	E	434	TRP	4.8
3	F	115	TRP	4.8
1	D	244	GLY	4.8
2	E	1080	GLY	4.7
2	E	879	ALA	4.7
2	E	98	TYR	4.7
2	E	588	ASP	4.6
2	E	713	SER	4.6
2	E	75	CYS	4.5
2	E	784	THR	4.5
2	B	28	PHE	4.5
1	D	299	THR	4.5
2	E	99	SER	4.5
2	E	802	LEU	4.5
2	E	720	TRP	4.4
2	E	120	THR	4.4
2	E	309	LEU	4.4
2	E	192	TYR	4.4
2	E	310	ILE	4.4
2	E	721	GLY	4.4
2	E	327	GLY	4.3
2	E	701	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
3	O	267	PHE	4.3
2	E	632	GLY	4.2
2	E	764	GLY	4.2
2	E	812	TRP	4.2
2	E	1063	TRP	4.2
2	E	572	GLN	4.2
3	O	111	PHE	4.2
2	E	794	GLY	4.1
2	E	830	ALA	4.1
2	E	252	HIS	4.1
2	E	454	VAL	4.1
1	D	101	GLN	4.0
2	E	63	PHE	4.0
2	E	185	ILE	4.0
2	E	339	PRO	4.0
2	E	576	TRP	4.0
1	D	322	PRO	4.0
2	E	717	ILE	4.0
2	E	261	ALA	4.0
2	E	317	ALA	4.0
2	E	809	HIS	3.9
2	E	374	ALA	3.9
2	E	756	ASP	3.9
2	E	599	SER	3.9
2	E	205	GLY	3.9
2	E	807	PRO	3.9
2	E	385	LEU	3.9
2	E	104	ASN	3.9
2	E	863	SER	3.9
2	E	1142	GLU	3.9
1	D	202	LEU	3.8
2	E	322	GLU	3.8
2	E	551	ASN	3.8
2	E	403	ASN	3.8
2	E	972	GLY	3.8
3	O	268	CYS	3.7
1	D	382	GLY	3.7
2	E	1141	GLY	3.7
1	D	63	VAL	3.7
3	F	213	ALA	3.7
2	E	618	ASN	3.7
3	O	134	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	348	THR	3.7
2	E	413	PRO	3.7
3	O	104	HIS	3.7
1	D	219	PRO	3.7
2	E	258	PRO	3.7
3	F	274	GLY	3.7
3	F	111	PHE	3.7
1	D	403	PRO	3.7
2	E	565	ASN	3.6
2	E	169	LEU	3.6
2	E	87	MET	3.6
2	E	284	HIS	3.6
2	E	593	ASN	3.6
2	E	1086	GLY	3.6
2	E	543	TYR	3.6
1	D	351	ILE	3.6
1	D	308	PRO	3.6
2	E	619	HIS	3.6
2	E	464	GLY	3.6
2	E	1077	ALA	3.6
2	E	80	PHE	3.5
1	D	69	GLY	3.5
2	E	85	VAL	3.5
2	E	627	ASN	3.5
3	F	255	CYS	3.5
2	E	882	TRP	3.5
2	E	690	TYR	3.5
2	E	770	ILE	3.5
3	O	109	ILE	3.5
2	E	810	PRO	3.4
2	E	1098	PRO	3.4
2	Q	429	GLY	3.4
2	E	569	GLY	3.4
2	E	574	SER	3.4
3	F	113	VAL	3.4
1	G	97	LYS	3.4
3	F	314	LEU	3.4
2	E	321	THR	3.4
2	E	33	PRO	3.3
2	E	765	ARG	3.3
3	O	165	TRP	3.3
2	E	968	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	243	GLU	3.3
2	E	235	GLY	3.3
2	E	826	GLY	3.3
1	D	86	PRO	3.3
2	E	180	TYR	3.3
2	E	119	TYR	3.3
2	E	831	TYR	3.3
2	E	938	ASN	3.3
1	D	256	THR	3.3
2	W	796	PRO	3.3
2	E	73	HIS	3.2
2	E	636	PHE	3.2
1	D	261	ALA	3.2
1	D	344	LEU	3.2
2	E	94	ASP	3.2
1	D	35	CYS	3.2
2	E	394	ARG	3.2
2	E	600	ALA	3.2
3	O	281	PHE	3.2
3	F	315	SER	3.2
2	E	1071	ASP	3.2
3	O	167	TRP	3.2
2	Q	457	GLY	3.2
2	E	931	TRP	3.2
2	E	866	PRO	3.2
3	F	215	LEU	3.2
1	D	320	PHE	3.2
3	F	281	PHE	3.2
2	E	334	THR	3.1
2	E	267	TRP	3.1
2	E	77	ILE	3.1
2	E	95	HIS	3.1
2	E	101	LEU	3.1
2	E	236	LYS	3.1
2	E	709	THR	3.1
2	E	402	PRO	3.1
1	D	39	GLN	3.1
2	E	696	PRO	3.1
2	E	549	THR	3.1
3	F	60	ALA	3.1
2	E	958	HIS	3.1
2	E	167	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	325	ASP	3.0
2	E	53	TYR	3.0
2	E	851	PRO	3.0
2	E	609	ALA	3.0
2	E	777	SER	3.0
2	E	562	TRP	3.0
2	E	617	TRP	3.0
2	E	716	PHE	3.0
2	E	70	ASN	3.0
3	O	289	PHE	3.0
2	E	204	GLN	3.0
1	D	393	THR	3.0
2	E	68	SER	3.0
2	E	264	GLY	3.0
2	E	462	LEU	3.0
2	E	181	ALA	3.0
2	E	658	ASN	3.0
2	E	299	SER	3.0
1	D	205	GLN	3.0
3	F	186	ALA	2.9
2	E	714	ASN	2.9
2	E	313	LYS	2.9
2	E	453	LEU	2.9
2	E	804	ARG	2.9
3	O	147	PRO	2.9
2	Q	476	ILE	2.9
1	D	237	ALA	2.9
2	E	955	HIS	2.9
3	F	320	ALA	2.9
2	E	315	PRO	2.9
3	O	236	LEU	2.9
2	E	861	ILE	2.9
2	E	862	VAL	2.9
1	D	267	ARG	2.9
2	E	893	SER	2.9
3	F	66	ALA	2.9
1	D	177	HIS	2.9
2	E	1068	HIS	2.9
1	D	68	TYR	2.9
3	F	110	TYR	2.9
2	E	584	TRP	2.9
2	E	700	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	825	THR	2.9
3	O	118	ALA	2.9
2	E	530	ASN	2.9
3	F	277	LEU	2.9
1	D	90	TRP	2.9
3	O	296	GLY	2.9
1	D	402	ARG	2.9
2	E	92	ASN	2.9
2	E	524	HIS	2.8
2	E	126	TYR	2.8
2	E	811	PHE	2.8
3	O	65	GLY	2.8
2	E	691	ALA	2.8
3	F	195	PHE	2.8
2	E	589	VAL	2.8
2	E	170	LEU	2.8
2	E	247	ALA	2.8
2	E	188	ILE	2.8
3	O	303	GLY	2.8
2	E	233	VAL	2.8
2	Q	440	GLY	2.8
3	F	267	PHE	2.8
2	E	230	LEU	2.8
2	E	566	TYR	2.8
2	E	742	ALA	2.8
1	D	266	ILE	2.8
2	E	685	THR	2.8
2	E	463	GLU	2.8
2	E	631	TYR	2.8
2	E	535	ALA	2.8
2	E	1023	TRP	2.8
2	E	583	GLY	2.8
2	E	1062	ASP	2.8
1	D	73	GLN	2.8
1	D	347	MET	2.8
2	E	624	LEU	2.8
1	V	202	LEU	2.7
2	E	511	LEU	2.7
2	E	766	ALA	2.7
2	E	293	MET	2.7
2	W	794	GLY	2.7
1	D	233	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	362	ILE	2.7
2	E	1087	PHE	2.7
2	E	652	THR	2.7
2	E	800	MET	2.7
2	E	964	ALA	2.7
3	F	134	ALA	2.7
2	E	1067	MET	2.7
1	D	143	ASN	2.7
2	E	111	ASN	2.7
2	E	268	SER	2.7
1	D	57	PHE	2.7
1	D	59	TRP	2.7
2	E	560	HIS	2.7
2	E	781	LYS	2.7
2	E	314	MET	2.7
2	E	430	ASP	2.7
2	E	529	VAL	2.7
3	F	276	PRO	2.7
1	D	264	GLY	2.7
3	F	212	ALA	2.7
3	O	286	SER	2.7
2	E	116	LEU	2.7
2	E	312	ASN	2.7
1	D	109	GLY	2.7
2	E	573	ALA	2.7
2	E	178	PHE	2.6
2	E	105	LYS	2.6
2	E	678	MET	2.6
2	E	779	THR	2.6
2	E	921	THR	2.6
2	E	1008	ASN	2.6
2	E	106	ALA	2.6
1	D	168	PHE	2.6
1	D	373	PHE	2.6
1	D	321	GLY	2.6
2	E	103	GLY	2.6
2	E	553	GLY	2.6
2	E	740	GLY	2.6
2	E	45	PRO	2.6
2	E	245	CYS	2.6
3	L	61	HIS	2.6
1	D	15	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	62	ASN	2.6
3	F	258	PHE	2.6
2	N	31	LEU	2.6
2	E	36	VAL	2.6
2	E	129	TYR	2.6
2	E	795	GLU	2.6
2	E	813	GLU	2.6
2	E	561	THR	2.6
2	T	305	THR	2.6
1	D	259	MET	2.6
2	E	575	LYS	2.6
3	X	296	GLY	2.6
2	E	234	ILE	2.6
2	E	324	MET	2.6
1	D	260	SER	2.6
2	E	426	GLU	2.6
3	C	120	ASP	2.6
1	D	149	ALA	2.6
2	E	878	ASN	2.6
2	E	189	THR	2.6
2	E	680	THR	2.6
1	D	375	MET	2.6
2	E	531	HIS	2.6
1	D	28	ALA	2.6
2	E	570	ASN	2.6
2	E	118	GLY	2.5
2	E	580	GLY	2.5
2	E	308	ASN	2.5
1	D	27	ALA	2.5
2	E	57	TYR	2.5
2	E	244	ASN	2.5
1	D	184	LEU	2.5
2	E	815	VAL	2.5
2	E	399	ASP	2.5
1	D	262	CYS	2.5
2	E	1022	ALA	2.5
3	O	112	GLN	2.5
3	O	139	PRO	2.5
1	D	32	ILE	2.5
2	E	409	ILE	2.5
2	W	934	ILE	2.5
3	O	271	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	894	TRP	2.5
3	F	265	VAL	2.5
1	D	158	TYR	2.5
3	O	102	ALA	2.5
1	D	214	CYS	2.5
2	E	69	PRO	2.5
2	E	109	ASN	2.5
3	C	302	ASN	2.5
1	D	391	VAL	2.5
2	E	679	SER	2.5
2	E	835	PRO	2.5
2	E	984	ARG	2.5
2	E	1069	GLN	2.5
1	D	16	PRO	2.5
2	E	711	SER	2.5
2	E	220	ARG	2.5
2	E	884	ASP	2.5
3	F	61	HIS	2.5
1	D	172	GLN	2.5
2	Q	450	GLY	2.5
2	E	856	TYR	2.5
2	E	622	ARG	2.5
3	O	282	VAL	2.5
3	O	151	PHE	2.5
1	D	186	ALA	2.5
3	F	165	TRP	2.5
2	E	734	ASP	2.4
2	E	1081	MET	2.4
3	F	254	GLY	2.4
2	E	49	TRP	2.4
1	D	239	TYR	2.4
1	D	401	ILE	2.4
2	E	115	CYS	2.4
2	E	542	TYR	2.4
2	W	65	TYR	2.4
3	O	136	LEU	2.4
3	O	138	PHE	2.4
2	E	956	GLN	2.4
3	O	234	GLU	2.4
1	D	170	TYR	2.4
2	E	601	LYS	2.4
1	D	71	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	653	ASN	2.4
3	U	302	ASN	2.4
2	E	76	ARG	2.4
2	E	177	ALA	2.4
2	E	525	TYR	2.4
2	E	643	PRO	2.4
2	E	486	LYS	2.4
2	E	136	ILE	2.4
3	O	114	ILE	2.4
3	O	166	HIS	2.4
2	E	44	TYR	2.4
2	E	139	GLY	2.4
2	E	757	ASN	2.4
2	E	712	CYS	2.4
2	E	1051	PHE	2.4
2	E	1096	THR	2.4
3	O	130	PHE	2.4
2	E	412	GLY	2.4
2	E	650	TRP	2.4
3	F	263	TRP	2.4
1	D	37	ALA	2.4
3	C	61	HIS	2.4
3	F	97	SER	2.4
2	E	46	ASP	2.4
2	E	295	ASP	2.4
2	E	897	THR	2.4
2	Q	434	TRP	2.4
3	O	302	ASN	2.4
1	D	234	LYS	2.4
2	E	286	LEU	2.4
2	E	337	TYR	2.3
1	D	43	MET	2.3
2	E	114	MET	2.3
2	B	1022	ALA	2.3
2	E	489	LEU	2.3
2	E	1024	ILE	2.3
2	E	693	PHE	2.3
2	E	953	GLY	2.3
2	E	768	VAL	2.3
2	E	206	TYR	2.3
3	F	292	ALA	2.3
2	T	30	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	555	PHE	2.3
3	O	76	GLY	2.3
1	D	193	TYR	2.3
2	E	854	THR	2.3
2	B	1021	SER	2.3
2	E	1046	GLY	2.3
2	E	416	HIS	2.3
3	O	103	ILE	2.3
1	D	113	GLY	2.3
2	Q	874	GLY	2.3
2	E	681	ASP	2.3
2	E	437	LYS	2.3
2	E	456	LYS	2.3
2	Q	542	TYR	2.3
2	E	113	ARG	2.3
2	E	920	HIS	2.3
2	E	212	ASP	2.3
2	E	259	ASP	2.3
1	D	251	GLY	2.3
2	E	628	THR	2.3
2	E	655	ASN	2.3
2	E	585	VAL	2.3
2	E	922	VAL	2.3
2	E	970	GLU	2.3
1	D	378	ASP	2.3
2	E	100	ASP	2.3
2	E	318	HIS	2.3
2	Q	629	PRO	2.3
2	E	229	GLY	2.3
1	D	85	SER	2.3
2	E	89	VAL	2.3
2	E	363	THR	2.3
2	E	932	ASN	2.2
2	E	88	ARG	2.2
1	D	276	PRO	2.2
1	D	342	MET	2.2
2	E	943	TYR	2.2
1	D	263	VAL	2.2
2	E	654	VAL	2.2
3	I	268	CYS	2.2
2	Q	1080	GLY	2.2
3	O	89	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	140	TRP	2.2
2	E	418	GLN	2.2
3	F	112	GLN	2.2
2	E	265	ARG	2.2
1	D	374	THR	2.2
2	E	338	SER	2.2
1	D	379	THR	2.2
2	E	274	GLY	2.2
2	T	1021	SER	2.2
2	W	264	GLY	2.2
1	D	381	ILE	2.2
2	Q	441	PRO	2.2
2	E	285	GLY	2.2
3	U	203	ASN	2.2
1	D	232	SER	2.2
3	F	246	SER	2.2
1	D	303	ILE	2.2
2	E	281	PRO	2.2
2	E	870	PRO	2.2
1	V	353	TYR	2.2
3	O	110	TYR	2.2
2	E	61	ARG	2.2
2	E	294	ASN	2.2
2	E	749	LEU	2.2
3	O	49	LEU	2.2
2	E	305	THR	2.2
2	Q	344	ALA	2.2
2	E	942	PRO	2.2
3	O	79	VAL	2.2
2	Q	584	TRP	2.2
1	D	380	VAL	2.2
2	E	432	VAL	2.2
1	D	199	GLY	2.2
2	E	386	LEU	2.2
1	D	31	ASN	2.2
1	D	296	GLN	2.2
2	E	559	SER	2.2
2	E	949	MET	2.2
3	U	147	PRO	2.2
1	D	70	GLY	2.1
2	E	1013	TYR	2.2
1	A	297	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	6	ASN	2.1
1	V	192	ILE	2.1
3	F	128	GLN	2.1
3	O	135	ALA	2.1
1	D	100	SER	2.1
2	E	397	PRO	2.1
2	E	466	PHE	2.1
2	E	586	ALA	2.1
2	E	890	ILE	2.1
1	V	24	HIS	2.1
2	E	107	THR	2.1
2	E	1106	THR	2.1
3	O	63	THR	2.1
1	D	353	TYR	2.1
2	K	403	ASN	2.1
2	E	985	PRO	2.1
2	E	662	HIS	2.1
2	E	131	LEU	2.1
2	E	939	PHE	2.1
2	Q	372	TYR	2.1
2	E	448	ASP	2.1
2	E	1061	ARG	2.1
2	E	400	ILE	2.1
2	E	785	CYS	2.1
1	D	370	GLY	2.1
3	F	101	LYS	2.1
1	D	281	THR	2.1
2	E	536	THR	2.1
2	E	544	LEU	2.1
2	E	548	LEU	2.1
2	E	769	TYR	2.1
3	F	244	LEU	2.1
2	Q	708	ILE	2.1
2	W	684	ILE	2.1
1	D	67	PRO	2.1
1	D	188	PRO	2.1
1	V	384	GLY	2.1
2	E	646	THR	2.1
2	E	695	PHE	2.1
2	E	797	GLY	2.1
3	O	156	GLY	2.1
2	E	612	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	338	LEU	2.1
2	E	383	PHE	2.1
3	O	204	TYR	2.1
1	D	227	GLY	2.1
2	E	182	SER	2.1
2	E	610	LEU	2.1
1	A	2	THR	2.1
1	D	148	THR	2.1
1	M	108	TYR	2.1
2	E	841	GLY	2.1
3	C	59	PRO	2.1
2	Q	806	TYR	2.0
3	O	60	ALA	2.0
2	E	67	CYS	2.0
2	E	370	LYS	2.0
2	E	1095	ASN	2.0
3	F	90	ASN	2.0
1	D	343	SER	2.0
2	E	644	SER	2.0
2	E	79	ALA	2.0
1	D	190	LYS	2.0
2	E	883	GLU	2.0
2	H	219	THR	2.0
3	F	63	THR	2.0
1	V	168	PHE	2.0
2	E	718	GLN	2.0
2	Q	260	GLN	2.0
2	N	1021	SER	2.0
3	O	116	ASP	2.0
2	E	451	GLU	2.0
2	E	867	TYR	2.0
2	E	498	VAL	2.0
1	V	62	ASN	2.0
2	E	83	ASN	2.0
2	E	772	ARG	2.0
2	E	615	ALA	2.0
2	E	376	TYR	2.0
2	E	926	TRP	2.0
3	F	167	TRP	2.0
1	D	395	VAL	2.0
3	F	264	THR	2.0
1	D	297	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	V	271	PHE	2.0
2	E	214	MET	2.0
2	E	442	LYS	2.0
2	E	1048	GLN	2.0
1	A	88	ASN	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(Å ²)	Q<0.9
9	CA	F	403	1/1	0.33	0.13	104,104,104,104	0
6	MD1	E	5801	47/47	0.73	0.29	75,111,136,150	0
9	CA	X	403	1/1	0.73	0.10	71,71,71,71	0
6	MD1	E	5802	47/47	0.82	0.27	80,117,133,137	0
9	CA	F	402	1/1	0.82	0.07	76,76,76,76	0
9	CA	I	403	1/1	0.85	0.10	69,69,69,69	0
8	HEM	F	401	43/43	0.85	0.30	77,97,112,116	0
9	CA	U	403	1/1	0.88	0.12	29,29,29,29	0
4	SF4	D	501	8/8	0.89	0.17	91,115,146,160	0
5	F3S	V	504	7/7	0.89	0.13	65,87,97,112	0
9	CA	O	402	1/1	0.90	0.09	61,61,61,61	0
8	HEM	X	401	43/43	0.91	0.23	59,75,81,89	0
7	MO	E	5803	1/1	0.92	0.06	139,139,139,139	0
9	CA	L	402	1/1	0.92	0.09	27,27,27,27	0
9	CA	C	403	1/1	0.92	0.13	35,35,35,35	0
9	CA	R	403	1/1	0.92	0.09	35,35,35,35	0
5	F3S	D	504	7/7	0.92	0.13	99,113,128,134	0
8	HEM	O	401	43/43	0.92	0.32	57,69,75,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MD1	Q	5802	47/47	0.93	0.23	30,43,56,59	0
4	SF4	D	503	8/8	0.93	0.16	107,133,158,166	0
7	MO	T	5803	1/1	0.93	0.14	37,37,37,37	0
4	SF4	E	5804	8/8	0.94	0.12	119,125,139,167	0
7	MO	Q	5803	1/1	0.94	0.11	46,46,46,46	0
9	CA	L	403	1/1	0.94	0.09	29,29,29,29	0
9	CA	C	402	1/1	0.94	0.09	33,33,33,33	0
4	SF4	D	502	8/8	0.94	0.08	112,118,142,149	0
9	CA	U	402	1/1	0.94	0.13	32,32,32,32	0
6	MD1	W	5802	47/47	0.94	0.20	28,47,62,72	0
8	HEM	I	401	43/43	0.94	0.19	38,55,65,66	0
4	SF4	W	5804	8/8	0.95	0.10	40,57,63,72	0
9	CA	O	403	1/1	0.95	0.07	73,73,73,73	0
9	CA	X	402	1/1	0.95	0.07	56,56,56,56	0
6	MD1	Q	5801	47/47	0.95	0.20	21,34,44,54	0
6	MD1	T	5802	47/47	0.96	0.19	22,31,41,45	0
6	MD1	W	5801	47/47	0.96	0.18	31,46,57,69	0
4	SF4	V	501	8/8	0.96	0.10	43,63,75,78	0
9	CA	I	402	1/1	0.96	0.09	46,46,46,46	0
4	SF4	N	5804	8/8	0.96	0.12	40,42,48,51	0
6	MD1	H	5802	47/47	0.96	0.21	15,30,36,47	0
6	MD1	K	5801	47/47	0.96	0.19	20,25,33,37	0
8	HEM	C	401	43/43	0.96	0.23	19,27,32,49	0
6	MD1	K	5802	47/47	0.96	0.22	15,29,38,45	0
6	MD1	N	5801	47/47	0.96	0.19	21,28,34,48	0
8	HEM	L	401	43/43	0.96	0.21	17,24,30,33	0
6	MD1	N	5802	47/47	0.96	0.19	26,34,44,46	0
6	MD1	B	5801	47/47	0.96	0.21	24,34,40,41	0
6	MD1	B	5802	47/47	0.96	0.18	28,42,50,56	0
6	MD1	T	5801	47/47	0.97	0.18	23,29,35,38	0
4	SF4	H	5804	8/8	0.97	0.11	15,35,41,43	0
9	CA	R	402	1/1	0.97	0.10	31,31,31,31	0
6	MD1	H	5801	47/47	0.97	0.19	16,24,36,38	0
8	HEM	R	401	43/43	0.97	0.21	23,33,40,46	0
8	HEM	U	401	43/43	0.97	0.19	23,30,34,43	0
4	SF4	M	502	8/8	0.97	0.08	58,64,82,84	0
7	MO	B	5803	1/1	0.97	0.13	45,45,45,45	0
4	SF4	J	502	8/8	0.98	0.08	24,36,52,52	0
4	SF4	V	502	8/8	0.98	0.08	62,72,89,95	0
4	SF4	V	503	8/8	0.98	0.09	50,65,72,83	0
4	SF4	K	5804	8/8	0.98	0.14	18,32,40,42	0
4	SF4	B	5804	8/8	0.98	0.12	22,38,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	F3S	M	504	7/7	0.98	0.10	46,67,69,70	0
4	SF4	J	501	8/8	0.98	0.09	16,26,33,33	0
7	MO	H	5803	1/1	0.98	0.14	38,38,38,38	0
7	MO	N	5803	1/1	0.98	0.14	30,30,30,30	0
4	SF4	P	502	8/8	0.98	0.10	37,47,60,63	0
4	SF4	Q	5804	8/8	0.98	0.10	26,43,57,67	0
7	MO	W	5803	1/1	0.98	0.13	61,61,61,61	0
4	SF4	S	503	8/8	0.99	0.07	28,33,41,47	0
4	SF4	T	5804	8/8	0.99	0.11	27,42,48,57	0
4	SF4	A	502	8/8	0.99	0.07	27,43,54,56	0
4	SF4	J	503	8/8	0.99	0.08	25,29,37,38	0
4	SF4	G	501	8/8	0.99	0.10	24,29,42,43	0
4	SF4	M	501	8/8	0.99	0.10	35,47,52,54	0
5	F3S	A	504	7/7	0.99	0.10	24,32,43,44	0
4	SF4	G	502	8/8	0.99	0.09	30,38,54,60	0
5	F3S	G	504	7/7	0.99	0.10	26,42,51,52	0
5	F3S	J	504	7/7	0.99	0.10	14,25,31,32	0
4	SF4	M	503	8/8	0.99	0.07	32,44,56,57	0
5	F3S	P	504	7/7	0.99	0.09	24,34,45,47	0
5	F3S	S	504	7/7	0.99	0.09	19,29,43,43	0
7	MO	K	5803	1/1	0.99	0.12	36,36,36,36	0
4	SF4	G	503	8/8	0.99	0.08	17,27,33,35	0
4	SF4	P	501	8/8	0.99	0.10	30,35,42,42	0
4	SF4	A	503	8/8	0.99	0.09	27,34,49,51	0
4	SF4	P	503	8/8	0.99	0.09	30,39,51,60	0
4	SF4	A	501	8/8	0.99	0.10	26,27,41,46	0
4	SF4	S	501	8/8	0.99	0.11	21,32,42,43	0
4	SF4	S	502	8/8	0.99	0.09	29,39,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.