Full wwPDB EM Validation Report ⓘ

Feb 24, 2024 – 08:24 PM EST

PDB ID	:	7KZO
EMDB ID	:	EMD-23084
Title	:	Outer dynein arm docking complex bound to doublet microtubules from C. reinhardtii
Authors	:	Walton, T.; Wu, H.; Brown, A.B.
Deposited on	:	2020-12-10
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

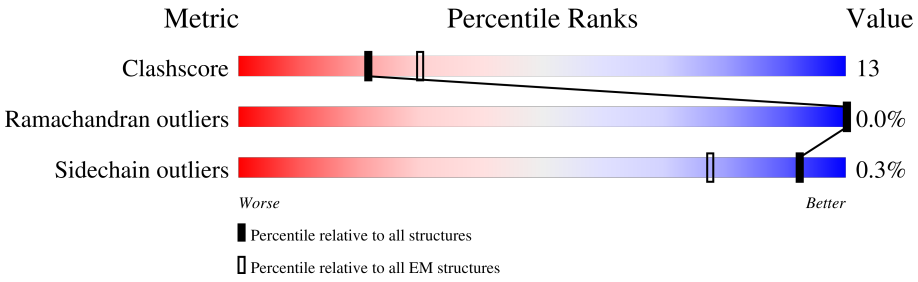
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



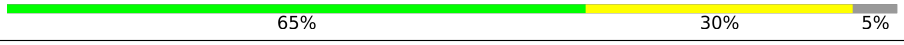
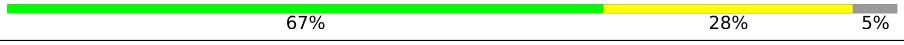
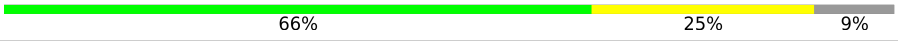
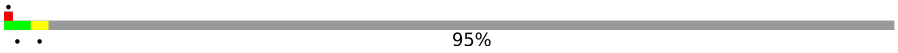
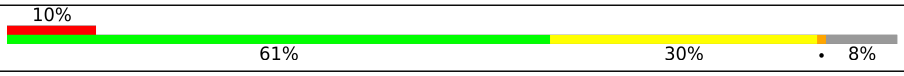
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	443	62% 34% ·
1	A3	443	64% 32% ·
1	A5	443	64% 32% ·
1	A7	443	68% 28% ·
1	B1	443	67% 28% 5%
1	B3	443	68% 25% 7%
1	B5	443	67% 29% ·
1	B7	443	8% 69% 27% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A2	451	
2	A4	451	
2	A6	451	
2	B2	451	
2	B4	451	
2	B6	451	
3	C	4485	
4	X	749	
4	X1	749	
5	Y	552	
5	Y1	552	
6	Z	184	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 54110 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A3	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B1	419	Total	C	N	O	S	0	0
			3298	2077	563	628	30		
1	B3	410	Total	C	N	O	S	0	0
			3227	2030	553	614	30		
1	B5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	430	Total	C	N	O	S	0	0
			3339	2114	568	636	21		
2	A4	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	A6	429	Total	C	N	O	S	0	0
			3335	2112	567	635	21		
2	B2	411	Total	C	N	O	S	0	0
			3204	2035	544	605	20		
2	B4	409	Total	C	N	O	S	0	0
			3193	2028	542	603	20		
2	B6	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 3 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	218	Total	C	N	O	S	0	0
			1771	1123	302	335	11		

- Molecule 4 is a protein called Outer dynein arm-docking complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	157	Total	C	N	O	S	0	0
			985	594	198	190	3		
4	X1	142	Total	C	N	O	S	0	0
			1178	715	223	235	5		

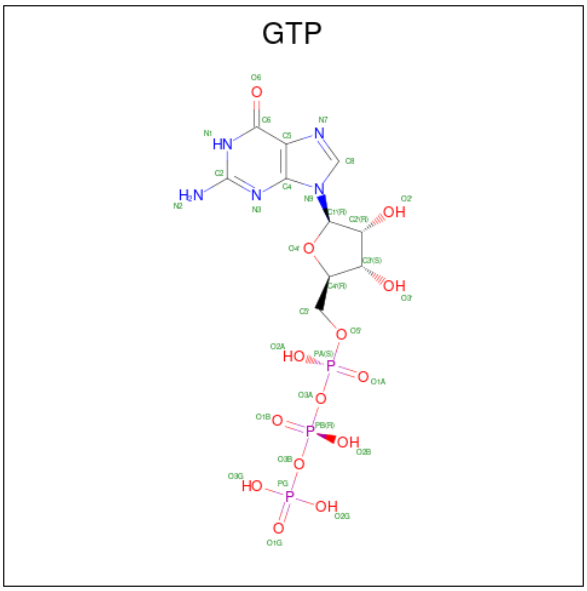
- Molecule 5 is a protein called Outer dynein arm protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	121	Total	C	N	O	S	0	0
			844	508	162	171	3		
5	Y1	147	Total	C	N	O	S	0	0
			1185	729	223	224	9		

- Molecule 6 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

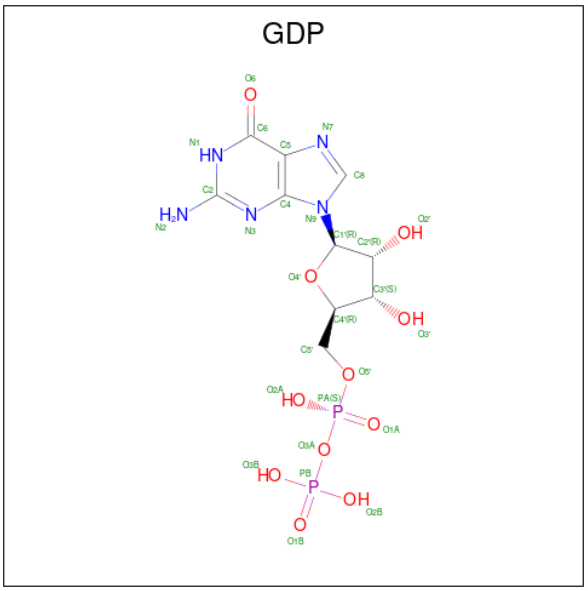


Mol	Chain	Residues	Atoms					AltConf
7	A1	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A3	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A5	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A7	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B5	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	A1	1	Total	Mg	0
			1	1	
8	A2	1	Total	Mg	0
			1	1	
8	A4	1	Total	Mg	0
			1	1	
8	A6	1	Total	Mg	0
			1	1	
8	B3	1	Total	Mg	0
			1	1	
8	B4	1	Total	Mg	0
			1	1	
8	B6	1	Total	Mg	0
			1	1	

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



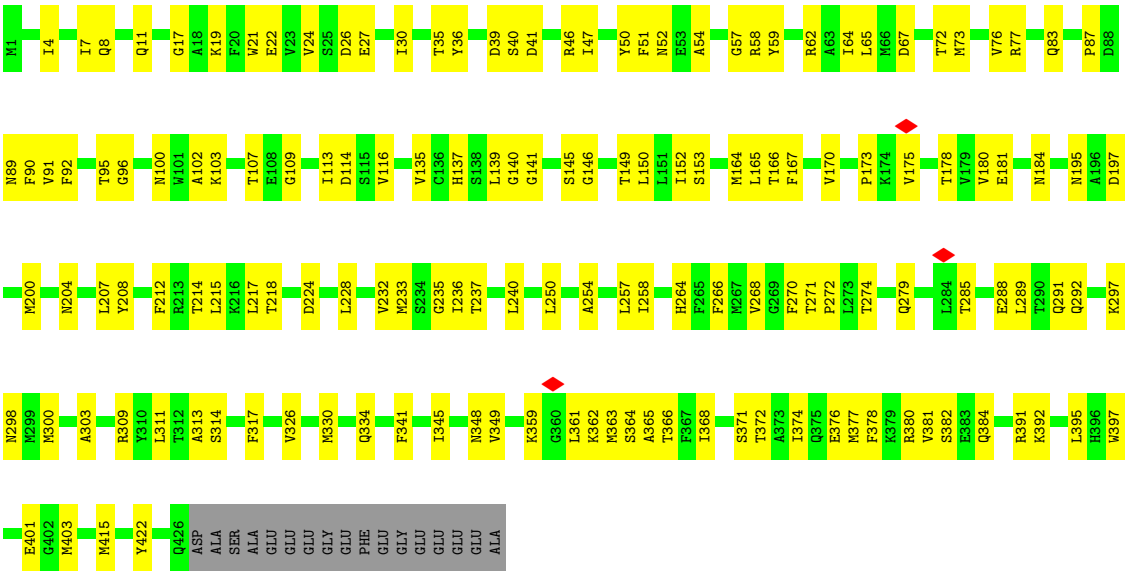
Mol	Chain	Residues	Atoms					AltConf
9	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

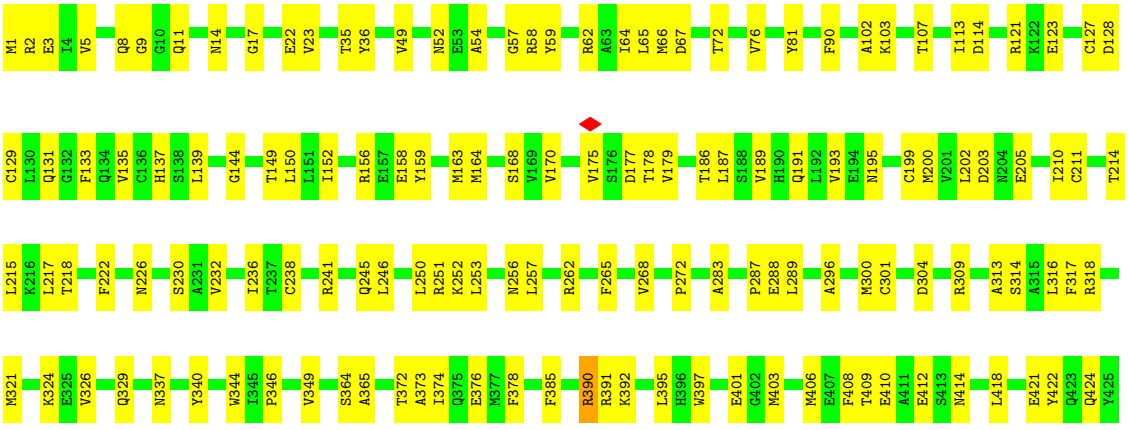
• Molecule 1: Tubulin beta

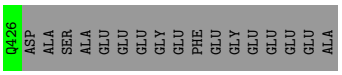
Chain A1:



• Molecule 1: Tubulin beta

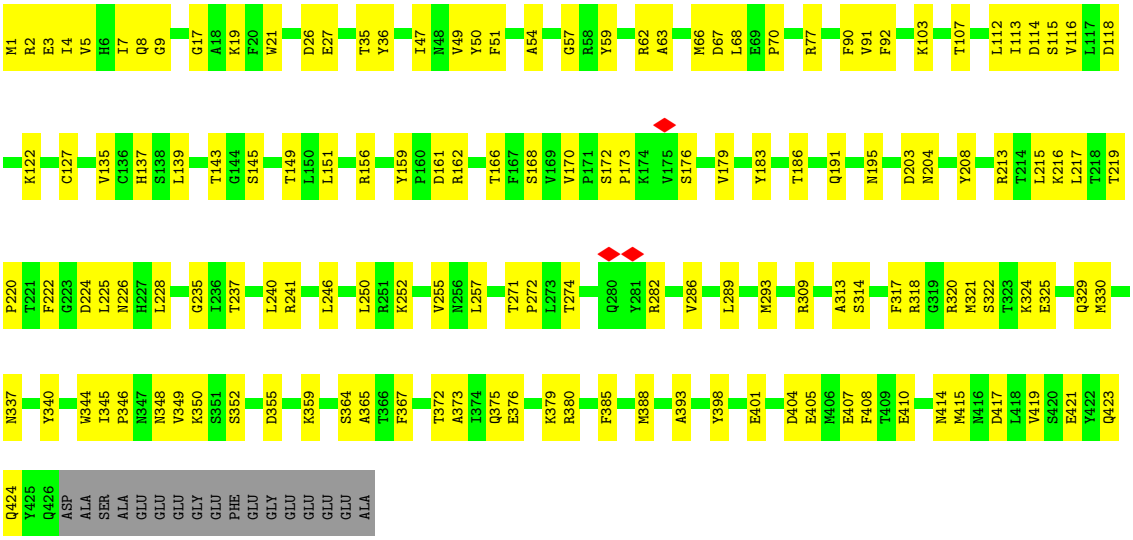
Chain A3:





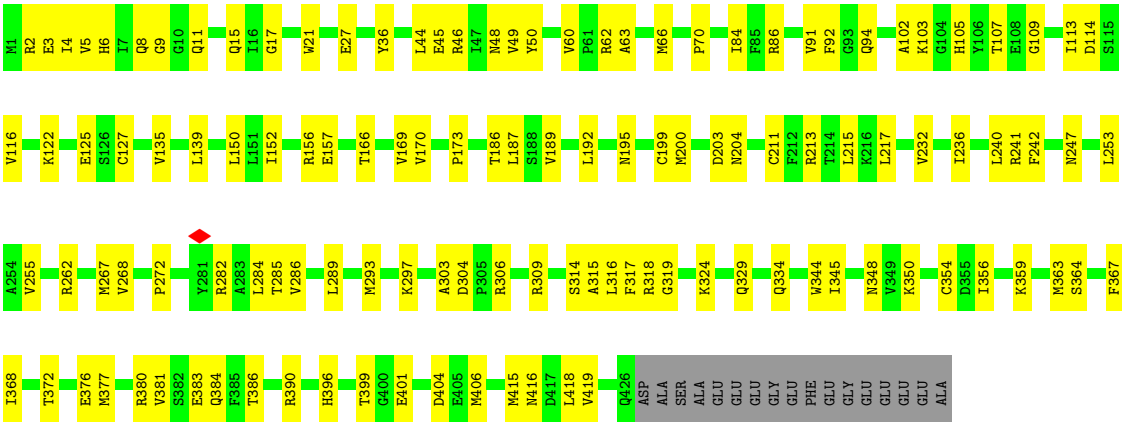
• Molecule 1: Tubulin beta

Chain A5:



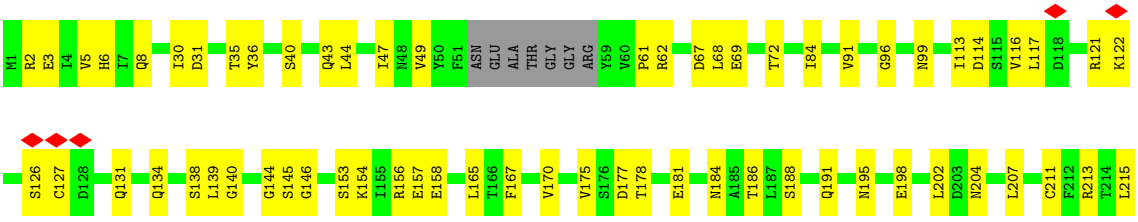
• Molecule 1: Tubulin beta

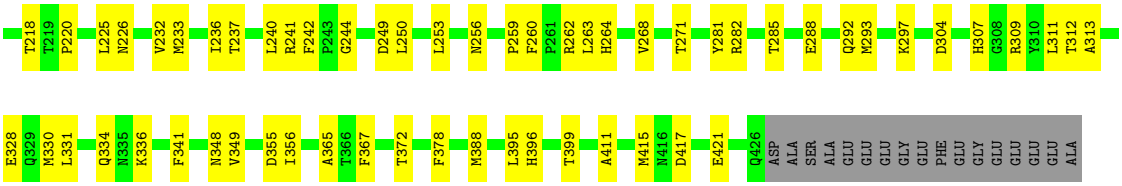
Chain A7:



• Molecule 1: Tubulin beta

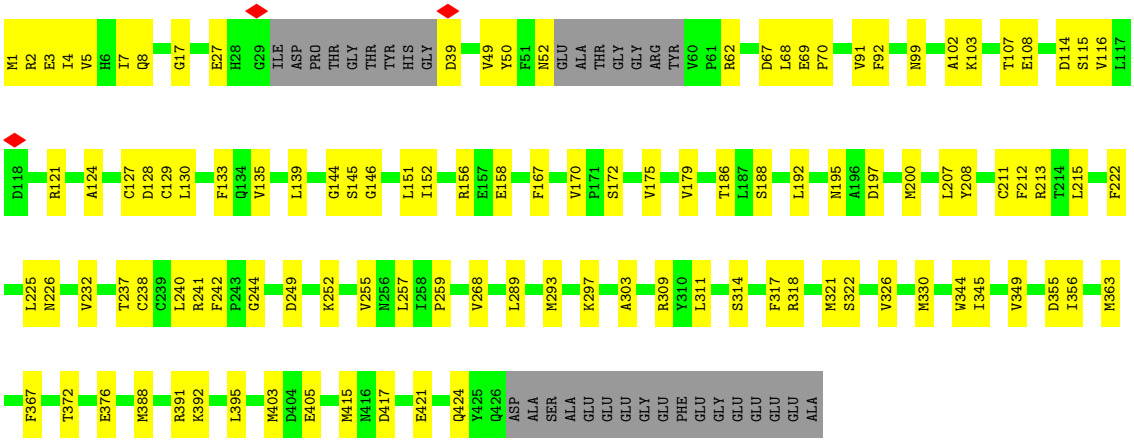
Chain B1:





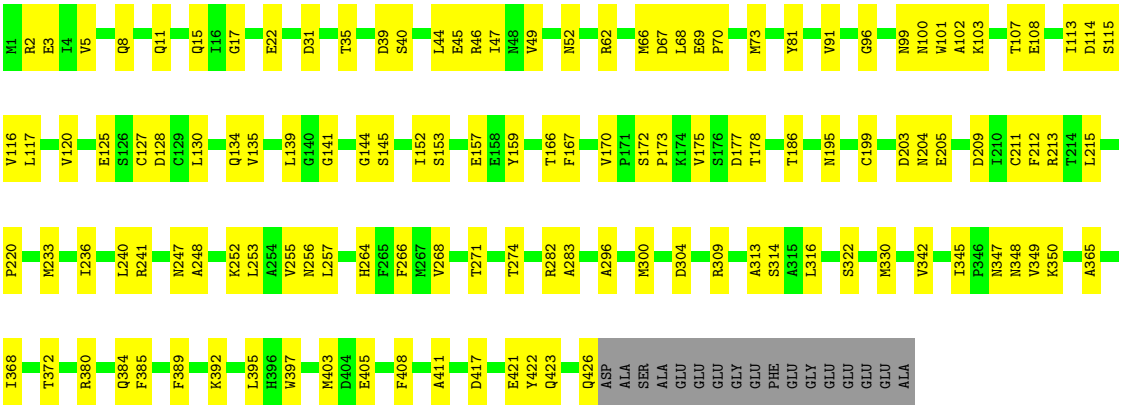
• Molecule 1: Tubulin beta

Chain B3:



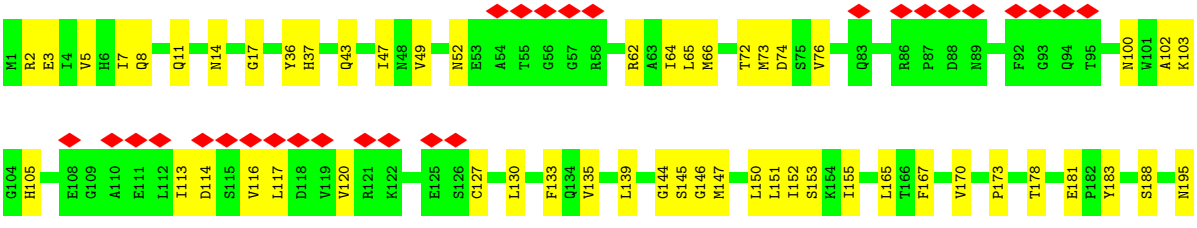
• Molecule 1: Tubulin beta

Chain B5:



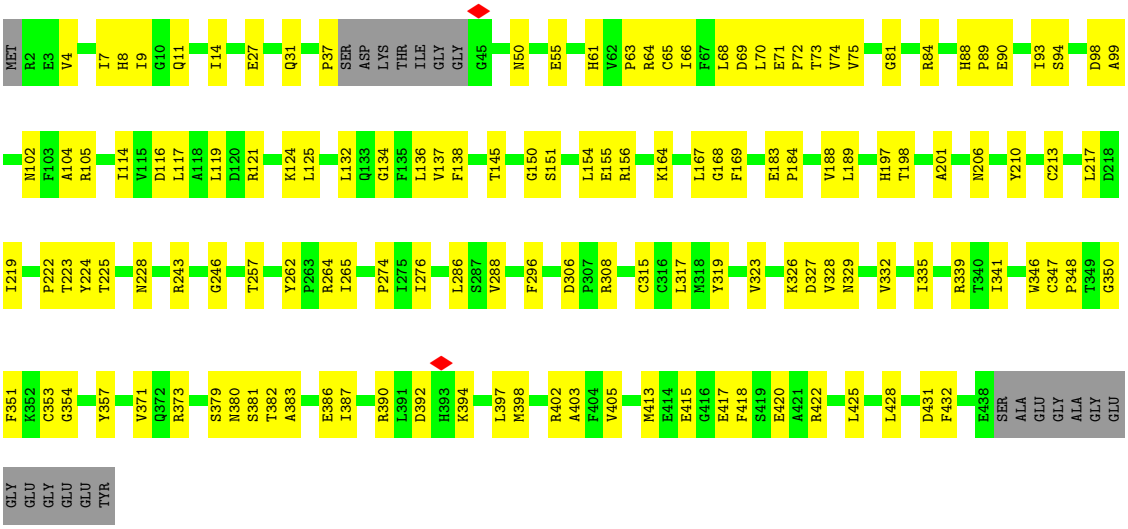
• Molecule 1: Tubulin beta

Chain B7:



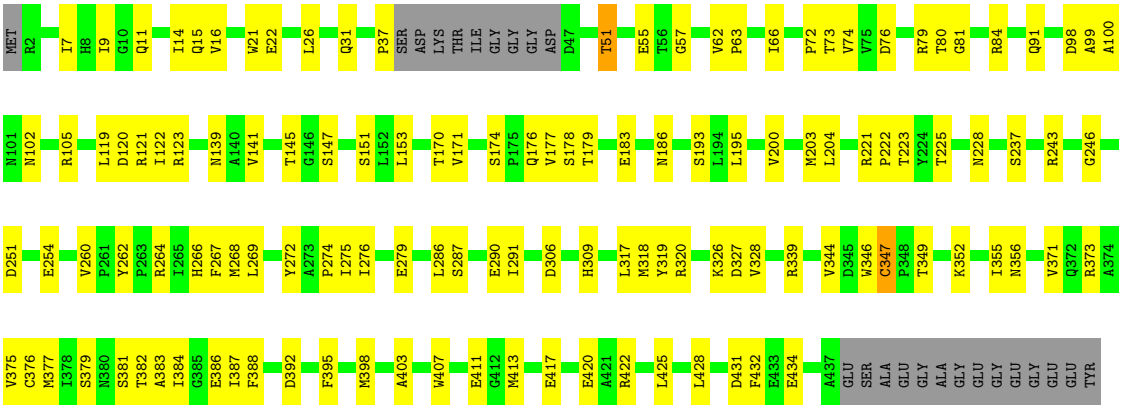
• Molecule 2: Tubulin alpha

Chain A2:



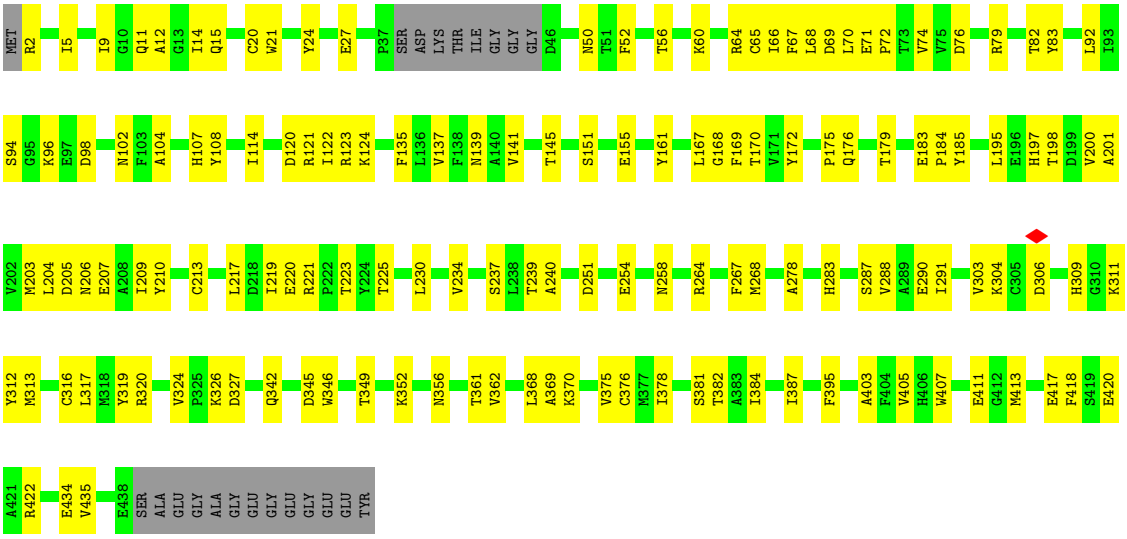
• Molecule 2: Tubulin alpha

Chain A4:



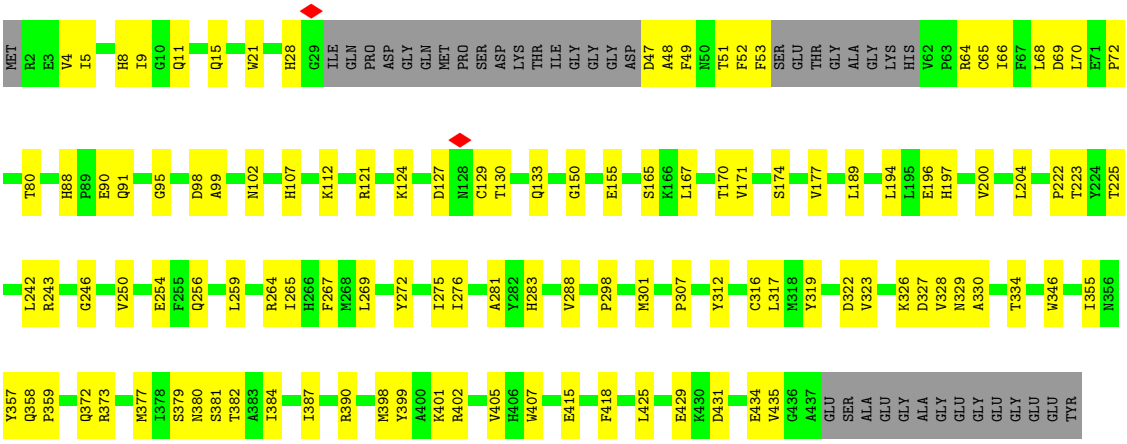
• Molecule 2: Tubulin alpha

Chain A6:



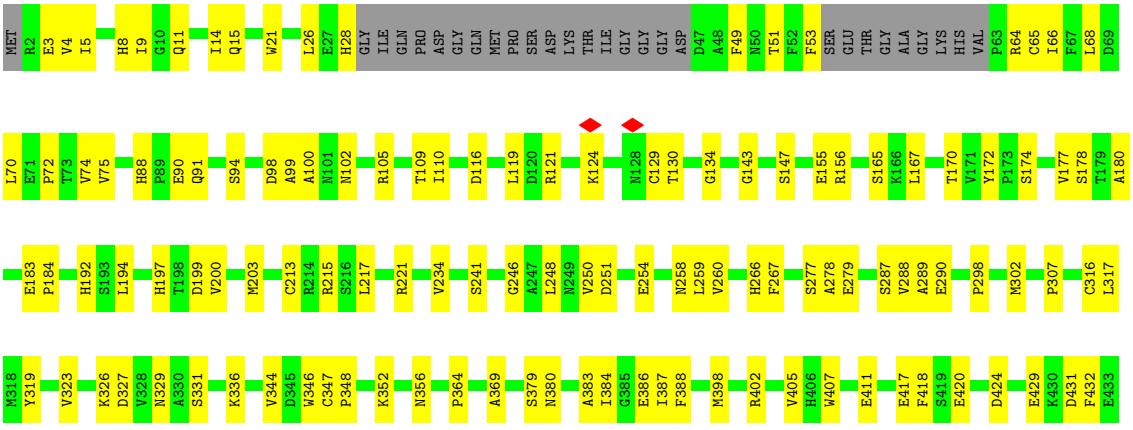
• Molecule 2: Tubulin alpha

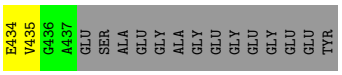
Chain B2:



• Molecule 2: Tubulin alpha

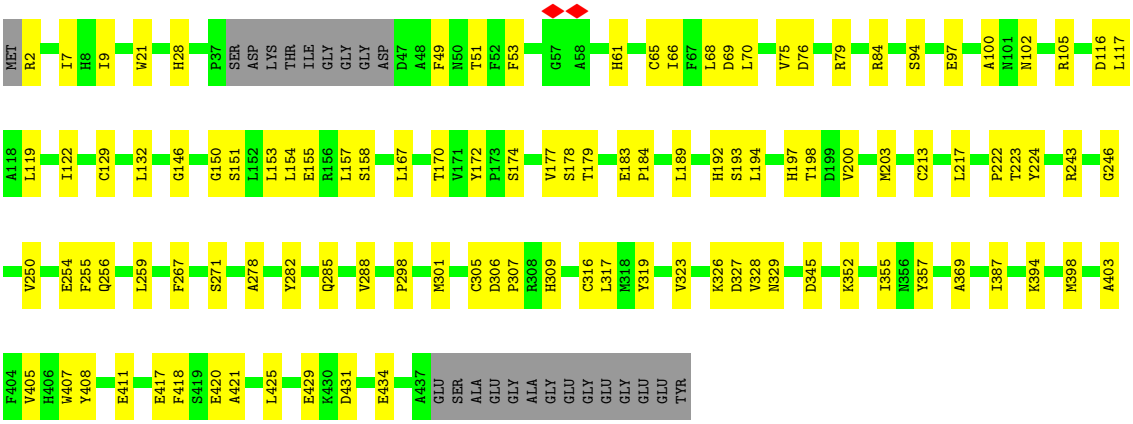
Chain B4:





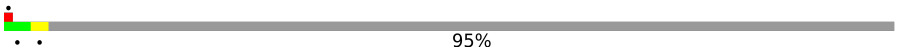
• Molecule 2: Tubulin alpha

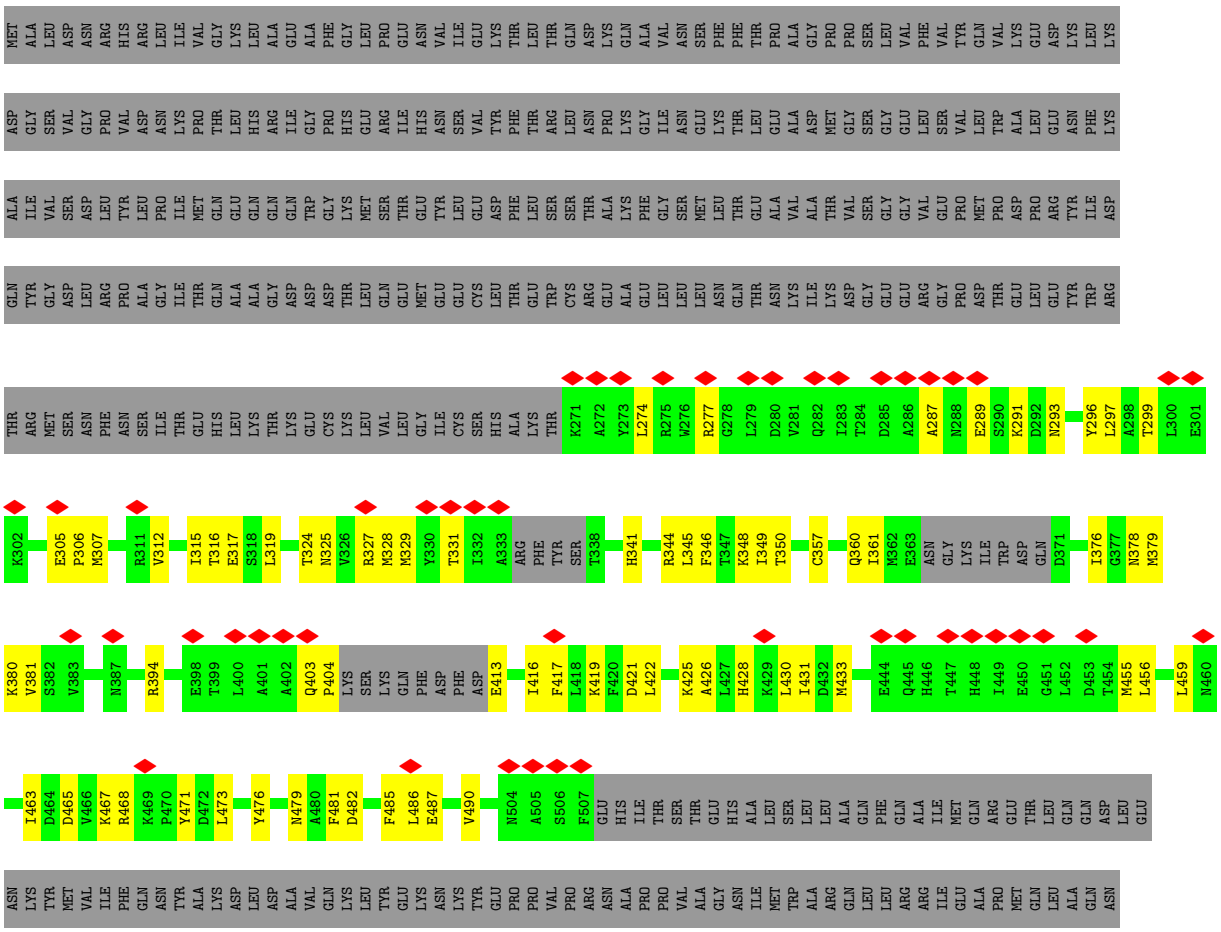
Chain B6:



• Molecule 3: Dynein gamma chain, flagellar outer arm

Chain C:





LYS ASN LEU LEU ALA ALA LYS GLU SER LYS LYS ASN ILE LYS THR TYR ASN LYS VAL ALA LYS ALA LEU ILE GLU PHE GLU THR LEU TRP HIS GLN ALA TRP ILE LYS SER ILE GLU GLN CYS LYS ALA GLY LEU ALA ALA PRO LEU LEU VAL GLN HIS PRO ASP THR GLY LYS ILE LEU

VAL ASN PHE ASP LYS GLU ILE MET GLN LEU VAL ARG GLU ALA LYS TYR MET GLN ARG PHE ASN ILE ARG CYS SER SER PRO SER GLN MET VAL LEU LEU GLN GLU GLU LYS PHE LYS PHE TYR HIS ASN GLN LEU THR HIS LEU VAL ARG GLU TYR GLU HIS VAL LEU GLY ARG GLY ALA

THR ILE LYS PRO LEU LEU ARG PRO HIS LEU ASP ASP MET GLU ARG LYS ILE ALA PRO GLY PHE ALA VAL LEU THR TRP THR SER LEU ASN ILE ASP GLY TYR LEU HIS ARG PHE LYS GLN GLY LEU ALA ARG LEU GLU GLU LEU VAL ARG LYS VAL VAL ASP LEU THR GLU ASN ARG VAL

ASP SER ASN LEU GLY ALA ILE SER SER THR LEU LEU VAL GLU LEU PRO THR ASP ARG SER PHE THR TYR GLU GLY PHE VAL GLU GLN ASN ARG PHE GLN LYS LYS GLN ALA GLU LEU LEU ALA ILE ARG ASN GLU GLU VAL ARG ARG ALA ILE GLU ASP LEU TYR THR LEU VAL ARG ASN

TYR PRO ARG GLU ASN THR GLU ASP VAL LEU ASP GLU LYS GLU VAL SER LEU LEU VAL ARG HIS TYR SER LYS ASN MET TYR ASN ALA ILE MET GLN CYS THR LEU ASN SER LEU GLN ALA MET LYS ARG ARG LEU GLY SER LYS THR THR THR GLY ILE PHE PHE MET GLU ARG PRO PHE

PHE ASP VAL ASP VAL GLU LEU LYS VAL PRO SER VAL CYS MET ASN PRO THR LEU GLU GLU ILE GLN ALA ALA ILE ASN GLN CYS ALA LYS LYS VAL LEU THR ILE SER LYS GLN LEU PRO ALA TRP GLY MET ASP ASN VAL ALA THR TYR HIS GLU MET MET ARG GLY ASP ARG ARG TRP

VAL LYS ALA VAL LEU ARG LEU THR GLY SER VAL GLU GLY ILE LYS THR GLN VAL GLY GLU TYR ILE ARG THR PHE ASP LYS TYR ASP PHE LEU TRP LYS GLU ASP LEU GLN ALA ALA TYR ASP HIS PHE MET ARG SER ASN PRO THR LEU GLU ALA PHE GLU ALA GLU LEU LYS LYS TYR

MET ALA ILE GLU THR GLU VAL THR MET ILE ASN GLY VAL ASN ASN ILE GLY ALA LEU SER LEU GLU THR HIS PRO LEU LYS ASN SER LEU LYS ALA GLU ALA VAL SER TRP LYS THR GLN PHE ALA GLN ASN LEU HIS LYS GLN CYS SER ASP ASP LEU LYS LEU ASP ASN TYR ILE ARG

ASP THR ASN SER LYS PHE HIS ARG LYS ILE GLU ASP LEU GLU ASP VAL ARG ASN VAL MET ALA VAL LEU LYS GLU VAL ARG GLU LYS GLU SER GLU ILE ASP ASN LEU ILE GLY PRO ILE GLU GLU MET TYR GLY LEU LEU MET ARG TYR GLU VAL ARG VAL PRO LYS GLU GLU THR THR

MET VAL SER ASP LEU ARG TYR GLY TRP LYS LYS LEU LYS LYS VAL ALA THR GLU VAL SER ASP ASN LEU THR ARG LEU GLN VAL GLY PHE LYS ARG GLU LEU ILE LYS GLU VAL LYS THR PHE VAL VAL ASP ALA GLN MET PHE ARG LYS ASP TRP GLU ALA ASN ALA MET VAL PRO GLY

LEU ASP PRO GLN GLU ALA VAL ASP ARG LEU ARG LYS PHE GLN GLN MET PHE GLU VAL ARG LYS ARG LYS TRP GLU ASN TYR SER SER GLY GLU GLU LEU PHE GLY LEU PRO VAL THR GLN TYR PRO GLU LEU GLU GLN THR GLU LYS GLU ILE GLN MET LEU ASP ARG LEU TYR SER LEU

TYR VAL ALA VAL ILE THR THR ILE LYS GLY TYR GLY ASP TYR PHE TRP VAL ASP VAL VAL GLU LYS ILE ASP GLU MET GLY GLU GLN VAL GLN GLN TYR GLN ASN GLN SER LYS LYS LEU PRO LYS LEU ARG ASP TRP PRO ALA TYR ASN ALA CYS ARG LYS THR ILE ASP ASP PHE LEU

GLU MET LEU PRO LEU PHE GLN ALA LEU THR HIS LYS SER MET ARG GLU ARG HIS TRP LYS GLU VAL MET ARG VAL THR GLY HIS GLU LEU ASN LEU ALA GLU ASP HIS PHE LYS LEU GLN HIS LEU LEU ASP CYS ASN VAL LEU ARG TYR ARG GLU ASP ILE GLU ASP LEU THR GLY ALA

ALA VAL LYS GLU GLU ILE ILE GLU VAL LYS LEU ASN GLN LEU LYS ALA ASP TRP ALA THR ALA ASN LEU ALA LEU ALA GLU TYR LYS ASN ARG GLY PRO VAL ILE LEU LYS PRO SER ASP THR SER GLU LEU MET GLU LYS LEU GLU GLU SER GLN MET THR LEU GLY SER MET ALA THR

ASN ARG TYR SER ALA PRO PHE ARG ASP GLU VAL GLN ALA TRP SER ILE LYS LEU SER THR VAL SER GLU ILE ILE GLU GLN TRP LEU MET VAL GLN SER MET TRP GLN TYR MET GLU ALA VAL PHE SER GLY GLY ASP ILE VAL LYS GLN LEU PRO GLN GLU ALA LYS ARG PHE LEU ASN

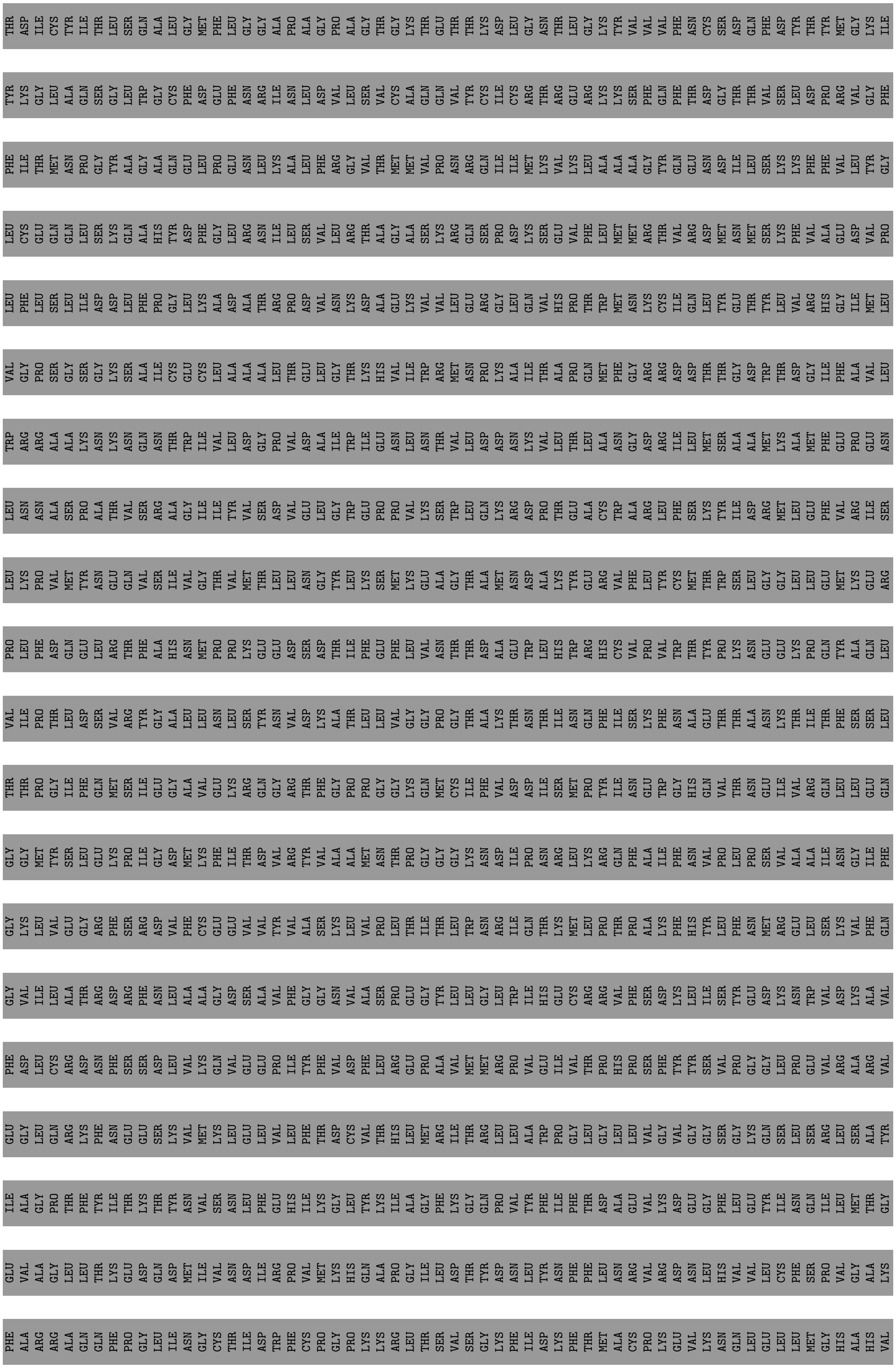
ILE ASP LYS ASN PHE MET LYS ILE VAL SER ASN ALA LEU GLU THR GLN ASN VAL ILE ASN THR CYS PHE GLY ASN GLU LEU MET LYS ASN MET LEU PRO HIS LEU HIS GLU GLN LEU GLU MET CYS GLN LYS SER LEU SER ALA TYR LEU GLU GLN LYS ARG ALA GLU PHE PRO ARG PHE

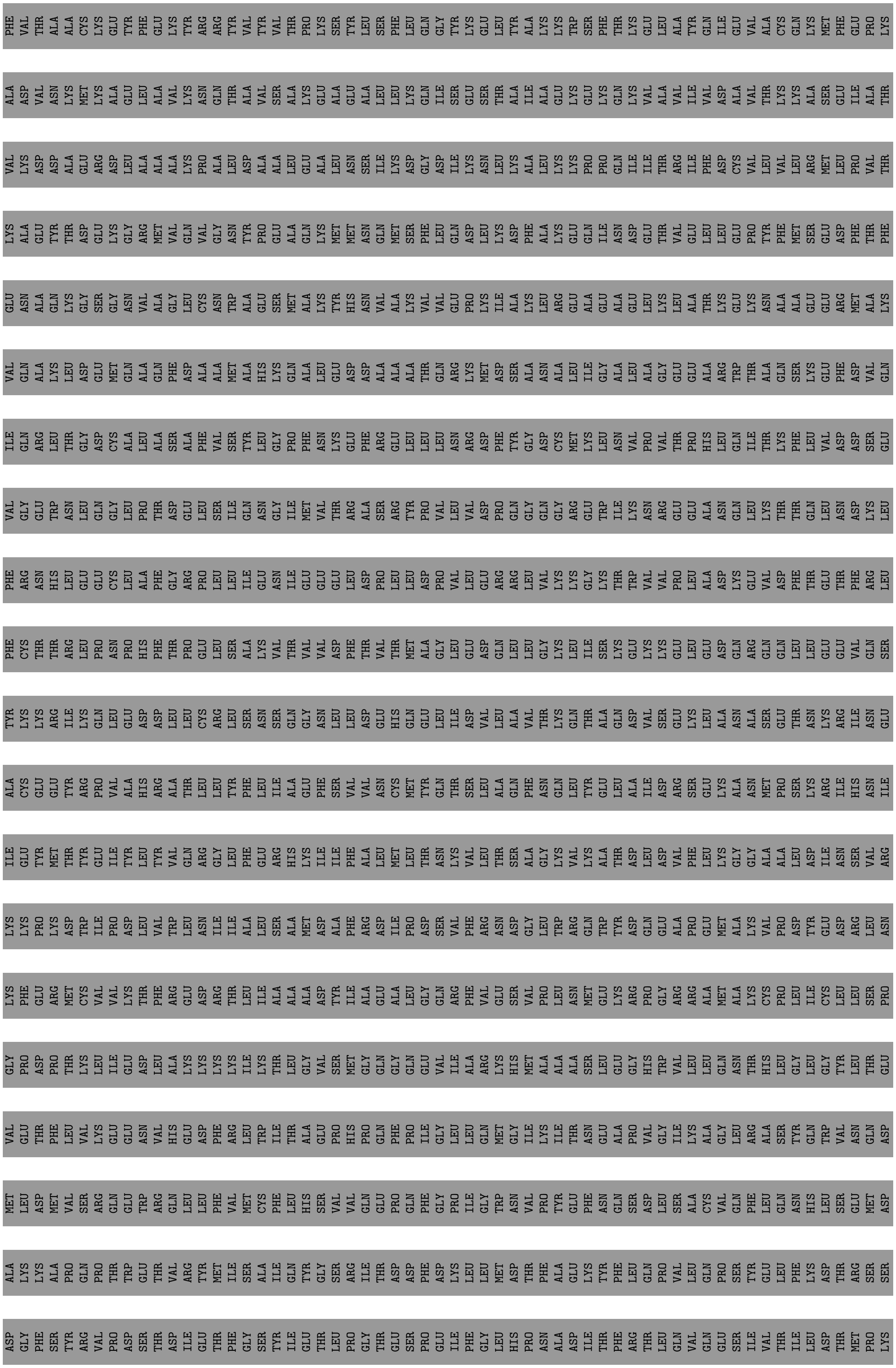
THR CYS VAL GLY PRO HIS LEU LEU GLU ILE CYS ARG TRP ALA HIS ASP PRO PRO SER VAL VAL PRO HIS PHE GLN SER GLY LEU PHE ASP SER LEU SER ASN VAL THR PHE ASP ARG ILE ASP LYS THR ARG MET THR GLU MET PHE SER GLN GLN ASN GLU LYS VAL GLU PHE GLU ARG

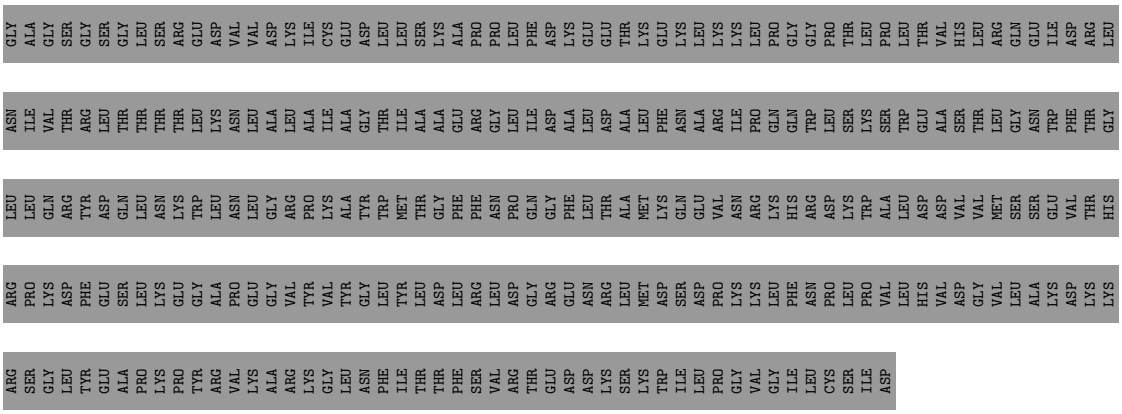
PRO VAL ASP ALA LYS GLY ASN ILE GLU VAL TRP LEU GLN ARG LEU VAL ASP GLY MET GLU ASP THR VAL LYS GLN ILE ILE LYS ARG ALA VAL ARG ASN VAL ALA GLU MET PRO LEU GLU ASP PHE VAL PHE GLY HIS PRO ALA GLN VAL SER LEU LEU GLY ILE GLN PHE GLN TRP THR

ALA GLU THR GLN MET ALA LEU SER SER ALA LYS VAL ASP LYS THR ILE MET ASN LYS ASN MET LYS LYS VAL ASP ALA LEU LEU ARG ASP MET VAL ASN ILE THR VAL ARG LEU ASP LEU THR LYS ASN GLN ARG THR ASN LEU GLU THR CYS ILE THR VAL HIS MET HIS GLN LYS GLU

SER THR GLU ASP LEU VAL LYS LYS LYS ILE LYS ASP PRO THR ASP PHE GLU TRP LEU LYS GLN VAL ARG PHE TYR TRP ARG ASP ASP LYS ASP THR VAL ILE ILE SER ILE CYS ASP VAL ASP PHE GLU TYR SER PHE GLU TYR LEU GLY VAL LYS GLU ARG LEU VAL ILE THR PRO LEU

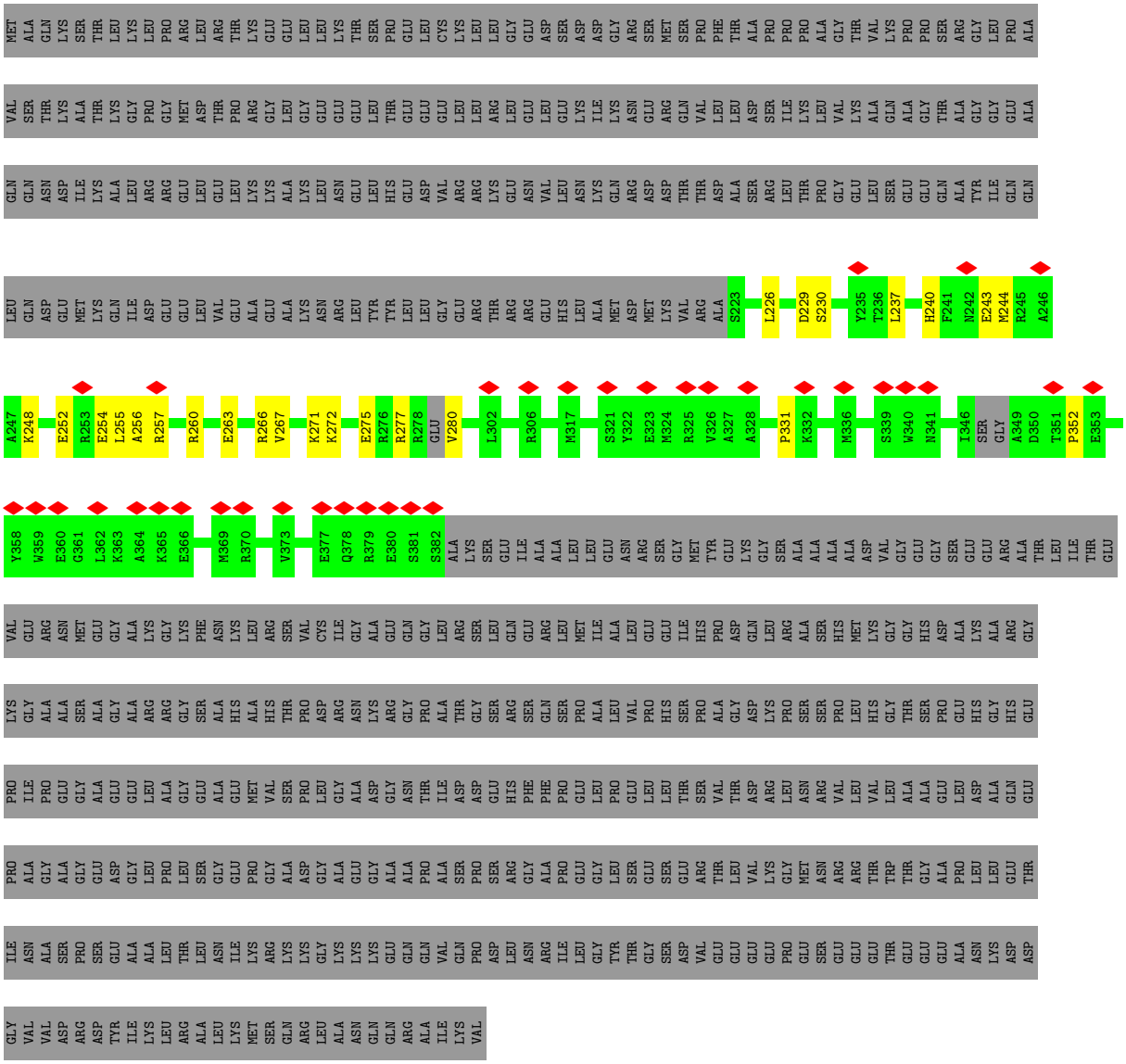

THR ASP ILE CYS TYR ILE THR LEU SER GLN ALA LEU GLY MET PHE LEU GLY GLY ALA PRO ALA GLY PRO ALA GLY THR GLY LYS THR GLU THR THR LYS ASP LEU GLY ASN THR LEU GLY LYS TYR VAL VAL VAL PHE ASN CYS SER ASP GLN PHE ASP TYR THR TYR MET GLY LYS ILE
TYR LYS GLY LEU ALA GLN SER GLY LEU TRP GLY CYS PHE ASP GLU PHE ASN ARG ILE ASN LEU ASP VAL LEU SER VAL CYS ALA GLN GLN VAL TYR CYS ILE CYS ARG THR ARG GLU ARG LYS LYS SER PHE GLN PHE THR ASP GLY THR THR VAL SER LEU ASP PRO ARG VAL GLY PHE
PHE ILE THR MET ASN PRO GLY TYR ALA GLY ALA GLN GLU LEU PRO GLU ASN LEU LYS ALA LEU PHE ARG GLY VAL THR MET MET VAL PRO ASN ARG GLN ILE ILE MET LYS VAL LYS LEU ALA ALA ALA GLY TYR GLN GLU ASN ASP ILE LEU SER LYS LYS PHE PHE VAL LEU TYR GLY
LEU CYS GLU GLN GLN LEU SER LYS GLN ALA HIS TYR ASP PHE GLY LEU ARG ASN ILE LEU SER VAL LEU ARG THR ALA GLY ALA SER LYS ARG GLN SER PRO ASP LYS SER GLU VAL PHE LEU MET MET ARG THR VAL ARG ASP MET ASN MET SER LYS PHE VAL ALA GLU ASP VAL PRO
LEU PHE LEU SER LEU ILE ASP ASP LEU PHE PRO GLY LEU LYS ALA ASP ALA THR ARG PRO ASP VAL ASN LYS ASP ALA GLU LYS VAL VAL LEU GLU ARG GLY LEU GLN VAL HIS PRO THR TRP MET ASN LYS CYS ILE GLN LEU TYR GLU THR TYR LEU VAL ARG HIS GLY ILE MET LEU
VAL GLY PRO SER GLY SER GLY LYS SER ALA ILE CYS GLU CYS LEU ALA ALA ALA LEU THR GLU LEU GLY THR LYS HIS VAL ILE TRP ARG MET ASN PRO LYS ALA ILE THR ALA PRO GLN MET PHE GLY ARG ARG ASP THR THR GLY ASP TRP THR ASP GLY ILE PHE ALA VAL LEU
TRP ARG ARG ALA ALA LYS ASN LYS ASN GLN ASN THR TRP ILE VAL LEU ASP GLY PRO VAL ASP ALA ILE TRP ILE GLU ASN LEU ASN THR VAL LEU ASP ASP ASN LYS VAL LEU THR LEU ALA ASN GLY ASP ARG ILE LEU MET SER ALA ALA MET LYS ALA MET PHE GLU PRO GLU ASN
LEU ASN ASN ALA SER PRO ALA THR VAL SER ARG ALA GLY ILE ILE TYR VAL SER ASP VAL GLU LEU GLY TRP GLU PRO PRO VAL LYS SER TRP LEU GLN LYS ARG ASP PRO THR GLU ALA CYS TRP ALA ARG LEU PHE SER LYS TYR ILE ASP ARG MET LEU GLU PHE VAL ARG ILE SER
LEU LYS PRO VAL MET TYR ASN GLU GLN VAL SER ILE VAL GLY THR VAL MET THR LEU LEU ASN GLY TYR LEU LYS SER MET LYS GLU ALA GLY THR ALA MET ASN ASP ALA LYS TYR GLU ARG VAL PHE LEU TYR CYS MET THR TRP SER LEU GLY GLY LEU LEU GLU MET LYS GLU ARG
PRO LEU PHE ASP GLN GLU LEU ARG THR PHE ALA HIS ASN MET PRO PRO LYS GLU GLU ASP SER ASP THR ILE PHE GLU PHE LEU VAL ASN THR THR ASP ALA GLU TRP LEU HIS TRP ARG HIS CYS VAL PRO VAL TRP THR TYR PRO LYS ASN GLU GLU LYS PRO GLN TYR ALA GLN LEU
VAL ILE PRO THR LEU ASP SER VAL ARG TYR GLY ALA LEU LEU ASN LEU SER TYR ASN VAL ASP LYS ALA THR LEU LEU VAL GLY GLY PRO GLY THR ALA LYS THR ASN THR ILE ASN GLN PHE ILE SER LYS PHE ASN ALA GLU THR THR ALA ASN LYS THR ILE THR PHE SER SER LEU
THR THR PRO GLY ILE PHE GLN MET SER ILE GLU GLY ALA VAL GLU LYS ARG GLN GLY ARG THR PHE GLY PRO PRO GLY GLY LYS GLN MET CYS ILE PHE VAL ASP ASP ILE SER MET PRO TYR ILE ASN GLU TRP GLY HIS GLN VAL THR ASN GLU ILE VAL ARG GLN LEU LEU GLU GLN
GLY GLY MET TYR SER LEU GLU LYS PRO ILE GLY ASP MET LYS PHE ILE THR ASP VAL ARG TYR VAL ALA ALA MET ASN THR PRO GLY GLY GLY LYS ASN ASP ILE PRO ASN ARG LEU LYS ARG GLN PHE ALA ILE PHE ASN VAL PRO LEU PRO SER VAL ALA ALA ILE ASN GLY ILE PHE
GLY LYS LEU VAL GLU GLY ARG PHE SER ARG ASP VAL PHE CYS GLU GLU VAL VAL TYR VAL ALA SER LYS LEU VAL PRO LEU THR ILE THR LEU TRP ASN ARG ILE GLN THR LYS MET LEU PRO THR PRO ALA LYS PHE HIS TYR LEU PHE ASN MET ARG GLU LEU SER LYS VAL PHE GLN
GLY VAL ILE LEU ALA THR ARG ASP ARG PHE ASN LEU ALA ALA GLY ASP SER ALA VAL PHE GLY GLY ASN VAL ALA SER PRO GLU GLY TYR LEU LEU GLY LEU TRP ILE HIS GLU CYS ARG ARG VAL PHE SER ASP LYS LEU ILE SER TYR GLU ASP LYS ASN TRP VAL ASP LYS ALA VAL
PHE ASP LEU CYS ARG ASP ASN PHE SER SER ASP LEU VAL LYS GLN VAL GLU GLU PRO ILE TYR PHE VAL ASP PHE LEU ARG GLU PRO ALA VAL MET MET ARG PRO VAL GLU ILE VAL THR PRO HIS PRO SER PHE TYR TYR SER VAL PRO GLY GLY LEU PRO GLU VAL ARG ALA ARG VAL
GLU GLY LEU GLN ARG LYS PHE ASN GLU GLU SER LYS VAL MET LYS LEU GLU LEU VAL LEU PHE THR ASP CYS VAL THR HIS LEU MET ARG ILE THR ARG LEU LEU ALA TRP PRO GLY LEU GLY LEU LEU VAL GLY VAL GLY GLY SER GLY LYS GLN SER LEU SER ARG LEU SER ALA TYR
ILE ALA GLY PRO THR PHE TYR ILE THR LYS THR TYR ASN VAL SER ASN LEU PHE GLU HIS ILE LYS GLY LEU TYR LYS ILE ALA GLY PHE LYS GLY GLN PRO VAL TYR PHE ILE PHE THR ASP ALA GLU VAL LYS ASP GLU GLY PHE LEU GLU TYR ILE ASN GLN ILE LEU MET THR GLY
GLU VAL ALA GLY LEU LEU THR LYS GLU ASP GLN ASN ASP MET ILE VAL ASN ASP ILE ARG PRO VAL MET LYS HIS GLN ALA PRO GLY ILE LEU ASP THR TYR ASP ASN LEU TYR ASN PHE PHE LEU ASN ARG VAL ARG ASP ASN LEU HIS VAL VAL LEU CYS PHE SER PRO VAL GLY ALA LYS
PHE ALA ARG ARG ALA GLN GLN PHE PRO GLY LEU ILE ASN GLY CYS THR ILE ASP TRP PHE CYS PRO GLY PRO LYS LYS ARG LEU THR SER VAL SER GLY LYS PHE ILE ASP LYS PHE THR MET ALA CYS PRO LYS GLU VAL LYS ASN GLN LEU GLU LEU LEU MET GLY HIS ALA HIS VAL


PHE VAL THR ALA ALA CYS LYS GLU TYR PHE GLU LYS TYR ARG ARG TYR VAL TYR VAL THR PRO LYS SER TYR LEU SER PHE LEU GLN GLY TYR LYS GLU LEU TYR ALA LYS LYS TRP SER PHE THR LYS GLU LEU ALA TYR GLN ILE GLU VAL ALA CYS GLN LYS MET PHE GLU PRO LYS
ALA ASP VAL ASN LYS MET LYS ALA GLU LEU ALA VAL LYS ASN GLN THR ALA VAL SER ALA LYS GLU ALA GLU ALA LEU LEU LYS GLN ILE SER GLU SER THR ALA ILE ALA GLU LYS GLU LYS GLN LYS VAL ALA VAL ILE VAL ASP ALA VAL THR LYS LYS ALA SER GLU ILE ALA THR
VAL LYS ASP ASP ALA GLU ARG ASP LEU ALA ALA ALA LYS PRO ALA LEU ASP ALA ALA LEU GLU ALA LEU ASN SER ILE LYS ASP GLY ASP ILE LYS ASN LEU LYS ALA LEU LYS LYS PRO PRO GLN ILE ILE THR ARG ILE PHE ASP CYS VAL LEU VAL LEU ARG MET LEU PRO VAL THR
LYS ALA GLU TYR THR ASP GLU LYS GLY ARG MET VAL GLN VAL GLY ASN TYR PRO GLU ALA GLN LYS MET MET ASN GLN MET SER PHE LEU GLN ASP LEU LYS ASP PHE ALA LYS GLU GLN ILE ASN ASP GLU THR VAL GLU LEU LEU GLU PRO TYR PHE MET SER GLU ASP PHE THR PHE
GLU ASN ALA GLN LYS GLY SER GLY ASN VAL ALA GLY LEU CYS ASN TRP ALA GLU SER MET ALA LYS TYR HIS ASN VAL ALA LYS VAL VAL GLU PRO LYS ILE ALA LYS LEU ARG GLU ALA GLU ALA GLU LEU LYS LEU ALA THR LYS GLU LYS ASN ALA ALA GLU GLU ARG MET ALA LYS
VAL GLN ALA LYS LEU ASP GLU MET GLN ALA GLN PHE ASP ALA ALA MET ALA HIS LYS GLN ALA LEU GLU ASP ASP ALA ALA ALA THR GLN ARG LYS MET ASP SER ALA ASN ALA LEU ILE GLY ALA LEU ALA GLY GLU GLU ALA ARG TRP THR ALA GLN SER LYS GLU PHE ASP VAL GLN
ILE GLN ARG LEU THR GLY ASP CYS ALA LEU ALA SER ALA PHE VAL SER TYR LEU GLY PRO PHE ASN LYS GLU PHE ARG GLU LEU LEU LEU ASN ARG ASP PHE TYR GLY ASP CYS MET LYS LEU ASN VAL PRO VAL THR PRO HIS LEU GLN ILE THR LYS PHE LEU VAL ASP ASP SER GLU
VAL GLY GLU TRP ASN LEU GLN GLY LEU PRO THR ASP GLU LEU SER ILE GLN ASN GLY ILE MET VAL THR ARG ALA SER ARG TYR PRO VAL LEU VAL ASP PRO GLN GLY GLN GLY ARG GLU TRP ILE LYS ASN ARG GLU GLU ALA ASN GLN LEU LYS THR THR GLN LEU ASN ASP LYS LEU
PHE ARG ASN HIS LEU GLU GLU CYS LEU ALA PHE GLY ARG PRO LEU LEU ILE GLU ASN ILE GLU GLU LEU ASP PRO LEU LEU ASP PRO VAL LEU GLU ARG ARG LEU VAL LYS LYS GLY LYS THR TRP VAL VAL PRO LEU ALA ASP LYS GLU VAL ASP PHE THR GLU THR PHE ARG LEU
PHE CYS THR THR ARG LEU PRO ASN PRO HIS PHE THR PRO GLU LEU SER ALA LYS VAL THR VAL VAL ASP PHE THR VAL THR MET ALA GLY LEU GLU ASP GLN LEU LEU GLY LYS LEU ILE SER LYS GLU LYS LYS GLU LEU GLU ASP GLN ARG GLN GLN LEU LEU GLU GLU VAL GLN SER
TYR LYS LYS ARG ILE LYS GLN LEU GLU ASP ASP LEU LEU CYS ARG LEU SER ASN SER GLN GLY ASN LEU LEU ASP GLU HIS GLN GLU LEU ILE ASP VAL LEU ALA VAL THR LYS GLN THR ALA GLN ASP VAL SER GLU LYS LEU ALA ASN ALA SER GLU THR ASN LYS ARG ILE ASN GLU
ALA CYS GLU GLU TYR ARG PRO VAL ALA HIS ARG ALA THR LEU LEU TYR PHE LEU ILE ALA GLU PHE SER VAL VAL ASN CYS MET TYR GLN THR SER LEU ALA GLN PHE ASN GLN LEU TYR GLU LEU ALA ILE ASP ARG SER GLU LYS ALA ASN MET PRO SER LYS ARG ILE HIS ASN ILE
ILE GLU TYR MET THR TYR GLU ILE TYR LEU TYR VAL GLN ARG GLY LEU PHE GLU ARG HIS LYS ILE ILE PHE ALA LEU MET LEU THR ASN LYS VAL LEU THR SER ALA GLY LYS VAL LYS ALA THR ASP LEU ASP VAL PHE LEU LYS GLY GLY ALA ALA LEU ASP ILE ASN SER VAL ARG
LYS LYS PRO LYS ASP TRP ILE PRO ASP LEU VAL TRP LEU ASN ILE ILE ALA LEU SER ALA MET ASP ALA PHE ARG ASP ILE PRO ASP SER VAL PHE ARG ASN ASP GLY LEU TRP ARG GLN TRP TYR ASP GLN GLU ALA PRO GLU MET ALA LYS VAL PRO ASP TYR GLU ASP ARG LEU ASN
LYS PHE GLU ARG MET CYS VAL VAL LYS THR PHE ARG GLU ASP ARG THR LEU ILE ALA ALA ASP TYR ILE ALA GLU ALA LEU GLY GLN ARG PHE VAL GLU SER VAL PRO LEU ASN MET GLU LYS ARG PRO GLY ARG ARG ALA MET ALA LYS CYS PRO LEU ILE CYS LEU LEU SER PRO
GLY PRO ASP PRO THR LYS LEU ILE GLU ASP LEU ALA LYS LYS LYS ILE LYS THR LEU GLY VAL SER MET GLY GLN GLY GLN GLU VAL ILE ALA ARG LYS HIS MET ALA ALA ALA SER LEU GLU GLY HIS TRP VAL LEU LEU GLN ASN THR HIS LEU GLY LEU GLY TYR LEU THR GLU
VAL GLU THR PHE LEU VAL LYS GLU GLU ASN VAL HIS GLU ASP PHE ARG LEU TRP ILE THR ALA GLU PRO HIS PRO GLN PHE PRO ILE GLY LEU LEU GLN MET GLY ILE LYS ILE THR ASN GLU ALA PRO VAL GLY ILE LYS ALA GLY LEU ARG ALA SER TYR GLN TRP VAL ASN GLN ASP
MET LEU ASP MET VAL SER ARG GLN GLU TRP ARG GLN LEU LEU PHE VAL MET CYS PHE LEU HIS SER VAL VAL GLN GLU PRO GLN PHE GLY PRO ILE GLY TRP ASN VAL PRO TYR GLU PHE ASN GLN SER ASP LEU SER ALA CYS VAL GLN PHE LEU GLN ASN HIS LEU SER GLU MET ASP
ALA LYS LYS ALA PRO GLN PRO THR TRP GLU THR VAL ARG TYR MET ILE SER ALA ILE GLN TYR GLY SER ARG ILE THR ASP ASP PHE ASP LYS LEU LEU MET ASP THR PHE ALA GLU LYS TYR PHE LEU GLN PRO VAL LEU GLN PRO SER TYR GLU LEU PHE LYS ASP THR ARG SER SER
ASP GLY PHE SER TYR ARG VAL PRO ASP SER THR ASP ILE GLU THR PHE GLY SER TYR ILE GLU THR LEU PRO GLY THR GLU SER PRO GLU ILE PHE GLY LEU HIS PRO ASN ALA ASP ILE THR PHE ARG THR LEU GLN VAL GLN GLU SER ILE VAL THR ILE LEU ASP THR MET PRO LYS



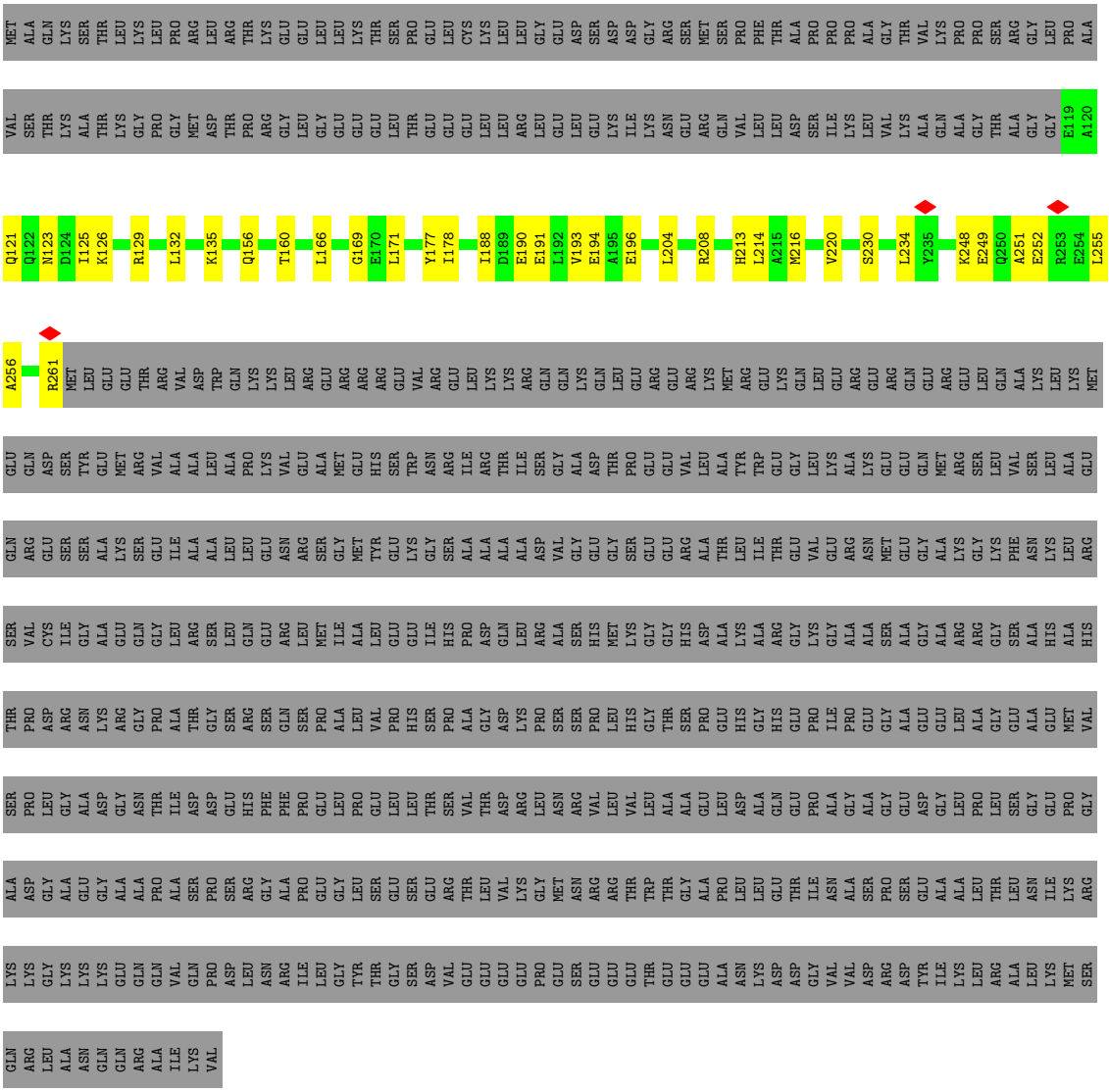
• Molecule 4: Outer dynein arm-docking complex subunit 1

Chain X:



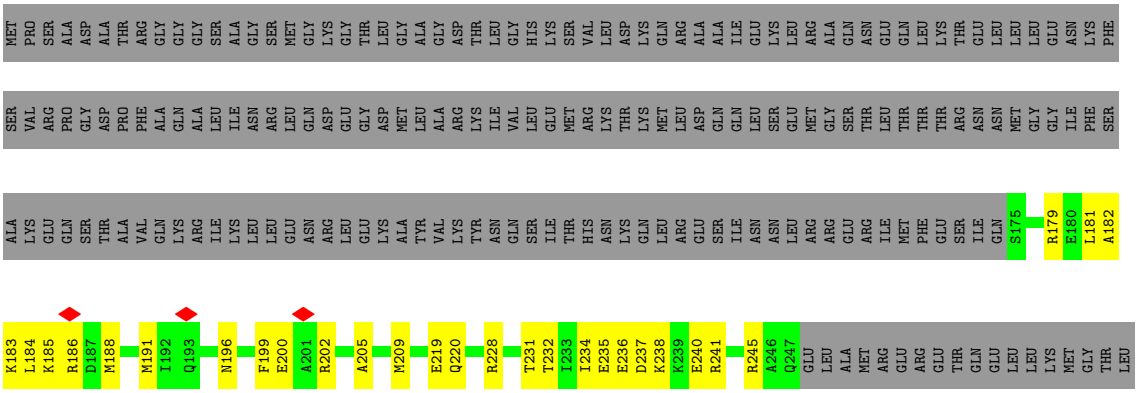
• Molecule 4: Outer dynein arm-docking complex subunit 1

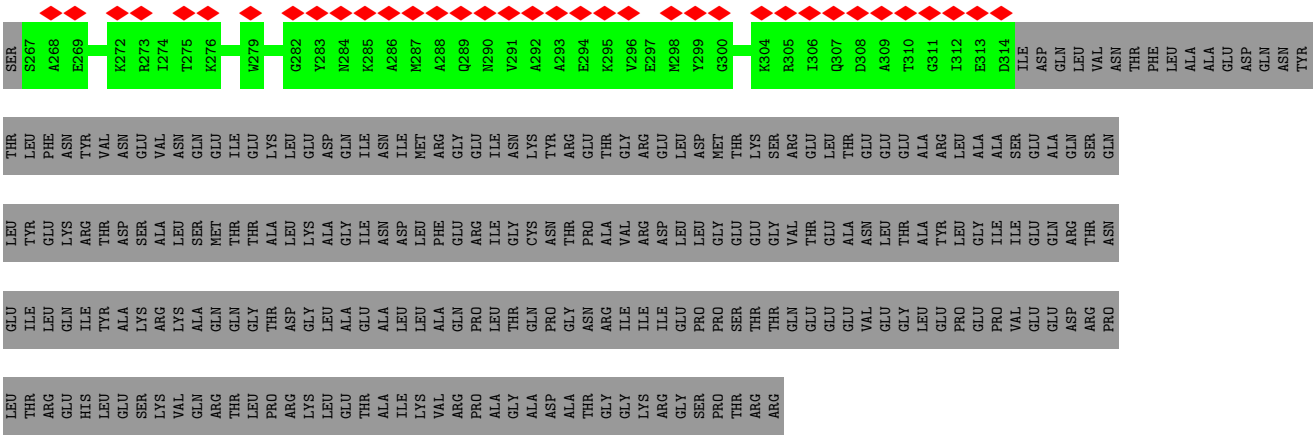
Chain X1:



• Molecule 5: Outer dynein arm protein 1

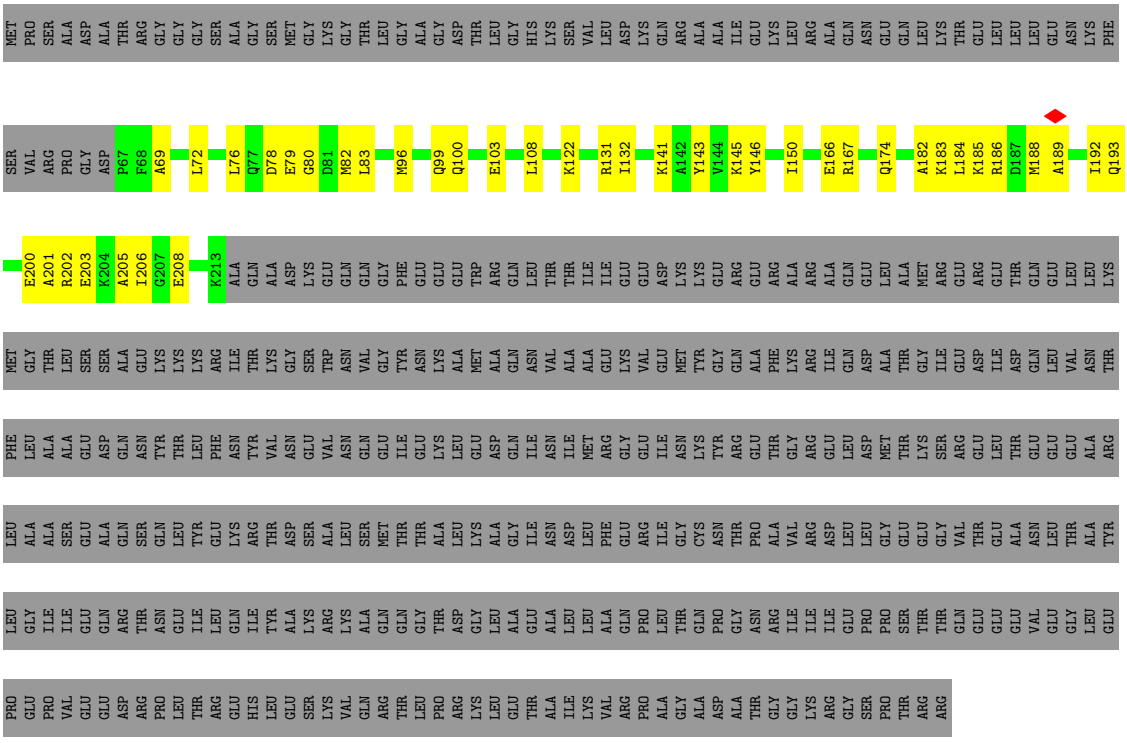
Chain Y:





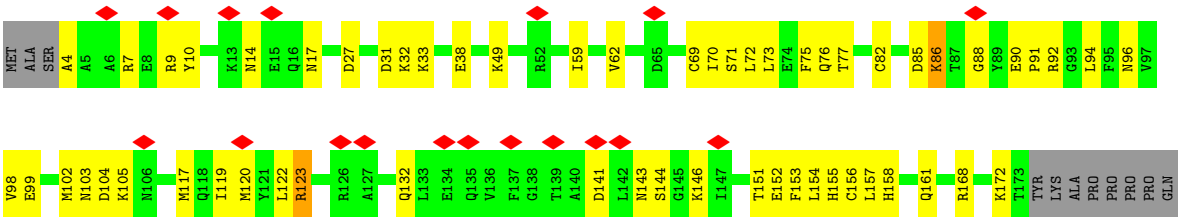
• Molecule 5: Outer dynein arm protein 1

Chain Y1:



• Molecule 6: Outer dynein arm-docking complex protein DC3

Chain Z:




LYS
ARG
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=82 Å, axial sym=C1	Depositor
Number of segments used	485694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61.48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	394.4, 394.4, 394.4	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP, MG

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	A1	0.28	0/3420	0.53	0/4628
1	A3	0.31	0/3420	0.54	0/4628
1	A5	0.30	0/3420	0.52	0/4628
1	A7	0.28	0/3420	0.51	0/4628
1	B1	0.29	0/3371	0.49	0/4561
1	B3	0.32	0/3295	0.49	0/4454
1	B5	0.31	0/3420	0.51	0/4628
1	B7	0.28	0/3420	0.50	0/4628
2	A2	0.31	0/3410	0.53	0/4623
2	A4	0.34	0/3389	0.58	0/4595
2	A6	0.31	0/3406	0.54	0/4618
2	B2	0.31	0/3271	0.52	0/4434
2	B4	0.32	0/3260	0.52	0/4418
2	B6	0.29	0/3389	0.50	0/4595
3	C	0.26	0/1796	0.50	0/2418
4	X	0.27	0/987	0.50	2/1341 (0.1%)
4	X1	0.31	0/1186	0.51	0/1582
5	Y	0.29	0/846	0.48	0/1132
5	Y1	0.29	0/1192	0.52	0/1585
6	Z	0.34	0/1403	0.67	0/1885
All	All	0.30	0/54721	0.52	2/74009 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	331	PRO	N-CA-CB	5.82	110.28	103.30
4	X	352	PRO	N-CA-CB	5.73	110.17	103.30

There are no chirality outliers.

There are no planarity outliers.

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	A1	3346	0	3238	107	0
1	A3	3346	0	3238	108	0
1	A5	3346	0	3238	103	0
1	A7	3346	0	3238	89	0
1	B1	3298	0	3196	82	0
1	B3	3227	0	3134	82	0
1	B5	3346	0	3238	106	0
1	B7	3346	0	3238	92	0
2	A2	3339	0	3272	104	0
2	A4	3318	0	3259	93	0
2	A6	3335	0	3269	105	0
2	B2	3204	0	3152	84	0
2	B4	3193	0	3141	106	0
2	B6	3318	0	3259	82	0
3	C	1771	0	1781	45	0
4	X	985	0	714	19	0
4	X1	1178	0	1179	28	0
5	Y	844	0	735	22	0
5	Y1	1185	0	1230	36	0
6	Z	1384	0	1359	46	0
7	A1	32	0	12	0	0
7	A3	32	0	12	1	0
7	A5	32	0	12	1	0
7	A7	32	0	12	4	0
7	B2	32	0	12	1	0
7	B5	32	0	12	0	0
7	B7	32	0	12	0	0
8	A1	1	0	0	0	0
8	A2	1	0	0	0	0
8	A4	1	0	0	0	0
8	A6	1	0	0	0	0
8	B3	1	0	0	0	0
8	B4	1	0	0	0	0
8	B6	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A1	28	0	12	0	0
9	A3	28	0	12	2	0
9	A5	28	0	12	0	0
9	A7	28	0	12	2	0
9	B1	28	0	12	3	0
9	B3	28	0	12	2	0
9	B5	28	0	12	1	0
9	B7	28	0	12	2	0
All	All	54110	0	52288	1396	0

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

All (1396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:215:LEU:HB3	1:A3:217:LEU:HD13	1.54	0.90
1:B5:175:VAL:HG22	2:B6:329:ASN:HD21	1.35	0.87
1:B3:330:MET:HE2	1:B3:349:VAL:HG11	1.55	0.86
1:B7:113:ILE:HD13	1:B7:150:LEU:HD11	1.55	0.85
1:A1:215:LEU:HB3	1:A1:217:LEU:HD13	1.59	0.84
1:A3:121:ARG:HD2	5:Y1:141:LYS:HZ2	1.41	0.84
1:B7:113:ILE:HD11	1:B7:147:MET:HG3	1.58	0.84
1:B5:173:PRO:HB3	1:B5:384:GLN:HE22	1.40	0.82
6:Z:59:ILE:HG13	6:Z:70:ILE:HD11	1.60	0.82
1:B5:256:ASN:HD22	1:B5:350:LYS:HD2	1.45	0.82
1:B3:175:VAL:HG12	2:B4:329:ASN:HD21	1.45	0.81
2:A2:417:GLU:HA	2:A2:420:GLU:HG2	1.62	0.81
6:Z:32:LYS:NZ	6:Z:71:SER:OG	2.13	0.81
1:A3:218:THR:O	2:A4:326:LYS:NZ	2.14	0.80
1:A5:309:ARG:H	1:A5:372:THR:HG22	1.44	0.79
2:A2:402:ARG:HH11	6:Z:168:ARG:HH22	1.29	0.79
1:A5:156:ARG:NH1	1:A5:195:ASN:O	2.14	0.79
2:A6:82:THR:HG23	2:A6:83:TYR:HD1	1.48	0.78
2:B4:88:HIS:CD2	2:B4:90:GLU:HG3	2.19	0.78
2:B4:155:GLU:HG2	2:B4:197:HIS:CE1	2.19	0.78
1:B7:100:ASN:HD22	1:B7:103:LYS:HG3	1.47	0.77
2:A4:11:GLN:OE1	2:A4:15:GLN:NE2	2.18	0.77
2:A2:75:VAL:HG11	2:A2:94:SER:HB2	1.67	0.77
1:B5:2:ARG:HE	1:B5:240:LEU:HD22	1.50	0.76
1:B3:5:VAL:HG23	1:B3:62:ARG:HG2	1.65	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:377:MET:SD	1:A1:380:ARG:NH2	2.59	0.76
1:A3:397:TRP:HH2	2:A4:260:VAL:HG23	1.51	0.76
2:B2:91:GLN:HG3	2:B2:121:ARG:HH21	1.51	0.76
1:A1:73:MET:HE1	1:A1:92:PHE:HB2	1.68	0.76
2:A6:71:GLU:OE1	1:A7:247:ASN:ND2	2.19	0.75
1:A1:268:VAL:HG23	1:A1:300:MET:HB2	1.69	0.75
2:B4:11:GLN:OE1	2:B4:15:GLN:NE2	2.20	0.74
5:Y:182:ALA:O	5:Y:186:ARG:HD3	1.86	0.74
1:A7:139:LEU:HD12	1:A7:170:VAL:HG12	1.70	0.74
2:B4:88:HIS:HD2	2:B4:90:GLU:HG3	1.53	0.73
1:A3:139:LEU:HD12	1:A3:170:VAL:HG12	1.70	0.73
2:A6:69:ASP:OD1	2:A6:70:LEU:N	2.22	0.73
1:B1:218:THR:O	2:B2:326:LYS:NZ	2.16	0.73
2:B4:178:SER:HB3	1:B5:347:ASN:HD21	1.52	0.73
2:B6:259:LEU:HD11	2:B6:316:CYS:HB2	1.70	0.73
1:A3:131:GLN:HE21	1:A3:250:LEU:HB2	1.54	0.73
1:B3:99:ASN:ND2	2:B4:254:GLU:OE1	2.22	0.73
1:B7:275:SER:HG	1:B7:278:SER:HG	1.36	0.73
4:X1:216:MET:HE1	5:Y1:167:ARG:HA	1.71	0.73
2:A4:102:ASN:ND2	2:A4:411:GLU:OE1	2.23	0.72
1:B5:107:THR:OG1	1:B5:108:GLU:OE1	2.06	0.72
2:A2:98:ASP:O	2:A2:105:ARG:NH2	2.21	0.72
2:B4:116:ASP:OD1	2:B4:156:ARG:NH1	2.21	0.72
1:B3:2:ARG:HE	1:B3:240:LEU:HD22	1.55	0.72
2:B4:75:VAL:HG11	2:B4:94:SER:HB2	1.72	0.72
2:B4:278:ALA:HA	2:B4:369:ALA:HB2	1.71	0.71
3:C:417:PHE:O	3:C:421:ASP:HB2	1.90	0.71
1:B1:99:ASN:ND2	2:B2:254:GLU:OE1	2.23	0.71
1:B3:52:ASN:OD1	1:B3:62:ARG:NH2	2.24	0.70
1:A3:36:TYR:HB2	1:A3:59:TYR:HE2	1.56	0.70
6:Z:152:GLU:O	6:Z:155:HIS:ND1	2.25	0.70
2:A6:82:THR:HG23	2:A6:83:TYR:CD1	2.25	0.70
1:B1:30:ILE:HD11	1:B1:47:ILE:HD11	1.72	0.70
2:B6:192:HIS:HD2	2:B6:421:ALA:HA	1.57	0.70
1:A1:175:VAL:HG13	2:A2:329:ASN:HD21	1.56	0.70
1:A5:375:GLN:HB2	1:A5:419:VAL:HG23	1.71	0.70
2:B2:288:VAL:HG13	2:B2:319:TYR:HE2	1.57	0.70
1:B3:293:MET:HG3	1:B3:367:PHE:HB2	1.74	0.70
2:A6:11:GLN:OE1	2:A6:15:GLN:NE2	2.24	0.69
1:A7:396:HIS:HA	1:A7:399:THR:HG22	1.74	0.69
2:B6:405:VAL:HG13	2:B6:418:PHE:HE2	1.55	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A4:51:THR:HG21	2:A4:243:ARG:HG2	1.75	0.69
2:A6:172:TYR:CE2	2:A6:203:MET:HG3	2.28	0.68
2:A4:317:LEU:HB3	2:A4:319:TYR:HE1	1.57	0.68
1:B5:175:VAL:HG22	2:B6:329:ASN:ND2	2.07	0.68
6:Z:103:ASN:ND2	6:Z:117:MET:SD	2.66	0.68
1:B1:2:ARG:HE	1:B1:240:LEU:HD22	1.59	0.68
1:B1:68:LEU:HB3	1:B1:96:GLY:HA2	1.75	0.68
2:B2:51:THR:HG21	2:B2:243:ARG:HG2	1.76	0.68
4:X:266:ARG:HH11	5:Y:219:GLU:HG2	1.57	0.68
1:A5:159:TYR:HB3	1:A5:162:ARG:HD3	1.74	0.68
1:B5:52:ASN:OD1	1:B5:62:ARG:NH2	2.26	0.68
2:A4:195:LEU:HD21	2:A4:264:ARG:HE	1.58	0.68
2:B4:259:LEU:HD11	2:B4:316:CYS:HB2	1.75	0.68
1:B5:248:ALA:HA	1:B5:252:LYS:HD2	1.76	0.67
1:B5:135:VAL:HG21	1:B5:152:ILE:HD11	1.76	0.67
1:B1:139:LEU:HD12	1:B1:170:VAL:HG12	1.75	0.67
2:B4:170:THR:HG21	2:B4:194:LEU:HD11	1.75	0.67
1:A5:172:SER:HB2	1:A5:380:ARG:HH12	1.59	0.67
1:A1:11:GLN:HG2	1:A1:72:THR:HG21	1.77	0.67
2:B4:178:SER:HB3	1:B5:347:ASN:ND2	2.09	0.67
1:A1:27:GLU:HA	1:A1:359:LYS:HD2	1.76	0.67
1:A1:113:ILE:HG21	1:A1:150:LEU:HD22	1.77	0.67
2:A2:72:PRO:HG3	1:A3:1:MET:HG2	1.76	0.67
1:B7:330:MET:HB3	1:B7:349:VAL:HG21	1.76	0.67
1:A3:65:LEU:HD12	1:A3:90:PHE:CE1	2.31	0.66
2:A6:176:GLN:NE2	2:A6:207:GLU:OE1	2.28	0.66
2:B6:102:ASN:ND2	2:B6:105:ARG:HG3	2.11	0.66
2:A2:262:TYR:HB2	2:A2:265:ILE:HD12	1.76	0.66
1:A7:9:GLY:HA2	1:A7:66:MET:HG3	1.76	0.66
1:B5:100:ASN:HD22	1:B5:103:LYS:HG3	1.61	0.66
6:Z:154:LEU:HB3	6:Z:158:HIS:HE1	1.60	0.66
2:A2:50:ASN:O	2:A2:64:ARG:NH2	2.28	0.66
2:A4:403:ALA:HB2	1:A5:344:TRP:HZ3	1.60	0.66
2:A4:274:PRO:HG3	2:A4:286:LEU:HD11	1.77	0.66
1:B5:139:LEU:HD12	1:B5:170:VAL:HG12	1.76	0.66
5:Y:205:ALA:O	5:Y:209:MET:HG2	1.96	0.66
1:B1:304:ASP:HB3	1:B1:307:HIS:CD2	2.30	0.66
5:Y1:122:LYS:HE3	5:Y1:122:LYS:HA	1.78	0.66
1:A1:311:LEU:HD11	1:A1:372:THR:HB	1.78	0.66
1:B1:165:LEU:HD21	1:B1:250:LEU:HD11	1.78	0.66
2:B6:75:VAL:HG11	2:B6:94:SER:HB2	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X1:216:MET:O	4:X1:220:VAL:HG23	1.94	0.66
1:A7:45:GLU:HG3	1:A7:46:ARG:HG2	1.78	0.66
1:B3:391:ARG:HH21	2:B4:346:TRP:HE1	1.44	0.66
1:B5:114:ASP:OD1	1:B5:115:SER:N	2.28	0.66
1:B1:49:VAL:HG11	1:B1:241:ARG:HG2	1.77	0.66
1:B5:220:PRO:HD2	2:B6:326:LYS:HD3	1.77	0.66
1:A1:77:ARG:NH1	1:A1:87:PRO:HG3	2.11	0.65
1:A1:107:THR:OG1	1:A1:401:GLU:OE2	2.13	0.65
1:B7:113:ILE:CD1	1:B7:150:LEU:HD11	2.23	0.65
5:Y:179:ARG:O	5:Y:183:LYS:HG3	1.97	0.65
2:A2:415:GLU:OE2	6:Z:168:ARG:NH1	2.29	0.65
2:A6:287:SER:N	2:A6:290:GLU:OE2	2.27	0.65
2:A2:71:GLU:HG3	1:A3:2:ARG:HH12	1.62	0.65
2:B4:5:ILE:HG22	2:B4:64:ARG:HB3	1.78	0.65
2:B6:222:PRO:O	1:B7:322:SER:OG	2.14	0.65
1:A1:215:LEU:HD11	1:A1:228:LEU:HD21	1.79	0.65
1:A3:49:VAL:HG11	1:A3:241:ARG:HG2	1.79	0.65
1:B3:388:MET:HE2	2:B4:348:PRO:HD2	1.79	0.65
1:A1:67:ASP:OD2	1:A1:72:THR:OG1	2.15	0.64
1:B7:135:VAL:HG21	1:B7:152:ILE:HD11	1.77	0.64
2:A6:172:TYR:HE2	2:A6:203:MET:HG3	1.62	0.64
1:A3:268:VAL:HG23	1:A3:300:MET:HB3	1.79	0.64
1:B3:213:ARG:HH12	1:B3:297:LYS:HD2	1.61	0.64
2:A2:27:GLU:OE1	2:A2:243:ARG:NH1	2.27	0.64
2:B4:180:ALA:O	1:B5:347:ASN:ND2	2.30	0.64
2:B6:271:SER:OG	2:B6:301:MET:SD	2.55	0.64
2:A6:56:THR:HA	2:B6:285:GLN:HB2	1.78	0.64
2:A4:76:ASP:OD1	2:A4:79:ARG:NH2	2.29	0.64
2:B2:259:LEU:HD11	2:B2:316:CYS:HB2	1.79	0.64
1:B7:183:TYR:HB3	1:B7:398:TYR:HE2	1.63	0.64
1:A1:36:TYR:HB2	1:A1:59:TYR:HE2	1.60	0.64
1:A1:235:GLY:HA3	1:A1:366:THR:HG21	1.79	0.64
1:A5:373:ALA:O	1:A5:376:GLU:HG3	1.98	0.64
1:B1:282:ARG:NH2	1:B1:292:GLN:OE1	2.31	0.64
1:B5:91:VAL:HG11	1:B5:116:VAL:HG12	1.80	0.64
1:B7:211:CYS:HA	1:B7:215:LEU:HB2	1.78	0.64
4:X:244:MET:HG3	5:Y:199:PHE:HE1	1.62	0.64
3:C:307:MET:HG3	3:C:315:ILE:HG12	1.79	0.64
2:A4:7:ILE:HG13	2:A4:66:ILE:HG13	1.80	0.63
2:A6:120:ASP:OD1	2:A6:121:ARG:N	2.31	0.63
1:B7:167:PHE:CE2	1:B7:233:MET:HG2	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:165:LEU:HD11	1:A1:250:LEU:HD23	1.79	0.63
1:B3:211:CYS:HA	1:B3:215:LEU:HB2	1.78	0.63
2:B4:279:GLU:OE1	2:B4:279:GLU:N	2.31	0.63
1:A7:345:ILE:O	1:A7:348:ASN:ND2	2.30	0.63
2:B2:174:SER:OG	2:B2:177:VAL:O	2.16	0.63
1:B5:99:ASN:ND2	2:B6:254:GLU:OE1	2.32	0.63
1:B3:139:LEU:HD12	1:B3:170:VAL:HG22	1.81	0.63
2:A2:14:ILE:HD11	2:A2:74:VAL:HG13	1.79	0.63
1:A1:374:ILE:HD11	1:A1:422:TYR:CZ	2.35	0.62
1:B1:156:ARG:HD2	1:B1:195:ASN:O	1.99	0.62
3:C:376:ILE:HG23	3:C:431:ILE:HD11	1.81	0.62
5:Y:181:LEU:O	5:Y:185:LYS:HG2	1.98	0.62
6:Z:75:PHE:HE1	6:Z:98:VAL:HG11	1.63	0.62
1:A5:49:VAL:HG11	1:A5:241:ARG:HG2	1.81	0.62
1:A5:173:PRO:HD2	1:A5:380:ARG:NH1	2.14	0.62
1:A1:73:MET:O	1:A1:76:VAL:HG22	2.00	0.62
2:A2:188:VAL:HG13	2:A2:425:LEU:HD12	1.80	0.62
1:A7:204:ASN:ND2	9:A7:502:GDP:O2'	2.33	0.62
1:B3:175:VAL:HG12	2:B4:329:ASN:ND2	2.13	0.62
6:Z:14:ASN:O	6:Z:17:ASN:ND2	2.32	0.62
1:A5:379:LYS:HG2	1:A5:419:VAL:HG21	1.82	0.62
1:A3:64:ILE:HD11	1:A3:123:GLU:HG3	1.82	0.62
6:Z:85:ASP:OD2	6:Z:90:GLU:HB2	2.00	0.62
1:B7:139:LEU:HD12	1:B7:170:VAL:HG12	1.82	0.62
1:B5:253:LEU:HD11	1:B5:316:LEU:HD21	1.81	0.61
1:B1:175:VAL:HG13	2:B2:329:ASN:ND2	2.15	0.61
2:A6:145:THR:OG1	7:A7:501:GTP:O1B	2.19	0.61
2:A6:20:CYS:HB3	2:A6:24:TYR:HE1	1.65	0.61
2:B4:267:PHE:HB2	2:B4:384:ILE:HD12	1.83	0.61
2:A2:383:ALA:O	2:A2:386:GLU:HG2	2.00	0.61
2:B6:189:LEU:HD11	2:B6:418:PHE:HE1	1.66	0.61
1:A3:222:PHE:O	1:A3:226:ASN:ND2	2.33	0.61
1:A5:220:PRO:HD2	2:A6:326:LYS:HD3	1.82	0.61
1:B1:211:CYS:HA	1:B1:215:LEU:HB2	1.83	0.61
1:B5:172:SER:OG	1:B5:380:ARG:NH1	2.34	0.61
1:A1:232:VAL:HG22	1:A1:270:PHE:HB2	1.82	0.61
2:A2:210:TYR:HH	2:A2:224:TYR:HE1	1.48	0.61
1:A7:376:GLU:O	1:A7:380:ARG:HG3	2.00	0.61
2:B2:107:HIS:O	2:B2:112:LYS:NZ	2.34	0.61
1:B1:131:GLN:HE21	1:B1:250:LEU:HB3	1.66	0.61
1:A1:77:ARG:HH12	1:A1:87:PRO:HG3	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:156:ARG:NE	1:A7:195:ASN:O	2.33	0.61
1:A7:200:MET:HE1	1:A7:368:ILE:HD12	1.83	0.61
1:B1:175:VAL:HG13	2:B2:329:ASN:HD21	1.65	0.61
3:C:422:LEU:HD13	3:C:425:LYS:HE2	1.83	0.61
2:B2:319:TYR:HB3	2:B2:323:VAL:HG11	1.81	0.60
1:B5:309:ARG:H	1:B5:372:THR:HG22	1.66	0.60
1:A5:222:PHE:O	1:A5:226:ASN:ND2	2.33	0.60
1:B5:186:THR:HG22	1:B5:411:ALA:HB1	1.84	0.60
1:B1:140:GLY:O	1:B1:184:ASN:ND2	2.34	0.60
2:B2:88:HIS:CE1	2:B2:90:GLU:HG2	2.36	0.60
4:X:254:GLU:O	4:X:257:ARG:HG2	2.02	0.60
1:A3:272:PRO:HD3	1:A3:364:SER:HA	1.82	0.60
1:B3:49:VAL:HG11	1:B3:241:ARG:HG2	1.82	0.60
2:B4:14:ILE:HD11	2:B4:74:VAL:HG13	1.83	0.60
2:B4:172:TYR:CD2	2:B4:203:MET:HG3	2.37	0.60
2:A2:413:MET:HB3	2:A2:417:GLU:OE2	2.02	0.60
2:B2:387:ILE:HG12	2:B2:390:ARG:HH22	1.67	0.60
6:Z:119:ILE:HD12	6:Z:123:ARG:HE	1.65	0.60
6:Z:132:GLN:O	6:Z:151:THR:OG1	2.17	0.60
2:A6:384:ILE:O	2:A6:387:ILE:HG22	2.02	0.60
2:A4:339:ARG:HG2	2:A4:339:ARG:HH11	1.67	0.60
2:A4:417:GLU:HA	2:A4:420:GLU:HG3	1.83	0.60
2:A2:379:SER:OG	2:A2:380:ASN:N	2.34	0.60
2:A4:98:ASP:OD1	2:A4:99:ALA:N	2.34	0.60
1:A7:173:PRO:HB3	1:A7:384:GLN:HE22	1.66	0.60
1:B7:113:ILE:HA	1:B7:116:VAL:HG22	1.84	0.60
5:Y:232:THR:HA	5:Y:235:GLU:HG2	1.83	0.60
1:A1:103:LYS:NZ	1:A1:397:TRP:O	2.34	0.60
2:B4:398:MET:HE2	1:B5:345:ILE:HD12	1.84	0.60
2:A2:224:TYR:O	2:A2:228:ASN:ND2	2.34	0.59
1:B7:282:ARG:NH1	1:B7:288:GLU:OE1	2.35	0.59
5:Y1:145:LYS:HE3	5:Y1:145:LYS:HA	1.83	0.59
1:A1:152:ILE:HG22	1:A1:195:ASN:HB3	1.84	0.59
2:A6:403:ALA:HB2	1:A7:344:TRP:HZ3	1.65	0.59
1:B3:5:VAL:HG12	1:B3:133:PHE:HD1	1.67	0.59
1:A3:128:ASP:OD1	1:A3:129:CYS:N	2.34	0.59
1:B3:257:LEU:HD21	1:B3:314:SER:HB3	1.84	0.59
1:A3:391:ARG:NH2	2:A4:262:TYR:OH	2.35	0.59
2:A6:251:ASP:H	2:A6:254:GLU:HG2	1.67	0.59
1:A3:289:LEU:HD11	1:A3:365:ALA:HB2	1.84	0.59
1:A3:392:LYS:HD2	1:A3:395:LEU:HD22	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:167:LEU:HD13	2:B2:200:VAL:HB	1.85	0.59
1:A1:345:ILE:O	1:A1:348:ASN:ND2	2.35	0.59
2:A4:14:ILE:HD11	2:A4:74:VAL:HG13	1.83	0.59
1:B7:165:LEU:HD23	1:B7:167:PHE:CZ	2.37	0.59
2:A4:31:GLN:HE22	2:A4:37:PRO:HG3	1.68	0.59
2:A4:286:LEU:O	2:A4:373:ARG:NH1	2.35	0.59
3:C:430:LEU:HD21	3:C:473:LEU:HD12	1.84	0.59
2:A2:394:LYS:HB2	1:A3:346:PRO:HG3	1.83	0.59
1:A3:121:ARG:HH11	5:Y1:141:LYS:NZ	2.01	0.59
2:A6:278:ALA:HA	2:A6:369:ALA:HB2	1.84	0.59
2:B2:358:GLN:OE1	2:B2:359:PRO:HD2	2.03	0.59
1:A1:208:TYR:HE2	2:A2:329:ASN:HD22	1.49	0.58
2:A4:222:PRO:HD2	1:A5:324:LYS:HE3	1.83	0.58
1:A7:113:ILE:HG21	1:A7:150:LEU:HD22	1.85	0.58
1:A1:153:SER:OG	1:A1:195:ASN:OD1	2.14	0.58
1:A1:361:LEU:HG	1:A1:363:MET:H	1.68	0.58
2:A2:155:GLU:HG2	2:A2:197:HIS:CD2	2.38	0.58
1:A3:5:VAL:HG12	1:A3:62:ARG:HD3	1.85	0.58
2:A4:120:ASP:OD1	2:A4:123:ARG:NH1	2.34	0.58
1:B1:139:LEU:HD22	1:B1:188:SER:HB3	1.85	0.58
6:Z:143:ASN:OD1	6:Z:144:SER:N	2.37	0.58
2:A6:405:VAL:HG13	2:A6:418:PHE:HE2	1.69	0.58
6:Z:153:PHE:O	6:Z:157:LEU:HD13	2.03	0.58
1:A5:337:ASN:HB3	1:A5:340:TYR:HD2	1.68	0.58
1:B1:61:PRO:HD3	1:B1:84:ILE:HG13	1.86	0.58
6:Z:154:LEU:O	6:Z:158:HIS:ND1	2.36	0.58
2:A2:286:LEU:O	2:A2:373:ARG:NH1	2.35	0.58
1:A5:286:VAL:HG12	1:A5:329:GLN:HG3	1.84	0.58
1:B1:262:ARG:NE	1:B1:421:GLU:OE2	2.36	0.58
2:B2:165:SER:HB3	2:B2:256:GLN:HE21	1.67	0.58
3:C:376:ILE:HG22	3:C:380:LYS:NZ	2.18	0.58
2:A2:288:VAL:HG21	2:A2:323:VAL:HG13	1.86	0.58
1:A3:113:ILE:HD12	1:A3:150:LEU:HD22	1.86	0.58
1:B7:8:GLN:NE2	1:B7:17:GLY:HA3	2.18	0.58
3:C:476:TYR:O	3:C:479:ASN:ND2	2.36	0.58
1:A3:121:ARG:NH2	1:A3:158:GLU:OE2	2.34	0.58
1:B5:256:ASN:ND2	1:B5:350:LYS:HD2	2.16	0.58
1:B7:105:HIS:HA	1:B7:150:LEU:HD23	1.86	0.58
1:A3:374:ILE:HD11	1:A3:422:TYR:CZ	2.39	0.57
1:B1:330:MET:SD	1:B1:349:VAL:HG11	2.44	0.57
1:B7:152:ILE:HG22	1:B7:195:ASN:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:254:ALA:O	1:A1:258:ILE:HG22	2.04	0.57
1:A7:309:ARG:H	1:A7:372:THR:HG22	1.68	0.57
2:B4:129:CYS:SG	2:B4:130:THR:N	2.76	0.57
3:C:360:GLN:O	3:C:378:ASN:ND2	2.37	0.57
2:A2:422:ARG:O	2:A2:422:ARG:NE	2.37	0.57
1:A3:102:ALA:HB2	1:A3:403:MET:HE2	1.85	0.57
2:B2:323:VAL:HG13	2:B2:355:ILE:HG23	1.86	0.57
6:Z:154:LEU:HB3	6:Z:158:HIS:CE1	2.38	0.57
1:A7:253:LEU:HD11	1:A7:316:LEU:HD21	1.87	0.57
1:B1:191:GLN:HG3	1:B1:195:ASN:HD22	1.69	0.57
1:B3:309:ARG:H	1:B3:372:THR:HG22	1.69	0.57
1:B5:178:THR:HG22	2:B6:352:LYS:HZ3	1.68	0.57
1:B7:100:ASN:ND2	1:B7:103:LYS:HG3	2.19	0.57
1:B7:238:CYS:SG	1:B7:318:ARG:NE	2.77	0.57
1:B3:303:ALA:HA	1:B3:376:GLU:OE2	2.05	0.57
1:A3:200:MET:SD	1:A3:268:VAL:HG11	2.43	0.57
1:A3:252:LYS:O	1:A3:256:ASN:ND2	2.37	0.57
2:B4:28:HIS:CE1	2:B4:49:PHE:HA	2.40	0.57
1:B5:100:ASN:ND2	1:B5:103:LYS:HG3	2.19	0.57
1:A1:39:ASP:OD1	1:A1:40:SER:N	2.35	0.57
1:B3:135:VAL:HG21	1:B3:152:ILE:HD11	1.86	0.57
1:B5:31:ASP:OD1	1:B5:35:THR:N	2.38	0.57
1:B7:248:ALA:HA	1:B7:252:LYS:HD2	1.86	0.57
1:A1:52:ASN:OD1	1:A1:62:ARG:NH2	2.38	0.56
1:A1:274:THR:OG1	1:A1:279:GLN:OE1	2.22	0.56
1:A1:376:GLU:HG3	1:A1:380:ARG:HH12	1.70	0.56
2:A4:237:SER:HA	2:A4:320:ARG:HD2	1.87	0.56
2:B4:417:GLU:HA	2:B4:420:GLU:HG2	1.87	0.56
2:B6:172:TYR:CE1	2:B6:203:MET:HG3	2.39	0.56
1:A5:203:ASP:OD1	1:A5:204:ASN:N	2.38	0.56
6:Z:85:ASP:O	6:Z:88:GLY:N	2.38	0.56
2:A4:328:VAL:HG21	2:A4:355:ILE:HD11	1.86	0.56
2:A4:398:MET:HE2	1:A5:346:PRO:HD2	1.86	0.56
1:B5:45:GLU:HG2	1:B5:46:ARG:HG2	1.86	0.56
2:A6:206:ASN:ND2	7:A7:501:GTP:O2'	2.38	0.56
2:B4:288:VAL:HG13	2:B4:319:TYR:HE2	1.69	0.56
2:B4:384:ILE:HD11	2:B4:432:PHE:CZ	2.40	0.56
1:B7:334:GLN:HE22	1:B7:347:ASN:H	1.52	0.56
1:A7:135:VAL:HB	1:A7:166:THR:HG22	1.87	0.56
2:B2:298:PRO:HB3	2:B2:307:PRO:HD2	1.88	0.56
2:A6:60:LYS:HD2	2:B6:282:TYR:CZ	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:376:ILE:HG22	3:C:380:LYS:HZ2	1.71	0.56
1:A3:193:VAL:HG11	1:A3:418:LEU:HD21	1.88	0.56
1:A5:179:VAL:HG23	2:A6:349:THR:O	2.06	0.56
2:A6:381:SER:OG	2:A6:382:THR:N	2.39	0.56
1:B7:183:TYR:HA	1:B7:385:PHE:HE1	1.71	0.56
2:A6:403:ALA:HB2	1:A7:344:TRP:CZ3	2.40	0.56
2:B2:72:PRO:HG2	1:B3:1:MET:SD	2.46	0.56
2:B6:9:ILE:HD13	2:B6:150:GLY:HA2	1.88	0.56
1:B7:36:TYR:O	1:B7:37:HIS:ND1	2.38	0.56
1:B7:394:PHE:HA	1:B7:397:TRP:CZ3	2.41	0.56
2:B2:401:LYS:HD3	1:B3:344:TRP:CG	2.41	0.56
2:B4:346:TRP:CH2	2:B4:435:VAL:HG13	2.41	0.56
1:B5:423:GLN:O	1:B5:426:GLN:HG3	2.05	0.56
1:B7:11:GLN:N	9:B7:502:GDP:O2B	2.35	0.56
2:A2:70:LEU:HD21	2:A2:114:ILE:HG21	1.87	0.55
1:A3:102:ALA:HB2	1:A3:403:MET:CE	2.36	0.55
2:A4:72:PRO:HG3	1:A5:1:MET:HE3	1.88	0.55
1:B1:175:VAL:HG11	1:B1:204:ASN:HB2	1.87	0.55
2:A4:383:ALA:O	2:A4:386:GLU:HG2	2.06	0.55
1:B1:293:MET:HG3	1:B1:367:PHE:HB2	1.88	0.55
2:B2:90:GLU:OE2	2:B2:121:ARG:NH1	2.39	0.55
3:C:324:THR:HG22	3:C:327:ARG:HH22	1.71	0.55
1:A1:218:THR:O	2:A2:326:LYS:NZ	2.39	0.55
1:A5:293:MET:HG3	1:A5:367:PHE:HB2	1.88	0.55
2:A6:9:ILE:HG22	2:A6:68:LEU:HD11	1.88	0.55
1:B5:209:ASP:OD2	1:B5:213:ARG:NH1	2.34	0.55
4:X1:251:ALA:O	4:X1:255:LEU:HG	2.06	0.55
1:A5:161:ASP:OD1	1:A5:162:ARG:HD2	2.06	0.55
1:A5:375:GLN:NE2	1:A5:423:GLN:OE1	2.30	0.55
1:A5:401:GLU:OE1	1:A5:401:GLU:N	2.39	0.55
2:A2:403:ALA:HB2	1:A3:344:TRP:HZ3	1.70	0.55
1:A3:3:GLU:CD	1:A3:127:CYS:HB2	2.26	0.55
2:B6:167:LEU:HD13	2:B6:200:VAL:HB	1.87	0.55
1:A1:83:GLN:O	1:B1:281:TYR:OH	2.16	0.55
1:A1:164:MET:HB3	1:A1:197:ASP:HB2	1.88	0.55
2:A2:415:GLU:CD	6:Z:168:ARG:HH12	2.10	0.55
1:B3:114:ASP:OD1	1:B3:115:SER:N	2.40	0.55
1:B5:101:TRP:HE1	1:B5:145:SER:HG	1.55	0.55
1:B5:211:CYS:HA	1:B5:215:LEU:HB2	1.86	0.55
1:A7:285:THR:O	1:A7:289:LEU:HD12	2.06	0.55
1:B3:226:ASN:OD1	9:B3:502:GDP:N1	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:66:ILE:HG13	2:B4:121:ARG:HH21	1.70	0.55
1:A1:102:ALA:HB2	1:A1:403:MET:HE3	1.87	0.55
1:A1:330:MET:HE2	1:A1:349:VAL:HG21	1.88	0.55
1:A3:3:GLU:OE2	1:A3:127:CYS:HB2	2.07	0.55
2:A4:7:ILE:HD13	2:A4:153:LEU:HD21	1.88	0.55
1:B1:3:GLU:HG3	1:B1:127:CYS:HB2	1.89	0.55
5:Y1:188:MET:O	5:Y1:192:ILE:HG12	2.07	0.55
1:A1:139:LEU:HD12	1:A1:170:VAL:HG22	1.89	0.55
1:A5:27:GLU:HA	1:A5:359:LYS:HE3	1.89	0.55
2:B2:124:LYS:HA	2:B2:127:ASP:HB2	1.88	0.54
2:B2:265:ILE:HG22	2:B2:380:ASN:HD21	1.72	0.54
1:B5:203:ASP:OD1	1:B5:204:ASN:N	2.40	0.54
2:A6:223:THR:HG23	2:A6:225:THR:H	1.72	0.54
1:B1:309:ARG:H	1:B1:372:THR:HG22	1.71	0.54
1:B5:173:PRO:HB3	1:B5:384:GLN:NE2	2.17	0.54
2:A2:317:LEU:HB3	2:A2:319:TYR:HE1	1.71	0.54
1:A7:293:MET:SD	1:A7:367:PHE:HB2	2.48	0.54
1:A1:382:SER:OG	1:A1:415:MET:HG2	2.07	0.54
2:A4:221:ARG:NH1	1:A5:325:GLU:OE2	2.39	0.54
1:A5:289:LEU:HD23	1:A5:365:ALA:HB2	1.89	0.54
1:A7:135:VAL:HG21	1:A7:152:ILE:HD11	1.89	0.54
1:B3:7:ILE:HG21	1:B3:151:LEU:HD21	1.89	0.54
2:B4:277:SER:OG	2:B4:278:ALA:N	2.39	0.54
1:A1:215:LEU:HB3	1:A1:217:LEU:CD1	2.34	0.54
2:A2:116:ASP:OD1	2:A2:117:LEU:N	2.37	0.54
2:A4:174:SER:HB3	2:A4:177:VAL:O	2.07	0.54
1:B7:5:VAL:HG23	1:B7:62:ARG:HG2	1.87	0.54
4:X1:248:LYS:HZ3	5:Y1:201:ALA:C	2.10	0.54
4:X1:125:ILE:HD13	5:Y1:72:LEU:HD23	1.89	0.54
1:A5:317:PHE:HB3	1:A5:321:MET:SD	2.48	0.54
1:B7:43:GLN:O	1:B7:47:ILE:HG23	2.08	0.54
1:A3:11:GLN:N	9:A3:502:GDP:O2B	2.35	0.54
1:A3:262:ARG:NH1	1:A3:421:GLU:OE1	2.39	0.54
2:A6:14:ILE:HD11	2:A6:74:VAL:HG22	1.89	0.54
1:A7:189:VAL:HA	1:A7:192:LEU:HG	1.89	0.54
1:A7:404:ASP:HB2	1:A7:406:MET:SD	2.47	0.54
2:B2:91:GLN:CG	2:B2:121:ARG:HH21	2.17	0.54
2:B4:11:GLN:NE2	1:B5:247:ASN:OD1	2.40	0.54
1:B1:177:ASP:N	1:B1:181:GLU:OE2	2.36	0.54
1:B3:128:ASP:OD1	1:B3:129:CYS:N	2.41	0.54
2:B6:9:ILE:HG12	2:B6:68:LEU:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:277:ARG:O	4:X:280:VAL:N	2.41	0.54
4:X1:160:THR:HG22	5:Y1:108:LEU:HD13	1.89	0.54
1:A3:373:ALA:O	1:A3:376:GLU:HG2	2.07	0.54
2:A2:206:ASN:O	2:A2:210:TYR:HD2	1.91	0.53
2:A4:407:TRP:CG	1:A5:255:VAL:HG23	2.44	0.53
2:B4:102:ASN:HD21	2:B4:411:GLU:HG3	1.72	0.53
1:A1:258:ILE:HD12	1:A1:264:HIS:HB3	1.91	0.53
2:A2:145:THR:OG1	7:A3:501:GTP:O1B	2.27	0.53
1:A3:215:LEU:HB3	1:A3:217:LEU:CD1	2.33	0.53
2:A4:318:MET:HB2	2:A4:376:CYS:HB3	1.90	0.53
1:B5:144:GLY:N	9:B5:502:GDP:O1B	2.34	0.53
1:B7:52:ASN:OD1	1:B7:62:ARG:NH2	2.41	0.53
1:B7:173:PRO:HB3	1:B7:384:GLN:OE1	2.08	0.53
4:X1:256:ALA:O	4:X1:261:ARG:NE	2.38	0.53
2:B4:298:PRO:HB3	2:B4:307:PRO:HD2	1.89	0.53
1:B5:39:ASP:OD1	1:B5:40:SER:N	2.42	0.53
1:B5:69:GLU:HG2	2:B6:2:ARG:HH22	1.73	0.53
2:B6:408:TYR:HD2	2:B6:418:PHE:HZ	1.56	0.53
1:B7:373:ALA:O	1:B7:376:GLU:HG2	2.08	0.53
1:A3:8:GLN:O	1:A3:66:MET:HG3	2.09	0.53
2:B6:203:MET:HE3	2:B6:267:PHE:HB3	1.91	0.53
2:B6:417:GLU:HA	2:B6:420:GLU:HG2	1.90	0.53
2:B2:264:ARG:NH1	2:B2:431:ASP:OD2	2.42	0.53
2:B4:66:ILE:CG1	2:B4:121:ARG:HH21	2.22	0.53
1:A1:35:THR:HA	1:A1:57:GLY:O	2.07	0.53
1:A5:2:ARG:HE	1:A5:240:LEU:HD22	1.74	0.53
2:B6:51:THR:HG21	2:B6:243:ARG:HG2	1.91	0.53
2:A2:381:SER:OG	2:A2:382:THR:N	2.42	0.53
1:A3:397:TRP:CH2	2:A4:260:VAL:HG23	2.37	0.53
1:A5:7:ILE:HD13	1:A5:151:LEU:HD21	1.91	0.53
1:A5:36:TYR:HB2	1:A5:59:TYR:HE2	1.74	0.53
2:B4:91:GLN:HA	2:B4:121:ARG:HH22	1.73	0.53
1:A1:217:LEU:HD21	1:A1:224:ASP:OD2	2.09	0.53
1:A1:232:VAL:O	1:A1:236:ILE:HD12	2.07	0.53
1:B5:117:LEU:HA	1:B5:120:VAL:HG12	1.90	0.53
5:Y1:183:LYS:O	5:Y1:186:ARG:HG3	2.08	0.53
2:A2:119:LEU:HD21	2:A2:156:ARG:HB3	1.91	0.53
1:A5:345:ILE:O	1:A5:348:ASN:ND2	2.42	0.53
1:B3:289:LEU:HD11	1:B3:363:MET:HG2	1.91	0.53
2:B4:221:ARG:HG2	1:B5:322:SER:HB3	1.90	0.53
2:B4:317:LEU:HB3	2:B4:319:TYR:HE1	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:407:TRP:O	2:B6:411:GLU:HG2	2.09	0.53
1:A1:314:SER:HB3	1:A1:368:ILE:HG23	1.92	0.53
1:A3:177:ASP:O	2:A4:352:LYS:HA	2.08	0.53
1:A3:210:ILE:O	1:A3:214:THR:OG1	2.24	0.53
2:A6:291:ILE:HD12	2:A6:375:VAL:HG13	1.91	0.53
1:A7:5:VAL:HG23	1:A7:62:ARG:HG2	1.91	0.53
2:B2:317:LEU:HB3	2:B2:319:TYR:HE1	1.74	0.53
1:B7:8:GLN:HB2	1:B7:65:LEU:HA	1.91	0.53
6:Z:33:LYS:HB3	6:Z:69:CYS:SG	2.49	0.53
1:A5:274:THR:HG21	1:A5:282:ARG:NE	2.24	0.52
1:B3:309:ARG:H	1:B3:372:THR:CG2	2.22	0.52
2:B4:431:ASP:O	2:B4:434:GLU:HG2	2.09	0.52
5:Y:199:PHE:O	5:Y:202:ARG:HG3	2.10	0.52
1:A1:114:ASP:OD1	1:A1:114:ASP:N	2.39	0.52
2:A4:183:GLU:HA	2:A4:186:ASN:HD22	1.72	0.52
2:A2:69:ASP:OD1	2:A2:70:LEU:N	2.42	0.52
2:A4:139:ASN:OD1	2:A4:170:THR:HG22	2.09	0.52
2:A4:306:ASP:HB3	2:A4:309:HIS:ND1	2.24	0.52
1:A7:186:THR:HG23	1:A7:187:LEU:HD12	1.90	0.52
1:B1:198:GLU:HA	1:B1:264:HIS:HB2	1.90	0.52
2:B6:102:ASN:HD22	2:B6:105:ARG:HG3	1.73	0.52
2:A2:387:ILE:HG12	2:A2:390:ARG:HH22	1.74	0.52
1:B1:417:ASP:O	1:B1:421:GLU:HG2	2.10	0.52
2:B2:223:THR:HG23	2:B2:225:THR:H	1.75	0.52
2:B4:319:TYR:HB3	2:B4:323:VAL:HG21	1.90	0.52
1:B5:125:GLU:OE1	1:B5:159:TYR:OH	2.19	0.52
2:A2:93:ILE:HD12	2:A2:117:LEU:HD21	1.90	0.52
1:A5:77:ARG:HE	1:A5:90:PHE:HE2	1.57	0.52
2:A6:317:LEU:HB3	2:A6:319:TYR:HE1	1.75	0.52
1:B5:102:ALA:HB2	1:B5:403:MET:HE3	1.92	0.52
2:B6:222:PRO:HD2	1:B7:324:LYS:HE3	1.92	0.52
4:X:263:GLU:O	4:X:267:VAL:HG23	2.09	0.52
2:A6:102:ASN:OD1	1:A7:255:VAL:HG11	2.10	0.52
1:B3:222:PHE:HE2	2:B4:248:LEU:HD11	1.74	0.52
1:B7:2:ARG:HE	1:B7:240:LEU:HD22	1.74	0.52
3:C:361:ILE:HA	3:C:378:ASN:HD22	1.75	0.52
2:A6:326:LYS:HG3	2:A6:327:ASP:N	2.25	0.52
1:B1:328:GLU:HA	1:B1:331:LEU:HG	1.91	0.52
1:A3:5:VAL:HG22	1:A3:133:PHE:HD1	1.75	0.52
2:B2:402:ARG:NH2	2:B2:415:GLU:OE2	2.42	0.52
1:B3:326:VAL:O	1:B3:330:MET:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:99:ALA:O	2:B4:105:ARG:HD3	2.09	0.52
2:B6:53:PHE:HB3	2:B6:61:HIS:HB3	1.91	0.52
2:A2:88:HIS:CE1	2:A2:90:GLU:HB2	2.45	0.52
2:A4:266:HIS:O	2:A4:266:HIS:ND1	2.43	0.52
1:A7:114:ASP:OD1	1:A7:114:ASP:N	2.43	0.52
1:B3:124:ALA:HB1	1:B3:130:LEU:HD11	1.91	0.52
1:A3:191:GLN:HG3	1:A3:195:ASN:ND2	2.24	0.52
1:A7:169:VAL:HG23	1:A7:203:ASP:HA	1.91	0.52
1:B3:238:CYS:SG	1:B3:318:ARG:NE	2.82	0.52
2:B4:172:TYR:CE2	2:B4:203:MET:HG3	2.44	0.52
2:B4:266:HIS:O	2:B4:266:HIS:ND1	2.43	0.52
1:B1:31:ASP:OD1	1:B1:35:THR:N	2.28	0.51
1:B7:334:GLN:HE22	1:B7:347:ASN:N	2.08	0.51
1:A1:7:ILE:HD13	1:A1:64:ILE:HB	1.92	0.51
2:A2:102:ASN:HB3	2:A2:105:ARG:HB2	1.92	0.51
1:A3:133:PHE:HZ	1:A3:159:TYR:HD2	1.57	0.51
1:A7:236:ILE:HD11	1:A7:368:ILE:HD11	1.91	0.51
1:A7:319:GLY:N	1:A7:354:CYS:O	2.37	0.51
2:B6:102:ASN:HD21	2:B6:411:GLU:HG3	1.74	0.51
3:C:482:ASP:O	3:C:486:LEU:HD13	2.11	0.51
1:A1:8:GLN:CD	1:A1:17:GLY:HA3	2.30	0.51
2:A4:105:ARG:HB2	2:A4:411:GLU:OE1	2.09	0.51
1:A7:334:GLN:OE1	1:A7:348:ASN:N	2.43	0.51
2:B2:11:GLN:NE2	2:B2:15:GLN:OE1	2.44	0.51
2:B4:241:SER:OG	2:B4:250:VAL:O	2.20	0.51
1:A3:72:THR:O	1:A3:76:VAL:HG23	2.09	0.51
2:A4:384:ILE:HD11	2:A4:432:PHE:CE1	2.45	0.51
2:A6:240:ALA:O	2:A6:356:ASN:ND2	2.43	0.51
1:B1:153:SER:O	1:B1:157:GLU:HG2	2.10	0.51
2:B2:407:TRP:CG	1:B3:255:VAL:HG23	2.46	0.51
1:B5:49:VAL:HG11	1:B5:241:ARG:HG2	1.91	0.51
2:B6:317:LEU:HB3	2:B6:319:TYR:HE1	1.75	0.51
1:A1:272:PRO:HD3	1:A1:364:SER:HA	1.92	0.51
2:A2:402:ARG:HH11	6:Z:168:ARG:NH2	2.03	0.51
2:A6:76:ASP:OD1	2:A6:79:ARG:NH2	2.44	0.51
6:Z:82:CYS:HA	6:Z:85:ASP:HB2	1.93	0.51
1:A7:4:ILE:HB	1:A7:50:TYR:HE1	1.74	0.51
1:B3:121:ARG:NH1	1:B3:158:GLU:OE2	2.44	0.51
1:B5:66:MET:SD	1:B5:116:VAL:HG11	2.51	0.51
1:B7:292:GLN:HG2	1:B7:298:ASN:ND2	2.25	0.51
3:C:346:PHE:HA	3:C:349:ILE:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y1:79:GLU:O	5:Y1:82:MET:HG3	2.10	0.51
2:A2:224:TYR:CE2	1:A3:246:LEU:HD11	2.45	0.51
2:B2:15:GLN:NE2	7:B2:501:GTP:O6	2.44	0.51
1:B5:212:PHE:HZ	2:B6:326:LYS:HG3	1.76	0.51
4:X:240:HIS:O	4:X:243:GLU:HG3	2.11	0.51
1:A3:8:GLN:CD	1:A3:17:GLY:HA3	2.32	0.51
1:A3:121:ARG:HH11	5:Y1:141:LYS:HZ1	1.58	0.51
2:B4:383:ALA:O	2:B4:386:GLU:HG2	2.11	0.51
1:B5:345:ILE:HG23	1:B5:348:ASN:OD1	2.11	0.51
4:X1:191:GLU:O	4:X1:194:GLU:HG3	2.11	0.51
2:A2:339:ARG:NH1	2:A2:339:ARG:HB2	2.26	0.51
1:B3:388:MET:HE1	2:B4:347:CYS:HA	1.93	0.51
1:A7:3:GLU:OE1	1:A7:127:CYS:HB2	2.11	0.51
1:A7:272:PRO:HD3	1:A7:364:SER:HA	1.93	0.51
1:B1:121:ARG:NH2	1:B1:158:GLU:OE2	2.43	0.51
1:B1:236:ILE:HG23	1:B1:237:THR:HG23	1.93	0.51
3:C:487:GLU:O	3:C:490:VAL:HG12	2.11	0.51
1:A1:65:LEU:HD12	1:A1:90:PHE:CE1	2.45	0.50
1:A3:2:ARG:HB3	1:A3:131:GLN:HB2	1.92	0.50
1:A3:317:PHE:HE2	1:A3:326:VAL:HG13	1.76	0.50
2:B2:66:ILE:O	2:B2:66:ILE:HG13	2.11	0.50
1:B3:27:GLU:OE1	1:B3:241:ARG:NH1	2.26	0.50
1:B5:177:ASP:O	2:B6:352:LYS:HA	2.10	0.50
4:X1:178:ILE:HD12	5:Y1:131:ARG:HG2	1.93	0.50
6:Z:104:ASP:O	6:Z:105:LYS:HD3	2.11	0.50
2:A2:151:SER:O	2:A2:155:GLU:HG3	2.11	0.50
1:A3:409:THR:O	1:A3:412:GLU:HG3	2.11	0.50
2:A4:274:PRO:HB2	2:A4:276:ILE:HG23	1.93	0.50
2:A6:151:SER:O	2:A6:155:GLU:HG3	2.12	0.50
1:B1:67:ASP:OD2	1:B1:72:THR:OG1	2.28	0.50
1:B3:186:THR:HG23	1:B3:415:MET:HG3	1.91	0.50
2:B4:167:LEU:HD22	2:B4:200:VAL:HB	1.94	0.50
2:A4:326:LYS:HG3	2:A4:327:ASP:N	2.26	0.50
1:A7:11:GLN:HG3	1:A7:15:GLN:HE22	1.77	0.50
2:B2:381:SER:OG	2:B2:382:THR:N	2.43	0.50
1:B5:342:VAL:HG12	1:B5:345:ILE:HG22	1.94	0.50
1:B7:199:CYS:HB3	1:B7:265:PHE:HD1	1.76	0.50
4:X1:135:LYS:NZ	5:Y1:80:GLY:O	2.35	0.50
2:A2:398:MET:SD	1:A3:346:PRO:HD2	2.52	0.50
2:A4:200:VAL:HG13	2:A4:268:MET:CE	2.42	0.50
4:X1:220:VAL:HG13	5:Y1:174:GLN:OE1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:91:VAL:HG11	1:A1:116:VAL:HB	1.93	0.50
2:A2:286:LEU:HD12	2:A2:371:VAL:HG23	1.93	0.50
1:A3:156:ARG:NH1	1:A3:195:ASN:O	2.44	0.50
1:A5:118:ASP:OD1	1:A5:122:LYS:NZ	2.44	0.50
2:A6:362:VAL:HG12	2:A6:368:LEU:HD12	1.93	0.50
2:B2:327:ASP:N	2:B2:327:ASP:OD1	2.45	0.50
2:B6:129:CYS:SG	2:B6:132:LEU:HB2	2.52	0.50
1:B1:378:PHE:HB3	1:B1:415:MET:HE3	1.94	0.50
2:B2:267:PHE:HB2	2:B2:384:ILE:HD12	1.94	0.50
6:Z:157:LEU:O	6:Z:161:GLN:HG2	2.12	0.50
1:A1:313:ALA:O	1:A1:349:VAL:HA	2.12	0.50
1:A5:246:LEU:HD22	1:A5:352:SER:HA	1.94	0.50
1:A5:337:ASN:HB3	1:A5:340:TYR:CD2	2.47	0.50
1:A7:2:ARG:HH21	1:A7:240:LEU:HA	1.77	0.50
1:B1:285:THR:HG23	1:B1:288:GLU:H	1.76	0.50
1:B3:212:PHE:CZ	2:B4:326:LYS:HE2	2.47	0.50
2:B4:251:ASP:H	2:B4:254:GLU:HG3	1.77	0.50
2:B6:116:ASP:OD1	2:B6:117:LEU:N	2.44	0.50
3:C:379:MET:HB2	3:C:431:ILE:HD13	1.94	0.50
6:Z:31:ASP:OD1	6:Z:32:LYS:N	2.43	0.50
6:Z:62:VAL:HG11	6:Z:94:LEU:HB3	1.93	0.50
1:A1:26:ASP:OD1	1:A1:359:LYS:NZ	2.44	0.50
1:A3:67:ASP:OD2	1:A3:72:THR:OG1	2.30	0.50
2:A6:21:TRP:HZ2	2:A6:65:CYS:HB3	1.77	0.50
2:A6:137:VAL:HG22	2:A6:168:GLY:HA2	1.94	0.50
1:A7:215:LEU:HB3	1:A7:217:LEU:HG	1.93	0.50
1:B1:36:TYR:CZ	1:B1:44:LEU:HD21	2.47	0.50
2:B2:69:ASP:OD1	2:B2:70:LEU:N	2.44	0.50
1:B3:39:ASP:OD1	1:B3:39:ASP:N	2.45	0.50
2:B4:98:ASP:OD1	2:B4:99:ALA:N	2.44	0.50
2:A6:21:TRP:CZ2	2:A6:65:CYS:HB3	2.47	0.50
2:A6:60:LYS:HD2	2:B6:282:TYR:CE2	2.47	0.50
5:Y1:82:MET:SD	5:Y1:83:LEU:HD12	2.52	0.50
1:A1:21:TRP:HA	1:A1:24:VAL:HG22	1.93	0.49
1:A7:27:GLU:OE2	1:A7:318:ARG:NH2	2.44	0.49
1:A7:211:CYS:HA	1:A7:215:LEU:HB2	1.94	0.49
1:B3:107:THR:OG1	1:B3:108:GLU:OE1	2.25	0.49
1:B5:113:ILE:HA	1:B5:116:VAL:HG22	1.94	0.49
2:B6:183:GLU:HG3	2:B6:184:PRO:HD3	1.94	0.49
3:C:471:TYR:CE2	3:C:481:PHE:HB3	2.47	0.49
2:A6:9:ILE:HG13	2:A6:139:ASN:HB3	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:31:ASP:OD2	1:B5:35:THR:OG1	2.30	0.49
2:B6:425:LEU:O	2:B6:429:GLU:HG2	2.12	0.49
1:B7:114:ASP:OD1	1:B7:114:ASP:N	2.45	0.49
3:C:422:LEU:HD12	3:C:476:TYR:HB2	1.94	0.49
1:A3:337:ASN:HB3	1:A3:340:TYR:HD2	1.77	0.49
2:A6:139:ASN:OD1	2:A6:170:THR:HG22	2.12	0.49
2:A6:183:GLU:HG2	2:A6:184:PRO:HD3	1.94	0.49
1:B1:260:PHE:HB2	1:B1:263:LEU:HD23	1.95	0.49
1:B3:3:GLU:HG3	1:B3:127:CYS:HB2	1.94	0.49
4:X:248:LYS:O	4:X:252:GLU:OE1	2.30	0.49
1:A5:173:PRO:O	1:A5:176:SER:OG	2.29	0.49
1:B1:271:THR:OG1	1:B1:365:ALA:HB3	2.13	0.49
1:B7:270:PHE:HD2	1:B7:273:LEU:HD21	1.78	0.49
5:Y:234:ILE:O	5:Y:238:LYS:HG2	2.12	0.49
5:Y1:96:MET:O	5:Y1:99:GLN:HG2	2.12	0.49
6:Z:27:ASP:HA	6:Z:38:GLU:OE1	2.13	0.49
1:A1:103:LYS:HA	1:A1:107:THR:HB	1.95	0.49
1:A1:334:GLN:HA	1:A1:341:PHE:CE2	2.47	0.49
2:A4:223:THR:HG23	2:A4:225:THR:H	1.77	0.49
2:A4:276:ILE:HD11	2:A4:371:VAL:HG22	1.95	0.49
2:A4:371:VAL:HG12	2:A4:373:ARG:H	1.78	0.49
1:B3:179:VAL:H	2:B4:258:ASN:ND2	2.10	0.49
1:A1:137:HIS:NE2	1:A1:166:THR:OG1	2.45	0.49
1:A3:203:ASP:OD1	1:A3:301:CYS:HA	2.13	0.49
1:A5:257:LEU:HD21	1:A5:314:SER:HB2	1.93	0.49
2:B2:129:CYS:SG	2:B2:130:THR:N	2.85	0.49
1:A1:167:PHE:CZ	1:A1:233:MET:HG3	2.48	0.49
1:A1:257:LEU:HB3	1:A1:266:PHE:HE2	1.77	0.49
1:A3:189:VAL:HG11	1:A3:378:PHE:HE1	1.76	0.49
1:A3:385:PHE:HZ	1:A3:408:PHE:HD1	1.59	0.49
1:B3:208:TYR:CD1	2:B4:326:LYS:HD3	2.48	0.49
2:B4:21:TRP:CZ2	2:B4:65:CYS:HB3	2.48	0.49
1:A1:200:MET:SD	1:A1:268:VAL:HG11	2.52	0.49
2:A2:7:ILE:HG13	2:A2:66:ILE:HG13	1.94	0.49
2:A4:384:ILE:O	2:A4:387:ILE:HG22	2.13	0.49
2:A6:20:CYS:O	2:A6:24:TYR:HD1	1.95	0.49
2:A6:185:TYR:HA	2:A6:395:PHE:CE1	2.48	0.49
1:B1:144:GLY:N	9:B1:501:GDP:O1B	2.38	0.49
1:B5:8:GLN:OE1	1:B5:17:GLY:HA3	2.13	0.49
1:B5:252:LYS:HG2	1:B5:350:LYS:HE2	1.93	0.49
2:B6:178:SER:OG	2:B6:183:GLU:OE2	2.22	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B7:100:ASN:HD21	1:B7:102:ALA:HB3	1.78	0.49
5:Y1:78:ASP:OD1	5:Y1:79:GLU:N	2.46	0.49
2:A2:132:LEU:HD23	2:A2:164:LYS:HD3	1.95	0.49
1:A3:211:CYS:HA	1:A3:215:LEU:HB2	1.94	0.49
2:A4:251:ASP:H	2:A4:254:GLU:HG3	1.78	0.49
2:B2:272:TYR:HB3	2:B2:275:ILE:HD11	1.95	0.49
2:B6:119:LEU:HA	2:B6:122:ILE:HG22	1.95	0.49
2:B6:172:TYR:CD1	2:B6:203:MET:HG3	2.48	0.49
2:B6:323:VAL:HG23	2:B6:355:ILE:HG23	1.94	0.49
2:A2:11:GLN:HG3	2:A2:74:VAL:HG21	1.93	0.49
1:A3:313:ALA:HB3	1:A3:349:VAL:HG22	1.95	0.49
1:B5:100:ASN:HD22	1:B5:103:LYS:H	1.59	0.49
2:B6:174:SER:HB3	2:B6:177:VAL:O	2.13	0.49
5:Y:237:ASP:O	5:Y:240:GLU:HG3	2.13	0.49
1:A3:22:GLU:HG3	1:A3:81:TYR:CD2	2.48	0.48
1:A3:421:GLU:O	1:A3:424:GLN:HG2	2.13	0.48
1:A5:7:ILE:HB	1:A5:135:VAL:HG22	1.94	0.48
1:A5:237:THR:HG22	1:A5:237:THR:O	2.13	0.48
2:A6:123:ARG:NH1	2:A6:161:TYR:OH	2.46	0.48
1:A7:49:VAL:HG11	1:A7:241:ARG:HG2	1.94	0.48
2:B4:91:GLN:HA	2:B4:121:ARG:NH2	2.27	0.48
2:B4:91:GLN:HG2	2:B4:121:ARG:HH12	1.78	0.48
1:B5:330:MET:SD	1:B5:349:VAL:HG11	2.53	0.48
2:B6:298:PRO:HB3	2:B6:307:PRO:HD2	1.95	0.48
1:B7:8:GLN:O	1:B7:66:MET:HG3	2.12	0.48
2:B4:384:ILE:O	2:B4:387:ILE:HG12	2.12	0.48
2:B4:407:TRP:CG	1:B5:255:VAL:HG23	2.48	0.48
1:B5:141:GLY:O	1:B5:145:SER:HB3	2.13	0.48
1:A5:67:ASP:OD1	1:A5:68:LEU:N	2.43	0.48
1:A5:272:PRO:HD3	1:A5:364:SER:HA	1.94	0.48
1:A7:70:PRO:HD3	1:A7:92:PHE:HZ	1.77	0.48
1:B1:334:GLN:HA	1:B1:341:PHE:CE2	2.48	0.48
2:B2:312:TYR:HD1	2:B2:381:SER:HB2	1.78	0.48
2:B4:287:SER:OG	2:B4:288:VAL:N	2.45	0.48
2:B6:403:ALA:HB2	1:B7:344:TRP:HZ3	1.79	0.48
4:X1:193:VAL:O	4:X1:196:GLU:HG2	2.12	0.48
6:Z:49:LYS:H	6:Z:146:LYS:NZ	2.11	0.48
2:A6:121:ARG:NH1	2:A6:124:LYS:HE2	2.29	0.48
2:A6:234:VAL:HG13	2:A6:376:CYS:SG	2.52	0.48
1:B7:49:VAL:HG11	1:B7:241:ARG:HG2	1.94	0.48
2:A2:88:HIS:CD2	2:A2:89:PRO:HD2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:3:GLU:OE1	1:A5:127:CYS:HB2	2.14	0.48
2:A6:287:SER:OG	2:A6:288:VAL:N	2.47	0.48
2:B2:170:THR:HG21	2:B2:194:LEU:HD21	1.96	0.48
2:B4:388:PHE:HB2	2:B4:429:GLU:OE2	2.14	0.48
1:B7:139:LEU:HD22	1:B7:188:SER:HB3	1.95	0.48
1:A1:54:ALA:HB3	1:A1:58:ARG:HB3	1.96	0.48
2:A2:137:VAL:HG22	2:A2:168:GLY:HA2	1.95	0.48
2:A4:16:VAL:HA	2:A4:228:ASN:HD22	1.78	0.48
1:A7:36:TYR:CZ	1:A7:44:LEU:HD21	2.48	0.48
1:B5:152:ILE:HG22	1:B5:195:ASN:HB3	1.94	0.48
1:A5:112:LEU:O	1:A5:115:SER:OG	2.27	0.48
2:A6:70:LEU:HG	2:A6:145:THR:HG22	1.94	0.48
2:A6:141:VAL:HG22	2:A6:172:TYR:HA	1.95	0.48
1:B5:153:SER:O	1:B5:157:GLU:HG2	2.14	0.48
6:Z:4:ALA:O	6:Z:7:ARG:HG2	2.14	0.48
2:A2:317:LEU:HB3	2:A2:319:TYR:CE1	2.48	0.48
1:B1:220:PRO:HD2	2:B2:326:LYS:HE2	1.96	0.48
2:B2:72:PRO:HG3	2:B2:95:GLY:O	2.13	0.48
1:B5:268:VAL:HG23	1:B5:300:MET:HB2	1.95	0.48
1:A1:178:THR:OG1	1:A1:181:GLU:HG3	2.14	0.48
1:A1:362:LYS:HE3	1:A1:362:LYS:HB2	1.62	0.48
1:A5:8:GLN:CD	1:A5:17:GLY:HA3	2.34	0.48
1:A7:309:ARG:H	1:A7:372:THR:CG2	2.27	0.48
2:B2:246:GLY:HA2	2:B2:357:TYR:CD2	2.49	0.48
1:B3:317:PHE:HB3	1:B3:321:MET:SD	2.53	0.48
2:A2:296:PHE:HZ	2:A2:351:PHE:HE1	1.60	0.48
2:A4:9:ILE:HD11	2:A4:139:ASN:HB3	1.96	0.48
2:B2:72:PRO:HD2	1:B3:2:ARG:NH1	2.29	0.48
3:C:465:ASP:HA	3:C:468:ARG:HH21	1.78	0.48
5:Y:196:ASN:O	5:Y:200:GLU:HG2	2.13	0.48
1:B1:259:PRO:HG3	1:B1:311:LEU:HD23	1.95	0.47
2:B2:250:VAL:HG23	2:B2:254:GLU:HG3	1.95	0.47
1:B5:67:ASP:OD1	1:B5:67:ASP:N	2.48	0.47
1:B5:102:ALA:HB2	1:B5:403:MET:CE	2.45	0.47
1:B5:134:GLN:HE21	1:B5:167:PHE:HE2	1.62	0.47
1:B7:7:ILE:HG12	1:B7:64:ILE:HD11	1.95	0.47
1:B7:8:GLN:OE1	1:B7:14:ASN:HA	2.14	0.47
1:B7:183:TYR:HA	1:B7:385:PHE:CE1	2.49	0.47
4:X:226:LEU:HA	4:X:229:ASP:OD2	2.14	0.47
4:X1:230:SER:HB3	5:Y1:184:LEU:HD22	1.96	0.47
4:X1:255:LEU:HD11	5:Y1:205:ALA:HB1	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:414:ASN:O	1:A3:418:LEU:HD23	2.14	0.47
2:A6:361:THR:HA	2:A6:370:LYS:NZ	2.30	0.47
2:B2:377:MET:SD	2:B2:379:SER:HB3	2.54	0.47
2:B6:250:VAL:HG11	2:B6:352:LYS:HE3	1.96	0.47
3:C:312:VAL:HG13	3:C:381:VAL:HG11	1.95	0.47
5:Y:232:THR:O	5:Y:236:GLU:HG2	2.13	0.47
1:A3:317:PHE:HB3	1:A3:321:MET:SD	2.54	0.47
1:A5:2:ARG:HH21	1:A5:240:LEU:HA	1.78	0.47
1:A5:139:LEU:HD12	1:A5:170:VAL:HG12	1.94	0.47
1:B3:244:GLY:HA2	1:B3:355:ASP:OD2	2.15	0.47
2:B4:307:PRO:HA	2:B4:383:ALA:HB2	1.97	0.47
2:B6:345:ASP:OD1	2:B6:345:ASP:N	2.47	0.47
5:Y:228:ARG:HA	5:Y:231:THR:HG22	1.97	0.47
4:X1:156:GLN:O	4:X1:160:THR:HG23	2.14	0.47
2:A6:50:ASN:O	2:A6:64:ARG:NH2	2.47	0.47
1:A7:169:VAL:HG21	1:A7:204:ASN:OD1	2.15	0.47
1:B1:117:LEU:HD11	1:B1:154:LYS:HB3	1.95	0.47
3:C:328:MET:O	3:C:331:THR:OG1	2.31	0.47
1:B7:178:THR:HG23	1:B7:181:GLU:HG3	1.96	0.47
1:A1:214:THR:HG23	1:A1:297:LYS:NZ	2.30	0.47
1:A7:282:ARG:HH12	1:A7:284:LEU:HD13	1.79	0.47
1:B3:392:LYS:HD2	1:B3:395:LEU:HD22	1.97	0.47
2:B6:69:ASP:OD1	2:B6:69:ASP:N	2.47	0.47
2:B6:79:ARG:O	2:B6:84:ARG:HG3	2.15	0.47
2:B6:194:LEU:O	2:B6:198:THR:HG22	2.15	0.47
1:B7:100:ASN:ND2	1:B7:103:LYS:H	2.13	0.47
1:A1:102:ALA:HB1	1:A1:401:GLU:OE1	2.15	0.47
1:A3:175:VAL:HG22	1:A3:205:GLU:HG3	1.97	0.47
2:A4:176:GLN:HG2	2:A4:177:VAL:N	2.30	0.47
1:A5:179:VAL:HG11	2:A6:258:ASN:HA	1.97	0.47
1:A5:208:TYR:HE1	1:A5:225:LEU:HD11	1.79	0.47
2:A6:237:SER:HA	2:A6:320:ARG:HD2	1.96	0.47
1:A7:105:HIS:CD2	1:A7:150:LEU:HD12	2.49	0.47
1:B1:309:ARG:H	1:B1:372:THR:CG2	2.28	0.47
1:B3:208:TYR:CE1	1:B3:225:LEU:HD11	2.48	0.47
1:B3:417:ASP:O	1:B3:421:GLU:HG3	2.14	0.47
2:B4:379:SER:OG	2:B4:380:ASN:N	2.48	0.47
1:B5:5:VAL:HG22	1:B5:62:ARG:HD3	1.96	0.47
1:B5:309:ARG:H	1:B5:372:THR:CG2	2.27	0.47
3:C:289:GLU:HG3	3:C:293:ASN:ND2	2.29	0.47
3:C:305:GLU:N	3:C:306:PRO:HD2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:19:LYS:HD2	1:A1:22:GLU:OE1	2.15	0.47
2:A6:206:ASN:OD1	7:A7:501:GTP:N2	2.48	0.47
1:B1:220:PRO:HD2	2:B2:326:LYS:CE	2.45	0.47
2:B4:100:ALA:HA	1:B5:252:LYS:HE3	1.97	0.47
1:B7:210:ILE:O	1:B7:214:THR:OG1	2.29	0.47
1:A1:8:GLN:NE2	1:A1:17:GLY:HA3	2.30	0.47
1:A1:73:MET:CE	1:A1:92:PHE:HB2	2.43	0.47
1:A3:238:CYS:SG	1:A3:318:ARG:NE	2.87	0.47
1:A5:213:ARG:O	1:A5:216:LYS:NZ	2.41	0.47
2:A6:198:THR:HG21	2:A6:201:ALA:HB2	1.96	0.47
1:B3:144:GLY:N	9:B3:502:GDP:O1B	2.38	0.47
2:B4:213:CYS:HA	2:B4:217:LEU:HB2	1.96	0.47
2:B6:9:ILE:HG22	2:B6:146:GLY:HA2	1.97	0.47
2:B6:306:ASP:HB3	2:B6:309:HIS:ND1	2.29	0.47
2:B6:431:ASP:O	2:B6:434:GLU:HG3	2.15	0.47
1:A1:291:GLN:N	1:A1:291:GLN:OE1	2.48	0.47
1:A3:287:PRO:HG3	1:A3:329:GLN:NE2	2.29	0.47
1:A3:364:SER:OG	1:A3:365:ALA:N	2.47	0.47
2:A4:81:GLY:O	2:A4:84:ARG:HG3	2.15	0.47
1:A5:4:ILE:HD11	1:A5:250:LEU:HD11	1.96	0.47
2:B6:28:HIS:CE1	2:B6:49:PHE:HA	2.50	0.47
3:C:467:LYS:HG3	3:C:467:LYS:O	2.15	0.47
2:A2:31:GLN:HG2	2:A2:37:PRO:HD3	1.97	0.46
1:A7:94:GLN:N	1:A7:94:GLN:OE1	2.48	0.46
1:A7:242:PHE:CD1	1:A7:356:ILE:HG13	2.51	0.46
1:B1:69:GLU:OE2	1:B1:96:GLY:HA3	2.15	0.46
2:B2:319:TYR:CZ	2:B2:328:VAL:HG23	2.50	0.46
4:X1:129:ARG:HG3	5:Y1:76:LEU:HD21	1.97	0.46
6:Z:90:GLU:HB3	6:Z:91:PRO:HD2	1.97	0.46
2:A6:220:GLU:HG2	2:A6:221:ARG:HG3	1.97	0.46
1:B1:113:ILE:HA	1:B1:116:VAL:HG22	1.96	0.46
1:B3:70:PRO:N	1:B3:92:PHE:HZ	2.13	0.46
2:B4:9:ILE:HG12	2:B4:68:LEU:HD21	1.96	0.46
1:B5:296:ALA:HB1	1:B5:304:ASP:OD1	2.15	0.46
1:B7:150:LEU:O	1:B7:153:SER:OG	2.29	0.46
3:C:350:THR:HB	3:C:419:LYS:NZ	2.30	0.46
1:A1:392:LYS:HD2	1:A1:395:LEU:HD22	1.96	0.46
2:A4:22:GLU:O	2:A4:26:LEU:HD23	2.16	0.46
1:A5:330:MET:SD	1:A5:349:VAL:HG11	2.55	0.46
2:A6:107:HIS:HB3	2:A6:108:TYR:CD2	2.50	0.46
1:A7:289:LEU:HD11	1:A7:363:MET:CE	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:3:GLU:HB2	1:B5:130:LEU:HA	1.96	0.46
2:A2:121:ARG:NH1	2:A2:124:LYS:HD2	2.30	0.46
2:A4:221:ARG:HG3	1:A5:325:GLU:OE2	2.16	0.46
1:A5:219:THR:HG23	2:A6:324:VAL:HG21	1.97	0.46
2:A6:5:ILE:HD11	2:A6:135:PHE:CE2	2.50	0.46
2:A6:316:CYS:SG	2:A6:352:LYS:HB3	2.55	0.46
1:A7:91:VAL:HG11	1:A7:116:VAL:HG23	1.97	0.46
1:A7:113:ILE:HA	1:A7:116:VAL:HG12	1.98	0.46
1:A1:100:ASN:OD1	2:A2:257:THR:HG21	2.16	0.46
1:A1:292:GLN:HG2	1:A1:298:ASN:ND2	2.30	0.46
2:A2:88:HIS:HD2	2:B2:283:HIS:HB2	1.80	0.46
1:A3:186:THR:HG23	1:A3:187:LEU:HD12	1.97	0.46
2:A4:243:ARG:HH11	2:A4:243:ARG:HG3	1.80	0.46
2:A4:317:LEU:HB3	2:A4:319:TYR:CE1	2.45	0.46
1:A5:135:VAL:O	1:A5:166:THR:HA	2.15	0.46
1:B1:134:GLN:HE21	1:B1:167:PHE:HE2	1.63	0.46
1:B1:388:MET:HG2	2:B2:346:TRP:O	2.16	0.46
1:B7:317:PHE:HE2	1:B7:326:VAL:HG13	1.81	0.46
3:C:394:ARG:NH1	3:C:413:GLU:OE1	2.48	0.46
1:A1:371:SER:OG	1:A1:372:THR:N	2.49	0.46
1:A3:54:ALA:HB3	1:A3:58:ARG:HB3	1.97	0.46
1:B1:178:THR:HG22	1:B1:181:GLU:HG3	1.97	0.46
1:B1:249:ASP:O	1:B1:253:LEU:HD13	2.15	0.46
2:B2:222:PRO:O	1:B3:322:SER:OG	2.33	0.46
2:B2:269:LEU:HD23	2:B2:301:MET:SD	2.55	0.46
1:B3:207:LEU:HB3	1:B3:225:LEU:HD22	1.97	0.46
1:A1:141:GLY:O	1:A1:145:SER:HB3	2.16	0.46
2:A6:213:CYS:HA	2:A6:217:LEU:HB2	1.97	0.46
1:A7:286:VAL:HG12	1:A7:329:GLN:HG3	1.97	0.46
1:B3:69:GLU:C	1:B3:92:PHE:HZ	2.18	0.46
2:B6:76:ASP:HA	2:B6:79:ARG:HD2	1.97	0.46
4:X:244:MET:HG3	5:Y:199:PHE:CE1	2.47	0.46
1:A3:191:GLN:HE21	1:A3:195:ASN:HD21	1.64	0.46
1:A3:390:ARG:HD3	1:A3:390:ARG:O	2.15	0.46
1:A5:114:ASP:N	1:A5:114:ASP:OD1	2.49	0.46
1:B1:242:PHE:CD1	1:B1:356:ILE:HG13	2.51	0.46
2:B2:399:TYR:O	2:B2:402:ARG:NH1	2.49	0.46
1:B7:117:LEU:HA	1:B7:120:VAL:HG12	1.98	0.46
6:Z:92:ARG:HH21	6:Z:92:ARG:HG3	1.81	0.46
1:A1:100:ASN:HB3	1:A1:103:LYS:HD3	1.97	0.46
2:A6:316:CYS:HB2	2:A6:378:ILE:HG23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:262:ARG:HH21	1:A7:418:LEU:HB3	1.81	0.46
1:B3:259:PRO:HG3	1:B3:311:LEU:HD23	1.97	0.46
1:B5:403:MET:HB2	1:B5:403:MET:HE2	1.47	0.46
2:A2:155:GLU:HG2	2:A2:197:HIS:NE2	2.31	0.46
2:A4:287:SER:N	2:A4:290:GLU:OE2	2.49	0.46
1:A5:4:ILE:HB	1:A5:50:TYR:HE1	1.80	0.46
1:A7:386:THR:O	1:A7:390:ARG:HG2	2.16	0.46
1:B1:232:VAL:HG11	1:B1:268:VAL:HG11	1.98	0.46
1:B5:11:GLN:HE21	1:B5:15:GLN:HE22	1.64	0.46
4:X1:249:GLU:HA	4:X1:252:GLU:OE2	2.15	0.46
2:A2:183:GLU:HG3	2:A2:184:PRO:HD3	1.98	0.45
2:A2:223:THR:HG23	2:A2:225:THR:H	1.81	0.45
2:A4:141:VAL:O	2:A4:147:SER:OG	2.30	0.45
2:A4:145:THR:OG1	7:A5:501:GTP:O1B	2.33	0.45
2:A6:395:PHE:HD2	2:A6:422:ARG:HH11	1.62	0.45
1:A7:315:ALA:HB1	1:A7:317:PHE:CE1	2.51	0.45
1:A7:377:MET:O	1:A7:381:VAL:HG22	2.16	0.45
1:B1:334:GLN:HE22	1:B1:348:ASN:H	1.64	0.45
2:B4:4:VAL:HG23	2:B4:134:GLY:O	2.16	0.45
2:B4:8:HIS:O	2:B4:68:LEU:HD23	2.16	0.45
2:B4:405:VAL:HG23	2:B4:418:PHE:CE2	2.50	0.45
1:B7:199:CYS:HB3	1:B7:265:PHE:CD1	2.51	0.45
1:A3:144:GLY:N	9:A3:502:GDP:O1B	2.49	0.45
2:A6:27:GLU:HG3	2:A6:361:THR:HG21	1.97	0.45
2:A6:185:TYR:HA	2:A6:395:PHE:HE1	1.81	0.45
2:A6:217:LEU:HB3	2:A6:219:ILE:HD12	1.97	0.45
1:B1:6:HIS:CD2	1:B1:8:GLN:HG2	2.51	0.45
1:B7:342:VAL:HG11	1:B7:345:ILE:HD13	1.99	0.45
4:X:255:LEU:HD13	5:Y:209:MET:SD	2.56	0.45
2:A2:98:ASP:OD1	2:A2:99:ALA:N	2.48	0.45
1:A3:114:ASP:OD1	1:A3:114:ASP:N	2.48	0.45
2:A4:339:ARG:HG2	2:A4:339:ARG:NH1	2.30	0.45
2:A6:306:ASP:HB3	2:A6:309:HIS:ND1	2.32	0.45
1:B1:395:LEU:HD23	1:B1:395:LEU:HA	1.79	0.45
2:B4:70:LEU:HD12	2:B4:99:ALA:HB2	1.97	0.45
2:B4:183:GLU:HG3	2:B4:184:PRO:HD3	1.98	0.45
2:B4:234:VAL:HG21	2:B4:302:MET:HE2	1.98	0.45
2:B6:246:GLY:HA2	2:B6:357:TYR:CD2	2.51	0.45
5:Y1:100:GLN:HA	5:Y1:103:GLU:HG3	1.98	0.45
2:A4:269:LEU:HD21	2:A4:384:ILE:HG22	1.98	0.45
2:A4:344:VAL:HG23	2:A4:347:CYS:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:68:LEU:HD12	1:A5:143:THR:HB	1.98	0.45
2:A6:195:LEU:HD21	2:A6:264:ARG:NH1	2.31	0.45
1:B7:152:ILE:HA	1:B7:155:ILE:HG22	1.98	0.45
3:C:433:MET:HB2	3:C:485:PHE:HE1	1.82	0.45
2:A2:136:LEU:HA	2:A2:167:LEU:O	2.16	0.45
2:A2:265:ILE:HG12	2:A2:432:PHE:CE1	2.51	0.45
2:A4:222:PRO:O	1:A5:322:SER:OG	2.34	0.45
2:A4:428:LEU:HD11	2:A4:432:PHE:HE2	1.82	0.45
2:A6:413:MET:HB3	2:A6:417:GLU:OE2	2.16	0.45
2:B2:88:HIS:ND1	2:B2:90:GLU:HG2	2.30	0.45
2:B4:289:ALA:HA	2:B4:331:SER:OG	2.17	0.45
3:C:428:HIS:HA	3:C:431:ILE:HG22	1.99	0.45
6:Z:96:ASN:O	6:Z:99:GLU:HG3	2.17	0.45
1:A1:271:THR:HG23	1:A1:292:GLN:OE1	2.16	0.45
2:A4:422:ARG:NH2	2:A4:425:LEU:HD23	2.31	0.45
2:A6:417:GLU:HA	2:A6:420:GLU:HG2	1.99	0.45
1:A7:103:LYS:HA	1:A7:107:THR:HB	1.98	0.45
1:B1:207:LEU:HB3	1:B1:225:LEU:HD22	1.98	0.45
2:B2:133:GLN:HG3	2:B2:242:LEU:HD11	1.98	0.45
2:B4:66:ILE:HD12	2:B4:121:ARG:HE	1.81	0.45
4:X:230:SER:HB2	5:Y:184:LEU:HD22	1.98	0.45
1:A1:47:ILE:HG22	1:A1:51:PHE:HB2	1.99	0.45
1:A7:102:ALA:HB3	1:A7:401:GLU:OE2	2.17	0.45
2:B4:192:HIS:ND1	2:B4:424:ASP:OD2	2.41	0.45
1:B5:417:ASP:O	1:B5:421:GLU:HG3	2.17	0.45
1:B7:165:LEU:HD23	1:B7:167:PHE:HZ	1.80	0.45
4:X:260:ARG:HD3	4:X:260:ARG:N	2.32	0.45
1:A1:272:PRO:HD2	1:A1:361:LEU:HD21	1.98	0.45
1:B1:312:THR:HG22	1:B1:313:ALA:N	2.32	0.45
1:B3:232:VAL:HG11	1:B3:268:VAL:HG11	1.99	0.45
2:B4:326:LYS:HA	2:B4:326:LYS:HD2	1.51	0.45
2:B6:305:CYS:HB3	2:B6:387:ILE:HD11	1.99	0.45
2:B6:319:TYR:CZ	2:B6:328:VAL:HG23	2.52	0.45
6:Z:96:ASN:HA	6:Z:99:GLU:HG3	1.99	0.45
2:A2:315:CYS:N	2:A2:350:GLY:O	2.48	0.45
1:A5:5:VAL:HG22	1:A5:62:ARG:HD3	1.99	0.45
1:A5:54:ALA:O	1:B5:283:ALA:HA	2.16	0.45
1:B7:73:MET:O	1:B7:76:VAL:HB	2.17	0.45
1:B7:150:LEU:HD12	1:B7:151:LEU:N	2.32	0.45
3:C:357:CYS:O	3:C:360:GLN:HG3	2.17	0.45
6:Z:73:LEU:HA	6:Z:76:GLN:OE1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:30:ILE:HD12	1:A1:36:TYR:HA	1.99	0.45
1:A1:180:VAL:HG23	1:A1:184:ASN:HD21	1.82	0.45
1:A3:9:GLY:HA2	1:A3:66:MET:O	2.17	0.45
1:A5:8:GLN:O	1:A5:66:MET:HG3	2.17	0.45
1:A5:47:ILE:HG22	1:A5:51:PHE:HB2	1.98	0.45
1:A5:388:MET:HB3	1:A5:393:ALA:HB3	1.97	0.45
1:A7:367:PHE:O	1:A7:368:ILE:HD13	2.17	0.45
2:B2:98:ASP:OD1	2:B2:99:ALA:N	2.48	0.45
2:B6:151:SER:HB2	2:B6:193:SER:OG	2.16	0.45
2:A4:398:MET:CE	1:A5:346:PRO:HD2	2.47	0.44
2:B2:434:GLU:OE2	2:B2:435:VAL:HG23	2.17	0.44
2:B4:119:LEU:HD21	2:B4:156:ARG:HD3	1.99	0.44
2:B4:246:GLY:HA3	2:B4:356:ASN:HA	1.99	0.44
1:B5:44:LEU:O	1:B5:47:ILE:HG12	2.17	0.44
1:B5:264:HIS:O	1:B5:264:HIS:ND1	2.48	0.44
1:B5:389:PHE:HZ	1:B5:405:GLU:HG3	1.83	0.44
2:B6:170:THR:HG21	2:B6:194:LEU:HD11	2.00	0.44
1:B7:296:ALA:HB1	1:B7:305:PRO:HD2	1.99	0.44
6:Z:72:LEU:O	6:Z:76:GLN:OE1	2.35	0.44
1:A1:95:THR:OG1	1:A1:96:GLY:N	2.50	0.44
1:A1:237:THR:HG22	1:A1:237:THR:O	2.18	0.44
1:A3:52:ASN:OD1	1:A3:62:ARG:NH2	2.49	0.44
1:A5:137:HIS:O	1:A5:168:SER:HA	2.17	0.44
2:A6:66:ILE:HD11	2:A6:122:ILE:HD11	1.99	0.44
1:A7:60:VAL:HG11	1:A7:86:ARG:NH2	2.31	0.44
1:B1:167:PHE:CZ	1:B1:233:MET:HG2	2.52	0.44
1:B1:204:ASN:OD1	9:B1:501:GDP:O2'	2.35	0.44
1:B7:144:GLY:N	9:B7:502:GDP:O1B	2.37	0.44
3:C:344:ARG:O	3:C:348:LYS:HE2	2.17	0.44
3:C:422:LEU:HB3	3:C:476:TYR:CG	2.51	0.44
1:A1:384:GLN:HB3	2:A2:348:PRO:HG3	1.99	0.44
2:A2:335:ILE:HG23	2:A2:341:ILE:HD11	1.98	0.44
2:A4:178:SER:HB2	2:A4:183:GLU:OE1	2.17	0.44
2:B2:4:VAL:HG13	2:B2:52:PHE:HE1	1.82	0.44
2:B4:260:VAL:HG23	2:B4:260:VAL:O	2.17	0.44
1:B5:209:ASP:CG	1:B5:213:ARG:HH12	2.18	0.44
2:B6:213:CYS:HA	2:B6:217:LEU:HB2	1.99	0.44
1:B7:224:ASP:OD1	1:B7:225:LEU:N	2.50	0.44
4:X:271:LYS:HA	4:X:271:LYS:HD3	1.84	0.44
1:A3:401:GLU:N	1:A3:401:GLU:OE1	2.50	0.44
2:A4:246:GLY:HA3	2:A4:356:ASN:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:91:VAL:HG11	1:B1:116:VAL:HG12	1.99	0.44
1:A1:208:TYR:O	1:A1:212:PHE:HD1	2.01	0.44
2:A2:402:ARG:NH1	6:Z:168:ARG:HH22	2.06	0.44
2:A4:203:MET:SD	2:A4:267:PHE:HB3	2.57	0.44
2:A4:392:ASP:OD1	2:A4:422:ARG:NH1	2.51	0.44
1:A5:113:ILE:HD11	1:A5:151:LEU:HB2	2.00	0.44
1:B5:70:PRO:HD2	2:B6:2:ARG:NH2	2.32	0.44
2:A2:346:TRP:CZ3	2:A2:347:CYS:HB2	2.53	0.44
1:A3:170:VAL:N	1:A3:202:LEU:O	2.49	0.44
1:A5:145:SER:O	1:A5:149:THR:OG1	2.18	0.44
1:A7:213:ARG:HD3	1:A7:297:LYS:HD2	1.99	0.44
2:B4:72:PRO:HD2	1:B5:2:ARG:NH1	2.33	0.44
2:B4:402:ARG:HD2	2:B4:405:VAL:HG11	1.99	0.44
6:Z:59:ILE:HG13	6:Z:70:ILE:CD1	2.37	0.44
1:A7:8:GLN:CD	1:A7:17:GLY:HA3	2.38	0.44
1:B3:91:VAL:CG1	1:B3:116:VAL:HG22	2.47	0.44
2:B4:72:PRO:HD2	1:B5:2:ARG:HH12	1.83	0.44
1:B7:100:ASN:OD1	1:B7:398:TYR:HE1	2.00	0.44
1:B7:130:LEU:HD21	1:B7:133:PHE:CE1	2.52	0.44
5:Y:241:ARG:HD2	5:Y:245:ARG:NH2	2.32	0.44
6:Z:70:ILE:HG22	6:Z:71:SER:N	2.33	0.44
1:A3:189:VAL:HG11	1:A3:378:PHE:CE1	2.53	0.44
2:A4:395:PHE:CE2	2:A4:422:ARG:HD2	2.53	0.44
2:A6:179:THR:O	1:A7:350:LYS:HD2	2.18	0.44
1:B1:91:VAL:CG1	1:B1:116:VAL:HG12	2.47	0.44
1:B1:186:THR:HG22	1:B1:411:ALA:HB1	1.99	0.44
2:B2:28:HIS:CE1	2:B2:49:PHE:HA	2.52	0.44
1:B7:105:HIS:CD2	1:B7:150:LEU:HB3	2.52	0.44
4:X:237:LEU:HB3	5:Y:191:MET:CE	2.48	0.44
1:A1:40:SER:OG	1:A1:41:ASP:N	2.51	0.44
1:A3:135:VAL:HG21	1:A3:152:ILE:HD11	2.00	0.44
1:A3:189:VAL:O	1:A3:193:VAL:HG23	2.18	0.44
2:A4:413:MET:HB3	2:A4:417:GLU:OE2	2.18	0.44
2:A6:407:TRP:O	2:A6:411:GLU:HG3	2.18	0.44
1:A7:113:ILE:HD13	1:A7:150:LEU:HD21	1.99	0.44
2:B2:47:ASP:OD1	2:B2:48:ALA:N	2.51	0.44
1:B3:249:ASP:OD1	1:B3:252:LYS:HB2	2.18	0.44
1:B5:22:GLU:HG3	1:B5:81:TYR:CD2	2.52	0.44
2:B6:179:THR:HG22	1:B7:327:ASP:OD1	2.18	0.44
3:C:315:ILE:O	3:C:319:LEU:HG	2.18	0.44
3:C:416:ILE:H	3:C:416:ILE:HD12	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:204:ASN:HA	1:A1:207:LEU:HD12	2.00	0.43
2:A2:81:GLY:O	2:A2:84:ARG:HG3	2.18	0.43
2:A2:150:GLY:O	2:A2:154:LEU:HD23	2.18	0.43
1:A3:103:LYS:HA	1:A3:107:THR:HB	1.99	0.43
1:A3:253:LEU:HD11	1:A3:316:LEU:HD21	1.99	0.43
1:A5:21:TRP:CZ2	1:A5:63:ALA:HB2	2.53	0.43
1:B5:274:THR:HG21	1:B5:282:ARG:HD2	2.00	0.43
2:B6:405:VAL:HG13	2:B6:418:PHE:CE2	2.44	0.43
4:X1:177:TYR:CD2	5:Y1:132:ILE:HD12	2.53	0.43
5:Y1:200:GLU:O	5:Y1:203:GLU:HG3	2.18	0.43
1:A1:309:ARG:H	1:A1:372:THR:HG22	1.83	0.43
2:A2:90:GLU:OE1	2:A2:121:ARG:NH2	2.50	0.43
1:A3:133:PHE:HD2	1:A3:164:MET:HE3	1.83	0.43
2:A4:387:ILE:HG23	2:A4:388:PHE:HD1	1.83	0.43
2:A6:72:PRO:HA	2:A6:94:SER:HB2	1.99	0.43
1:A7:122:LYS:HA	1:A7:125:GLU:HG3	1.99	0.43
1:B1:5:VAL:HG22	1:B1:62:ARG:HD3	2.01	0.43
2:B2:21:TRP:CZ2	2:B2:65:CYS:HB3	2.54	0.43
2:B2:196:GLU:OE2	2:B2:197:HIS:NE2	2.51	0.43
1:B3:91:VAL:HG11	1:B3:116:VAL:HG22	2.00	0.43
2:B4:203:MET:HE3	2:B4:267:PHE:HB3	1.99	0.43
1:B7:267:MET:CE	1:B7:299:MET:HG3	2.48	0.43
3:C:403:GLN:HG2	3:C:404:PRO:HD3	1.99	0.43
1:A5:385:PHE:HZ	1:A5:408:PHE:HD2	1.65	0.43
2:A6:70:LEU:CD2	2:A6:114:ILE:HD12	2.48	0.43
2:A6:434:GLU:OE1	2:A6:435:VAL:HG23	2.18	0.43
1:B1:122:LYS:O	1:B1:126:SER:OG	2.33	0.43
1:B3:152:ILE:HG22	1:B3:195:ASN:HB3	2.01	0.43
2:B6:278:ALA:HA	2:B6:369:ALA:HB2	2.00	0.43
4:X1:123:ASN:HA	4:X1:126:LYS:HG2	1.99	0.43
2:A2:189:LEU:HD11	2:A2:418:PHE:HE1	1.82	0.43
1:A5:271:THR:CG2	1:A5:365:ALA:HB3	2.49	0.43
2:A6:52:PHE:HE1	2:A6:239:THR:HG21	1.83	0.43
2:A6:200:VAL:HG13	2:A6:268:MET:CE	2.48	0.43
1:B1:114:ASP:OD1	1:B1:114:ASP:N	2.50	0.43
1:B1:170:VAL:HG22	1:B1:202:LEU:O	2.18	0.43
1:B5:3:GLU:HB2	1:B5:130:LEU:HD12	2.01	0.43
1:B7:74:ASP:OD1	1:B7:74:ASP:N	2.49	0.43
1:B7:263:LEU:HD22	1:B7:422:TYR:CZ	2.53	0.43
1:A1:258:ILE:O	1:A1:258:ILE:HG23	2.18	0.43
2:A2:9:ILE:HG12	2:A2:68:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:283:HIS:CG	2:A6:283:HIS:O	2.70	0.43
1:B1:213:ARG:NH1	1:B1:297:LYS:HE2	2.34	0.43
2:B4:102:ASN:HB3	2:B4:105:ARG:HB3	2.00	0.43
2:B4:287:SER:HB3	2:B4:290:GLU:OE2	2.18	0.43
1:B5:205:GLU:OE1	1:B5:205:GLU:N	2.52	0.43
1:B5:236:ILE:HD13	1:B5:368:ILE:HD11	1.99	0.43
2:B6:326:LYS:HE2	2:B6:326:LYS:HB3	1.92	0.43
3:C:325:ASN:O	3:C:329:MET:HG2	2.19	0.43
5:Y1:146:TYR:O	5:Y1:150:ILE:HG12	2.19	0.43
2:A4:21:TRP:CZ3	2:A4:63:PRO:HB3	2.53	0.43
1:A7:173:PRO:HB3	1:A7:384:GLN:NE2	2.31	0.43
1:A7:192:LEU:HD13	1:A7:199:CYS:SG	2.58	0.43
4:X:266:ARG:HH12	5:Y:220:GLN:HA	1.84	0.43
1:B1:40:SER:O	1:B1:43:GLN:HG2	2.19	0.43
1:B1:220:PRO:HD2	2:B2:326:LYS:HD3	2.00	0.43
2:B4:66:ILE:CB	2:B4:121:ARG:HH21	2.32	0.43
2:B4:121:ARG:HD2	2:B4:121:ARG:C	2.39	0.43
1:B5:113:ILE:HD12	1:B5:116:VAL:HG21	2.00	0.43
1:B5:397:TRP:CH2	2:B6:256:GLN:HB3	2.54	0.43
1:A1:4:ILE:HB	1:A1:50:TYR:HE1	1.83	0.43
2:A2:387:ILE:HG12	2:A2:390:ARG:NH2	2.32	0.43
1:A3:8:GLN:NE2	1:A3:17:GLY:HA3	2.34	0.43
1:A3:296:ALA:HB1	1:A3:304:ASP:OD1	2.18	0.43
2:A4:431:ASP:O	2:A4:434:GLU:HG3	2.19	0.43
2:A6:52:PHE:CE1	2:A6:239:THR:HG21	2.54	0.43
1:A7:200:MET:CE	1:A7:368:ILE:HD12	2.47	0.43
2:B4:143:GLY:O	2:B4:147:SER:HB3	2.19	0.43
2:B6:7:ILE:HD12	2:B6:153:LEU:HD23	2.00	0.43
2:A2:265:ILE:HG23	2:A2:432:PHE:HE1	1.82	0.43
1:A3:391:ARG:NH2	2:A4:262:TYR:CZ	2.87	0.43
2:A4:171:VAL:HA	2:A4:204:LEU:O	2.18	0.43
2:A6:12:ALA:HB2	7:A7:501:GTP:C8	2.54	0.43
2:A6:102:ASN:ND2	2:A6:411:GLU:OE2	2.51	0.43
1:A7:314:SER:OG	1:A7:368:ILE:HB	2.18	0.43
1:B1:395:LEU:O	1:B1:399:THR:HG23	2.19	0.43
2:B2:372:GLN:OE1	2:B2:372:GLN:HA	2.19	0.43
1:B3:392:LYS:HE3	1:B3:405:GLU:OE1	2.19	0.43
1:B5:175:VAL:HG23	1:B5:205:GLU:CD	2.40	0.43
1:B5:271:THR:OG1	1:B5:365:ALA:HB3	2.19	0.43
2:B6:70:LEU:HB3	2:B6:97:GLU:O	2.19	0.43
2:A2:353:CYS:SG	2:A2:354:GLY:N	2.91	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:155:GLU:HG2	2:A6:197:HIS:CD2	2.54	0.43
1:B3:242:PHE:CD1	1:B3:356:ILE:HG13	2.54	0.43
1:B7:293:MET:SD	1:B7:367:PHE:HB2	2.59	0.43
3:C:316:THR:OG1	3:C:317:GLU:OE1	2.34	0.43
3:C:471:TYR:CZ	3:C:481:PHE:HB3	2.53	0.43
4:X:272:LYS:O	4:X:275:GLU:HG2	2.19	0.43
1:A1:215:LEU:HD23	1:A1:215:LEU:HA	1.86	0.42
1:A1:378:PHE:HA	1:A1:381:VAL:HG22	2.00	0.42
2:A4:100:ALA:HB1	1:A5:252:LYS:HA	2.00	0.42
2:A4:291:ILE:HD12	2:A4:375:VAL:HG23	2.01	0.42
1:A5:215:LEU:HB3	1:A5:217:LEU:HG	2.01	0.42
1:A7:383:GLU:HA	1:A7:386:THR:HG22	2.01	0.42
2:B2:288:VAL:HG13	2:B2:319:TYR:CE2	2.45	0.42
2:B4:258:ASN:CG	2:B4:352:LYS:HD3	2.39	0.42
2:B6:394:LYS:HB2	1:B7:346:PRO:HG3	2.01	0.42
5:Y:234:ILE:HB	5:Y:238:LYS:NZ	2.34	0.42
1:A5:35:THR:HA	1:A5:57:GLY:O	2.19	0.42
2:A6:311:LYS:HG2	2:A6:342:GLN:HG3	2.00	0.42
2:B4:53:PHE:C	2:B4:64:ARG:HH22	2.22	0.42
1:B5:3:GLU:HG3	1:B5:127:CYS:HB2	1.99	0.42
1:B5:166:THR:OG1	1:B5:199:CYS:SG	2.52	0.42
2:B6:2:ARG:HE	2:B6:2:ARG:HB3	1.68	0.42
3:C:455:MET:SD	3:C:456:LEU:N	2.92	0.42
4:X:256:ALA:O	4:X:260:ARG:HG2	2.19	0.42
4:X1:248:LYS:HD3	5:Y1:202:ARG:HG2	2.01	0.42
1:A1:146:GLY:O	1:A1:149:THR:HG22	2.20	0.42
2:A2:4:VAL:HG23	2:A2:134:GLY:O	2.19	0.42
1:A3:191:GLN:HG3	1:A3:195:ASN:HD22	1.84	0.42
1:A3:309:ARG:H	1:A3:372:THR:HG22	1.84	0.42
1:A5:271:THR:OG1	1:A5:272:PRO:HA	2.20	0.42
1:A5:421:GLU:HA	1:A5:424:GLN:HG3	2.01	0.42
2:A6:71:GLU:HB2	2:A6:98:ASP:OD1	2.19	0.42
2:A6:345:ASP:OD1	2:A6:346:TRP:N	2.51	0.42
1:A7:11:GLN:N	9:A7:502:GDP:O2B	2.45	0.42
1:A7:232:VAL:HG11	1:A7:268:VAL:HG11	2.01	0.42
2:B2:9:ILE:HD13	2:B2:150:GLY:HA2	2.01	0.42
2:B2:102:ASN:OD1	1:B3:255:VAL:HG21	2.19	0.42
2:B4:336:LYS:NZ	2:B4:348:PRO:O	2.28	0.42
2:B4:344:VAL:HG13	2:B4:346:TRP:H	1.84	0.42
1:B5:257:LEU:HD21	1:B5:314:SER:HB2	2.01	0.42
2:B6:155:GLU:HG2	2:B6:197:HIS:CD2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X1:169:GLY:O	4:X1:171:LEU:HD12	2.20	0.42
2:A2:8:HIS:CD2	2:A2:138:PHE:HD2	2.37	0.42
2:A2:326:LYS:HB3	2:A2:326:LYS:HE2	1.70	0.42
2:A2:328:VAL:O	2:A2:332:VAL:HG23	2.19	0.42
2:A4:377:MET:SD	2:A4:379:SER:HB3	2.60	0.42
1:A5:19:LYS:HA	1:A5:19:LYS:HD3	1.85	0.42
1:A7:267:MET:SD	1:A7:303:ALA:HB3	2.60	0.42
1:B1:3:GLU:HG3	1:B1:127:CYS:CB	2.49	0.42
2:B2:8:HIS:O	2:B2:68:LEU:HD23	2.19	0.42
1:B3:3:GLU:HG3	1:B3:127:CYS:SG	2.59	0.42
1:B3:67:ASP:OD1	1:B3:68:LEU:N	2.51	0.42
1:B3:192:LEU:HD23	1:B3:192:LEU:HA	1.91	0.42
1:B5:68:LEU:HB3	1:B5:96:GLY:HA2	2.02	0.42
1:B5:175:VAL:N	1:B5:205:GLU:OE2	2.51	0.42
1:B5:385:PHE:HZ	1:B5:408:PHE:HD1	1.67	0.42
1:B7:145:SER:OG	1:B7:146:GLY:N	2.53	0.42
1:B7:367:PHE:O	1:B7:368:ILE:HD13	2.18	0.42
6:Z:99:GLU:HA	6:Z:102:MET:HG2	2.00	0.42
1:A1:64:ILE:HA	1:A1:89:ASN:HB3	2.02	0.42
1:A1:175:VAL:HG13	2:A2:329:ASN:ND2	2.29	0.42
1:A3:406:MET:O	1:A3:410:GLU:HG3	2.18	0.42
2:A6:67:PHE:HB2	2:A6:92:LEU:HD23	2.01	0.42
2:A6:313:MET:HE3	2:A6:382:THR:HG22	2.02	0.42
1:B3:67:ASP:CG	1:B3:68:LEU:H	2.22	0.42
1:B3:208:TYR:CG	2:B4:326:LYS:HD3	2.55	0.42
5:Y1:182:ALA:HA	5:Y1:185:LYS:HG2	2.01	0.42
6:Z:7:ARG:HD3	6:Z:120:MET:HA	2.00	0.42
1:A1:334:GLN:HA	1:A1:341:PHE:HE2	1.83	0.42
2:A2:104:ALA:HB2	2:A2:413:MET:SD	2.60	0.42
2:A2:198:THR:HG21	2:A2:201:ALA:HB2	2.01	0.42
2:A4:422:ARG:HH22	2:A4:425:LEU:HD23	1.85	0.42
1:A5:103:LYS:HD2	1:A5:107:THR:OG1	2.20	0.42
2:B2:171:VAL:HA	2:B2:204:LEU:O	2.19	0.42
1:B5:69:GLU:CG	2:B6:2:ARG:HH22	2.32	0.42
5:Y1:78:ASP:OD1	5:Y1:79:GLU:HG2	2.20	0.42
1:A3:317:PHE:CE2	1:A3:326:VAL:HG13	2.54	0.42
2:A6:209:ILE:HG23	2:A6:230:LEU:HD11	2.01	0.42
1:B3:103:LYS:HA	1:B3:107:THR:OG1	2.20	0.42
2:B4:26:LEU:HD21	2:B4:364:PRO:HD2	2.01	0.42
2:B4:91:GLN:CA	2:B4:121:ARG:HH22	2.32	0.42
2:B4:174:SER:HB3	2:B4:177:VAL:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:223:THR:OG1	2:B6:224:TYR:N	2.53	0.42
1:B7:64:ILE:HG13	1:B7:64:ILE:O	2.20	0.42
4:X:230:SER:OG	5:Y:184:LEU:HD13	2.20	0.42
1:A1:173:PRO:HG3	1:A1:380:ARG:HD2	2.02	0.42
2:A2:213:CYS:HA	2:A2:217:LEU:HB2	2.01	0.42
1:A5:149:THR:HG22	1:A5:191:GLN:HG2	2.01	0.42
2:A6:422:ARG:HA	2:A6:422:ARG:HD2	1.88	0.42
1:A7:293:MET:CG	1:A7:367:PHE:HB2	2.50	0.42
1:B1:138:SER:O	1:B1:139:LEU:HD23	2.20	0.42
1:B1:336:LYS:HE2	1:B1:336:LYS:HB3	1.87	0.42
2:B2:330:ALA:O	2:B2:334:THR:HG23	2.20	0.42
2:B2:402:ARG:O	2:B2:405:VAL:HG12	2.19	0.42
1:B7:203:ASP:O	1:B7:207:LEU:HG	2.20	0.42
4:X1:188:ILE:HG13	5:Y1:143:TYR:CE1	2.55	0.42
2:A2:425:LEU:HD23	2:A2:425:LEU:HA	1.85	0.42
1:A3:232:VAL:O	1:A3:236:ILE:HG12	2.20	0.42
2:A4:267:PHE:HB2	2:A4:384:ILE:CD1	2.50	0.42
1:A5:112:LEU:HD12	1:A5:112:LEU:HA	1.93	0.42
1:A7:109:GLY:O	1:A7:113:ILE:HG12	2.19	0.42
1:B1:145:SER:OG	1:B1:146:GLY:N	2.52	0.42
2:B2:80:THR:HG22	2:B2:80:THR:O	2.20	0.42
1:B3:8:GLN:CD	1:B3:17:GLY:HA3	2.40	0.42
2:B4:121:ARG:O	2:B4:124:LYS:HG2	2.19	0.42
1:B5:2:ARG:NE	1:B5:240:LEU:HD22	2.27	0.42
1:A1:109:GLY:O	1:A1:113:ILE:HG12	2.20	0.42
1:A1:317:PHE:CE2	1:A1:326:VAL:HG13	2.54	0.42
1:A3:137:HIS:O	1:A3:168:SER:HA	2.20	0.42
1:A3:149:THR:HG23	1:A3:191:GLN:HG2	2.02	0.42
1:A7:21:TRP:CZ2	1:A7:63:ALA:HB2	2.55	0.42
2:B6:157:LEU:HD23	2:B6:157:LEU:HA	1.88	0.42
1:A3:163:MET:HE2	1:A3:251:ARG:HG3	2.02	0.41
1:A3:245:GLN:C	1:A3:246:LEU:HD12	2.39	0.41
1:A5:224:ASP:O	1:A5:228:LEU:HG	2.20	0.41
2:B2:425:LEU:O	2:B2:429:GLU:HG2	2.20	0.41
1:B3:172:SER:HB3	1:B3:175:VAL:HG22	2.02	0.41
2:B4:3:GLU:HA	2:B4:51:THR:OG1	2.19	0.41
2:B6:66:ILE:O	2:B6:66:ILE:HG13	2.19	0.41
2:B6:150:GLY:O	2:B6:154:LEU:HD23	2.20	0.41
1:B7:170:VAL:HG22	1:B7:202:LEU:O	2.19	0.41
1:B7:253:LEU:HD11	1:B7:316:LEU:HD21	2.02	0.41
2:B2:53:PHE:O	2:B2:64:ARG:NH2	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:398:MET:HE2	1:B3:345:ILE:HG23	2.01	0.41
1:B3:156:ARG:NH2	1:B3:197:ASP:OD1	2.52	0.41
1:B5:392:LYS:HD2	1:B5:395:LEU:HD22	2.01	0.41
2:B6:255:PHE:N	2:B6:255:PHE:CD1	2.88	0.41
1:B7:167:PHE:CD2	1:B7:233:MET:HG2	2.54	0.41
5:Y:184:LEU:O	5:Y:188:MET:HG2	2.20	0.41
2:A2:210:TYR:OH	2:A2:224:TYR:HE1	2.01	0.41
1:A5:67:ASP:CG	1:A5:68:LEU:H	2.22	0.41
1:A5:186:THR:HG23	1:A5:415:MET:SD	2.60	0.41
2:A6:267:PHE:HB2	2:A6:384:ILE:HD12	2.02	0.41
1:A7:203:ASP:OD1	1:A7:204:ASN:N	2.53	0.41
1:A7:289:LEU:HD11	1:A7:363:MET:HE3	2.01	0.41
2:B2:51:THR:CG2	2:B2:243:ARG:HG2	2.49	0.41
2:B2:317:LEU:HB3	2:B2:319:TYR:CE1	2.55	0.41
1:B3:167:PHE:CE2	1:B3:200:MET:HE2	2.55	0.41
1:B7:359:LYS:HD2	1:B7:359:LYS:HA	1.88	0.41
5:Y1:205:ALA:O	5:Y1:208:GLU:HG3	2.19	0.41
1:A1:391:ARG:O	1:A1:391:ARG:HG2	2.20	0.41
2:A2:63:PRO:HB2	2:A2:65:CYS:SG	2.61	0.41
2:A2:66:ILE:HG13	2:A2:66:ILE:O	2.21	0.41
2:A2:264:ARG:NH1	2:A2:431:ASP:OD2	2.54	0.41
2:A2:274:PRO:HB2	2:A2:276:ILE:HG12	2.02	0.41
1:A3:35:THR:HA	1:A3:57:GLY:O	2.20	0.41
2:A6:167:LEU:HB3	2:A6:169:PHE:CE1	2.55	0.41
1:A7:60:VAL:HG23	1:A7:84:ILE:O	2.20	0.41
2:B2:189:LEU:HD11	2:B2:418:PHE:CE1	2.56	0.41
1:B7:267:MET:HE1	1:B7:299:MET:HG3	2.02	0.41
1:B7:310:TYR:CD1	1:B7:371:SER:HB2	2.55	0.41
3:C:296:TYR:O	3:C:299:THR:OG1	2.32	0.41
4:X1:166:LEU:HD23	4:X1:166:LEU:HA	1.86	0.41
4:X1:190:GLU:O	4:X1:193:VAL:HG12	2.20	0.41
2:A2:222:PRO:HD2	1:A3:324:LYS:HD3	2.01	0.41
2:A2:392:ASP:OD1	2:A2:422:ARG:NH1	2.53	0.41
1:A5:325:GLU:O	1:A5:329:GLN:HG2	2.20	0.41
2:A6:9:ILE:HG22	2:A6:68:LEU:CD1	2.49	0.41
2:A6:66:ILE:HG21	2:A6:121:ARG:HG3	2.02	0.41
2:A6:104:ALA:HB3	2:A6:411:GLU:OE1	2.20	0.41
1:A7:48:ASN:OD1	1:A7:48:ASN:N	2.54	0.41
1:B3:421:GLU:HA	1:B3:424:GLN:HB3	2.02	0.41
1:B5:128:ASP:OD1	1:B5:128:ASP:N	2.41	0.41
1:B7:305:PRO:HA	1:B7:373:ALA:CB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:297:LEU:HD21	3:C:345:LEU:HD21	2.02	0.41
3:C:425:LYS:HG3	3:C:426:ALA:N	2.36	0.41
3:C:455:MET:SD	3:C:456:LEU:HG	2.61	0.41
1:A1:289:LEU:HD11	1:A1:365:ALA:HB2	2.03	0.41
1:A3:23:VAL:HG11	1:A3:230:SER:HB2	2.03	0.41
1:A3:257:LEU:HD13	1:A3:314:SER:OG	2.20	0.41
2:A4:80:THR:HA	2:A4:84:ARG:HG2	2.02	0.41
2:A4:179:THR:O	1:A5:350:LYS:HA	2.20	0.41
2:B2:155:GLU:HG2	2:B2:197:HIS:NE2	2.35	0.41
1:B3:3:GLU:HB2	1:B3:130:LEU:HD23	2.03	0.41
2:B4:178:SER:CB	1:B5:347:ASN:ND2	2.82	0.41
2:B4:215:ARG:HG2	2:B4:215:ARG:HH11	1.84	0.41
2:B4:327:ASP:OD1	2:B4:327:ASP:N	2.51	0.41
2:B6:21:TRP:CZ2	2:B6:65:CYS:HB3	2.55	0.41
6:Z:86:LYS:HB2	6:Z:86:LYS:HE2	1.81	0.41
1:A1:46:ARG:HA	1:A1:46:ARG:HD3	1.86	0.41
1:A1:135:VAL:HG12	1:A1:137:HIS:HD2	1.86	0.41
1:A1:285:THR:HG22	1:A1:288:GLU:OE1	2.20	0.41
2:A2:55:GLU:OE1	2:A2:61:HIS:ND1	2.54	0.41
2:A2:428:LEU:HD21	2:A2:432:PHE:HE2	1.84	0.41
1:A5:183:TYR:HD2	1:A5:398:TYR:CE2	2.39	0.41
1:B5:172:SER:HB3	1:B5:205:GLU:OE2	2.21	0.41
1:B7:167:PHE:N	1:B7:167:PHE:CD1	2.88	0.41
4:X1:234:LEU:HD13	5:Y1:188:MET:HE1	2.02	0.41
5:Y1:189:ALA:O	5:Y1:193:GLN:HG2	2.21	0.41
5:Y1:202:ARG:HE	5:Y1:206:ILE:HD11	1.86	0.41
6:Z:172:LYS:HA	6:Z:172:LYS:HD3	1.84	0.41
1:A5:376:GLU:O	1:A5:380:ARG:HB2	2.20	0.41
1:A7:416:ASN:O	1:A7:419:VAL:HG22	2.21	0.41
2:B2:326:LYS:HB2	2:B2:326:LYS:HE3	1.82	0.41
1:B3:50:TYR:OH	1:B3:237:THR:HG21	2.21	0.41
2:B6:288:VAL:HG21	2:B6:327:ASP:CG	2.41	0.41
1:B7:292:GLN:HG2	1:B7:298:ASN:HD22	1.85	0.41
6:Z:152:GLU:HA	6:Z:155:HIS:ND1	2.36	0.41
2:A4:91:GLN:NE2	2:A4:121:ARG:HH21	2.19	0.41
2:A4:119:LEU:HA	2:A4:122:ILE:HG22	2.01	0.41
2:A4:151:SER:HB2	2:A4:193:SER:OG	2.21	0.41
2:A4:272:TYR:HD2	2:A4:275:ILE:HD11	1.85	0.41
2:A4:381:SER:OG	2:A4:382:THR:N	2.54	0.41
1:A5:9:GLY:HA2	1:A5:66:MET:O	2.21	0.41
1:A5:404:ASP:CG	1:A5:405:GLU:H	2.25	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:6:HIS:CE1	1:A7:8:GLN:HG2	2.56	0.41
1:A7:105:HIS:CD2	1:A7:150:LEU:HB2	2.55	0.41
1:A7:152:ILE:HD13	1:A7:152:ILE:HA	1.90	0.41
1:A7:415:MET:O	1:A7:418:LEU:HG	2.21	0.41
1:B1:396:HIS:HA	1:B1:399:THR:OG1	2.21	0.41
2:B2:276:ILE:HG23	2:B2:281:ALA:HB2	2.02	0.41
2:B2:322:ASP:HB2	2:B2:373:ARG:HH21	1.85	0.41
2:B2:387:ILE:HG12	2:B2:390:ARG:NH2	2.33	0.41
1:B3:139:LEU:HD22	1:B3:188:SER:HB2	2.03	0.41
1:B3:391:ARG:HE	2:B4:346:TRP:HE1	1.69	0.41
2:B4:91:GLN:CG	2:B4:121:ARG:HH12	2.33	0.41
2:B4:165:SER:HA	2:B4:199:ASP:OD2	2.21	0.41
1:B5:313:ALA:N	1:B5:348:ASN:O	2.53	0.41
2:B6:155:GLU:O	2:B6:158:SER:OG	2.38	0.41
3:C:287:ALA:O	3:C:291:LYS:HG2	2.20	0.41
3:C:341:HIS:O	3:C:345:LEU:HB2	2.20	0.41
4:X1:132:LEU:HD12	5:Y1:83:LEU:HD22	2.03	0.41
4:X1:188:ILE:HG13	5:Y1:143:TYR:HE1	1.85	0.41
2:A2:327:ASP:OD1	2:A2:327:ASP:N	2.54	0.41
2:A4:121:ARG:HA	2:A4:121:ARG:HD2	1.94	0.41
1:A5:135:VAL:HG12	1:A5:137:HIS:HD2	1.86	0.41
1:A5:320:ARG:NH1	1:A5:355:ASP:HB3	2.36	0.41
1:A7:200:MET:HE1	1:A7:268:VAL:HG22	2.03	0.41
1:B3:391:ARG:NH2	2:B4:346:TRP:HE1	2.15	0.41
2:A2:405:VAL:HG21	6:Z:168:ARG:NH2	2.36	0.40
1:A3:36:TYR:HB2	1:A3:59:TYR:CE2	2.45	0.40
1:A3:178:THR:HG22	1:A3:179:VAL:H	1.86	0.40
1:A3:283:ALA:HB3	1:A3:288:GLU:OE2	2.21	0.40
1:A5:91:VAL:CG1	1:A5:116:VAL:HG22	2.51	0.40
1:A5:313:ALA:HB3	1:A5:349:VAL:HG22	2.02	0.40
1:A5:407:GLU:O	1:A5:410:GLU:HG2	2.21	0.40
1:A7:359:LYS:HE2	1:A7:359:LYS:HB3	1.83	0.40
1:B3:145:SER:OG	1:B3:146:GLY:N	2.53	0.40
1:B5:233:MET:O	1:B5:236:ILE:HG22	2.20	0.40
2:B6:100:ALA:HA	1:B7:252:LYS:HE3	2.03	0.40
1:B7:267:MET:HG2	1:B7:369:GLY:O	2.21	0.40
1:B7:314:SER:OG	1:B7:368:ILE:HB	2.21	0.40
3:C:274:LEU:HA	3:C:277:ARG:NE	2.36	0.40
4:X:237:LEU:HD23	4:X:237:LEU:HA	1.84	0.40
4:X1:121:GLN:OE1	5:Y1:69:ALA:HB3	2.21	0.40
6:Z:85:ASP:CG	6:Z:90:GLU:HB2	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:140:GLY:O	1:A1:184:ASN:ND2	2.54	0.40
1:A1:152:ILE:HG23	1:A1:164:MET:SD	2.61	0.40
2:A2:167:LEU:HB3	2:A2:169:PHE:CE1	2.57	0.40
1:A3:14:ASN:OD1	1:A3:65:LEU:HD22	2.22	0.40
2:A4:55:GLU:HG3	2:A4:57:GLY:H	1.87	0.40
1:A5:26:ASP:O	1:A5:359:LYS:NZ	2.38	0.40
2:A6:203:MET:O	2:A6:204:LEU:HD23	2.21	0.40
2:A6:210:TYR:CG	1:A7:324:LYS:HG3	2.55	0.40
1:B3:4:ILE:HB	1:B3:50:TYR:HE1	1.86	0.40
2:B4:221:ARG:HG2	1:B5:322:SER:CB	2.52	0.40
1:B5:8:GLN:CD	1:B5:17:GLY:HA3	2.42	0.40
1:B5:73:MET:CE	1:B5:73:MET:HA	2.50	0.40
2:B6:398:MET:HG2	1:B7:344:TRP:O	2.21	0.40
1:B7:3:GLU:HG3	1:B7:127:CYS:HB2	2.04	0.40
1:B7:150:LEU:HD12	1:B7:150:LEU:C	2.41	0.40
1:B7:286:VAL:HB	1:B7:287:PRO:HD3	2.03	0.40
1:B7:399:THR:HA	1:B7:403:MET:O	2.21	0.40
3:C:459:LEU:O	3:C:463:ILE:HG12	2.22	0.40
1:A1:240:LEU:HD11	1:A1:250:LEU:HD13	2.03	0.40
1:A1:303:ALA:HB2	1:A1:377:MET:HE2	2.03	0.40
2:A2:155:GLU:HA	2:A2:197:HIS:CE1	2.56	0.40
2:A2:246:GLY:HA2	2:A2:357:TYR:CD2	2.56	0.40
2:A2:397:LEU:HD22	1:A3:346:PRO:HD3	2.03	0.40
1:A3:199:CYS:HB3	1:A3:265:PHE:CD1	2.56	0.40
2:A4:407:TRP:CD1	1:A5:255:VAL:HG23	2.57	0.40
1:A5:70:PRO:HG2	2:A6:2:ARG:NH2	2.36	0.40
1:A5:235:GLY:HA2	1:A5:318:ARG:HH11	1.85	0.40
2:A6:123:ARG:HA	2:A6:123:ARG:NE	2.37	0.40
2:A6:175:PRO:HG2	2:A6:176:GLN:OE1	2.21	0.40
1:A7:304:ASP:OD2	1:A7:306:ARG:HG2	2.22	0.40
1:B1:178:THR:CG2	1:B1:181:GLU:HG3	2.51	0.40
1:B1:244:GLY:HA2	1:B1:355:ASP:OD2	2.20	0.40
2:B2:5:ILE:HG22	2:B2:64:ARG:HD3	2.02	0.40
6:Z:73:LEU:O	6:Z:77:THR:HG23	2.22	0.40
6:Z:155:HIS:CG	6:Z:156:CYS:N	2.89	0.40
2:A2:8:HIS:O	2:A2:68:LEU:HD23	2.21	0.40
2:A2:219:ILE:HG13	2:A2:219:ILE:O	2.21	0.40
1:A3:135:VAL:HG12	1:A3:137:HIS:HD2	1.86	0.40
1:A7:157:GLU:HA	1:A7:157:GLU:OE1	2.21	0.40
1:B1:226:ASN:OD1	9:B1:501:GDP:N1	2.39	0.40
1:B1:256:ASN:O	1:B1:312:THR:HG21	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:109:THR:HG22	2:B4:110:ILE:HD13	2.04	0.40
1:B5:266:PHE:HB3	1:B5:368:ILE:HG23	2.03	0.40
1:B5:372:THR:HA	1:B5:422:TYR:HD1	1.87	0.40
1:A1:271:THR:HG21	1:A1:289:LEU:HA	2.02	0.40
2:A2:125:LEU:HD23	2:A2:125:LEU:HA	1.93	0.40
2:A2:306:ASP:OD2	2:A2:308:ARG:HB2	2.22	0.40
2:A2:339:ARG:HB2	2:A2:339:ARG:HH11	1.86	0.40
1:A3:421:GLU:HA	1:A3:424:GLN:HG2	2.02	0.40
2:A4:73:THR:CG2	1:A5:2:ARG:HH22	2.34	0.40
2:A4:279:GLU:HA	2:A4:279:GLU:OE2	2.21	0.40
2:A4:403:ALA:HB2	1:A5:344:TRP:CZ3	2.48	0.40
1:A5:70:PRO:N	1:A5:92:PHE:HZ	2.19	0.40
1:A5:414:ASN:HA	1:A5:417:ASP:OD2	2.22	0.40
2:A6:96:LYS:HE3	2:A6:96:LYS:HB3	1.90	0.40
2:A6:205:ASP:CB	2:A6:303:VAL:HA	2.52	0.40
2:A6:304:LYS:HA	2:A6:304:LYS:HD3	1.74	0.40
2:A6:312:TYR:HD1	2:A6:381:SER:HB2	1.86	0.40
1:B3:102:ALA:HB2	1:B3:403:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A1	424/443 (96%)	399 (94%)	25 (6%)	0	100	100
1	A3	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	A5	424/443 (96%)	407 (96%)	17 (4%)	0	100	100
1	A7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	B1	415/443 (94%)	396 (95%)	19 (5%)	0	100	100
1	B3	404/443 (91%)	392 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B5	424/443 (96%)	403 (95%)	21 (5%)	0	100	100
1	B7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
2	A2	426/451 (94%)	402 (94%)	24 (6%)	0	100	100
2	A4	423/451 (94%)	409 (97%)	14 (3%)	0	100	100
2	A6	425/451 (94%)	408 (96%)	17 (4%)	0	100	100
2	B2	405/451 (90%)	391 (96%)	14 (4%)	0	100	100
2	B4	403/451 (89%)	385 (96%)	18 (4%)	0	100	100
2	B6	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
3	C	210/4485 (5%)	204 (97%)	6 (3%)	0	100	100
4	X	151/749 (20%)	151 (100%)	0	0	100	100
4	X1	140/749 (19%)	140 (100%)	0	0	100	100
5	Y	117/552 (21%)	116 (99%)	1 (1%)	0	100	100
5	Y1	145/552 (26%)	145 (100%)	0	0	100	100
6	Z	168/184 (91%)	156 (93%)	10 (6%)	2 (1%)	13	42
All	All	6799/13521 (50%)	6526 (96%)	271 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Z	86	LYS
6	Z	141	ASP

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 PDB entries followed by that with respect to all EM entries.

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	A1	367/379 (97%)	367 (100%)	0	100	100
1	A3	367/379 (97%)	366 (100%)	1 (0%)	92	96
1	A5	367/379 (97%)	367 (100%)	0	100	100
1	A7	367/379 (97%)	367 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B1	363/379 (96%)	363 (100%)	0	100 100
1	B3	356/379 (94%)	356 (100%)	0	100 100
1	B5	367/379 (97%)	367 (100%)	0	100 100
1	B7	367/379 (97%)	366 (100%)	1 (0%)	92 96
2	A2	361/374 (96%)	360 (100%)	1 (0%)	92 96
2	A4	359/374 (96%)	354 (99%)	5 (1%)	67 82
2	A6	361/374 (96%)	361 (100%)	0	100 100
2	B2	347/374 (93%)	347 (100%)	0	100 100
2	B4	346/374 (92%)	346 (100%)	0	100 100
2	B6	359/374 (96%)	359 (100%)	0	100 100
3	C	197/3945 (5%)	197 (100%)	0	100 100
4	X	50/618 (8%)	50 (100%)	0	100 100
4	X1	125/618 (20%)	121 (97%)	4 (3%)	39 67
5	Y	63/462 (14%)	63 (100%)	0	100 100
5	Y1	128/462 (28%)	127 (99%)	1 (1%)	81 89
6	Z	150/162 (93%)	146 (97%)	4 (3%)	44 71
All	All	5767/11543 (50%)	5750 (100%)	17 (0%)	92 96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A2	73	THR
1	A3	390	ARG
2	A4	51	THR
2	A4	62	VAL
2	A4	346	TRP
2	A4	347	CYS
2	A4	349	THR
1	B7	72	THR
4	X1	204	LEU
4	X1	208	ARG
4	X1	213	HIS
4	X1	214	LEU
5	Y1	166	GLU
6	Z	9	ARG
6	Z	10	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	Z	122	LEU
6	Z	123	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	A2	11	GLN
2	A2	101	ASN
2	A2	329	ASN
1	A3	6	HIS
1	A3	131	GLN
1	A3	134	GLN
1	A3	195	ASN
1	A3	256	ASN
2	A4	91	GLN
2	A4	102	ASN
2	A4	228	ASN
1	A7	204	ASN
1	B1	6	HIS
1	B1	131	GLN
2	B2	256	GLN
2	B2	329	ASN
1	B3	15	GLN
1	B3	190	HIS
2	B4	88	HIS
2	B4	102	ASN
2	B4	258	ASN
2	B4	329	ASN
1	B5	15	GLN
1	B5	99	ASN
1	B5	100	ASN
1	B5	347	ASN
1	B5	384	GLN
2	B6	102	ASN
2	B6	329	ASN
1	B7	100	ASN
1	B7	334	GLN
1	B7	375	GLN
3	C	378	ASN
4	X1	240	HIS
6	Z	17	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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
9	GDP	B5	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
7	GTP	A5	501	8	26,34,34	1.22	2 (7%)	32,54,54	1.66	7 (21%)
9	GDP	A7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	5 (16%)
9	GDP	A3	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	5 (16%)
9	GDP	A5	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	5 (16%)
9	GDP	A1	503	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
9	GDP	B3	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
7	GTP	A7	501	8	26,34,34	1.20	2 (7%)	32,54,54	1.66	7 (21%)
7	GTP	A1	501	8	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
7	GTP	B5	501	8	26,34,34	1.21	2 (7%)	32,54,54	1.62	7 (21%)
9	GDP	B7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	5 (16%)
7	GTP	A3	501	8	26,34,34	1.17	2 (7%)	32,54,54	1.72	7 (21%)
7	GTP	B2	501	8	26,34,34	1.19	2 (7%)	32,54,54	1.73	7 (21%)
9	GDP	B1	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GTP	B7	501	8	26,34,34	1.20	2 (7%)	32,54,54	1.58	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B5	502	-	-	4/12/32/32	0/3/3/3
7	GTP	A5	501	8	-	6/18/38/38	0/3/3/3
9	GDP	A7	502	-	-	4/12/32/32	0/3/3/3
9	GDP	A3	502	-	-	1/12/32/32	0/3/3/3
9	GDP	A5	502	-	-	1/12/32/32	0/3/3/3
9	GDP	A1	503	-	-	3/12/32/32	0/3/3/3
9	GDP	B3	502	-	-	3/12/32/32	0/3/3/3
7	GTP	A7	501	8	-	7/18/38/38	0/3/3/3
7	GTP	A1	501	8	-	5/18/38/38	0/3/3/3
7	GTP	B5	501	8	-	7/18/38/38	0/3/3/3
9	GDP	B7	502	-	-	6/12/32/32	0/3/3/3
7	GTP	A3	501	8	-	7/18/38/38	0/3/3/3
7	GTP	B2	501	8	-	4/18/38/38	0/3/3/3
9	GDP	B1	501	-	-	2/12/32/32	0/3/3/3
7	GTP	B7	501	8	-	6/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A7	501	GTP	C5-C6	-4.28	1.38	1.47
7	B5	501	GTP	C5-C6	-4.27	1.38	1.47
7	A5	501	GTP	C5-C6	-4.25	1.38	1.47
7	B7	501	GTP	C5-C6	-4.23	1.38	1.47
7	B2	501	GTP	C5-C6	-4.16	1.39	1.47
7	A3	501	GTP	C5-C6	-4.04	1.39	1.47
7	A1	501	GTP	C5-C6	-3.96	1.39	1.47
9	B5	502	GDP	C6-N1	-2.64	1.33	1.37
9	A3	502	GDP	C6-N1	-2.63	1.34	1.37
9	B1	501	GDP	C6-N1	-2.58	1.34	1.37
9	B3	502	GDP	C6-N1	-2.54	1.34	1.37
9	A7	502	GDP	C6-N1	-2.52	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B7	502	GDP	C6-N1	-2.50	1.34	1.37
9	A5	502	GDP	C6-N1	-2.43	1.34	1.37
9	A1	503	GDP	C6-N1	-2.42	1.34	1.37
7	A1	501	GTP	C2-N3	2.20	1.38	1.33
7	B7	501	GTP	C2-N3	2.18	1.38	1.33
7	A3	501	GTP	C2-N3	2.18	1.38	1.33
7	B5	501	GTP	C2-N3	2.14	1.38	1.33
7	A5	501	GTP	C2-N3	2.09	1.38	1.33
7	B2	501	GTP	C2-N3	2.06	1.38	1.33
7	A7	501	GTP	C2-N3	2.05	1.38	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B2	501	GTP	PB-O3B-PG	-4.99	115.69	132.83
7	A5	501	GTP	PA-O3A-PB	-4.67	116.80	132.83
7	A3	501	GTP	PB-O3B-PG	-4.46	117.50	132.83
7	A3	501	GTP	PA-O3A-PB	-4.46	117.53	132.83
7	A7	501	GTP	PA-O3A-PB	-4.45	117.54	132.83
7	B5	501	GTP	PA-O3A-PB	-4.33	117.95	132.83
7	A1	501	GTP	PA-O3A-PB	-4.06	118.89	132.83
7	A1	501	GTP	PB-O3B-PG	-3.97	119.19	132.83
9	B3	502	GDP	PA-O3A-PB	-3.94	119.31	132.83
7	B2	501	GTP	PA-O3A-PB	-3.85	119.61	132.83
7	A7	501	GTP	PB-O3B-PG	-3.82	119.71	132.83
9	B7	502	GDP	PA-O3A-PB	-3.65	120.30	132.83
7	B7	501	GTP	PB-O3B-PG	-3.63	120.37	132.83
9	B5	502	GDP	PA-O3A-PB	-3.52	120.75	132.83
7	B5	501	GTP	C5-C6-N1	3.45	120.04	113.95
9	B1	501	GDP	PA-O3A-PB	-3.44	121.04	132.83
7	A3	501	GTP	C5-C6-N1	3.42	119.98	113.95
7	B7	501	GTP	PA-O3A-PB	-3.41	121.14	132.83
7	A5	501	GTP	PB-O3B-PG	-3.37	121.28	132.83
7	A5	501	GTP	C5-C6-N1	3.34	119.85	113.95
7	B2	501	GTP	C5-C6-N1	3.32	119.81	113.95
7	B7	501	GTP	C5-C6-N1	3.30	119.78	113.95
7	A7	501	GTP	C5-C6-N1	3.27	119.72	113.95
9	B1	501	GDP	C3'-C2'-C1'	3.25	105.88	100.98
9	A1	503	GDP	PA-O3A-PB	-3.24	121.72	132.83
7	A1	501	GTP	C5-C6-N1	3.21	119.62	113.95
9	B7	502	GDP	C3'-C2'-C1'	3.17	105.75	100.98
9	A3	502	GDP	PA-O3A-PB	-3.16	122.00	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B5	501	GTP	PB-O3B-PG	-3.16	122.00	132.83
9	A5	502	GDP	PA-O3A-PB	-3.11	122.14	132.83
7	B2	501	GTP	C8-N7-C5	3.10	108.89	102.99
7	A1	501	GTP	C8-N7-C5	3.05	108.80	102.99
9	A1	503	GDP	C3'-C2'-C1'	3.04	105.56	100.98
7	A3	501	GTP	C8-N7-C5	3.04	108.78	102.99
9	A3	502	GDP	C3'-C2'-C1'	3.03	105.54	100.98
7	A3	501	GTP	C2-N1-C6	-3.03	119.52	125.10
7	A7	501	GTP	C8-N7-C5	3.02	108.75	102.99
7	B5	501	GTP	C2-N1-C6	-3.02	119.54	125.10
9	A5	502	GDP	C3'-C2'-C1'	3.01	105.52	100.98
7	B7	501	GTP	C2-N1-C6	-3.00	119.57	125.10
7	A5	501	GTP	C8-N7-C5	3.00	108.70	102.99
7	B7	501	GTP	C8-N7-C5	2.98	108.66	102.99
7	B5	501	GTP	C8-N7-C5	2.97	108.65	102.99
7	B2	501	GTP	C2-N1-C6	-2.96	119.65	125.10
9	A7	502	GDP	PA-O3A-PB	-2.96	122.68	132.83
7	A5	501	GTP	C2-N1-C6	-2.94	119.68	125.10
7	A7	501	GTP	C2-N1-C6	-2.93	119.70	125.10
7	B2	501	GTP	O4'-C1'-C2'	-2.87	102.73	106.93
7	A1	501	GTP	C2-N1-C6	-2.85	119.85	125.10
9	B3	502	GDP	C3'-C2'-C1'	2.85	105.27	100.98
9	A7	502	GDP	C3'-C2'-C1'	2.85	105.27	100.98
9	B5	502	GDP	C3'-C2'-C1'	2.77	105.16	100.98
7	B5	501	GTP	C3'-C2'-C1'	2.70	105.04	100.98
7	A5	501	GTP	C3'-C2'-C1'	2.58	104.86	100.98
7	A5	501	GTP	O6-C6-C5	-2.55	119.38	124.37
7	A1	501	GTP	C3'-C2'-C1'	2.53	104.78	100.98
7	A7	501	GTP	C3'-C2'-C1'	2.49	104.73	100.98
7	A3	501	GTP	C3'-C2'-C1'	2.46	104.68	100.98
9	A3	502	GDP	C5-C6-N1	2.45	118.28	113.95
9	B1	501	GDP	C8-N7-C5	2.41	107.58	102.99
9	B5	502	GDP	C5-C6-N1	2.40	118.19	113.95
7	A7	501	GTP	O6-C6-C5	-2.38	119.72	124.37
9	A1	503	GDP	C5-C6-N1	2.38	118.16	113.95
9	B1	501	GDP	C5-C6-N1	2.38	118.15	113.95
9	A5	502	GDP	C5-C6-N1	2.38	118.15	113.95
9	A5	502	GDP	C8-N7-C5	2.38	107.52	102.99
9	B3	502	GDP	C5-C6-N1	2.37	118.13	113.95
7	B7	501	GTP	C3'-C2'-C1'	2.37	104.54	100.98
9	A7	502	GDP	C8-N7-C5	2.34	107.44	102.99
9	A1	503	GDP	C8-N7-C5	2.33	107.42	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B3	502	GDP	C8-N7-C5	2.32	107.41	102.99
9	A7	502	GDP	C5-C6-N1	2.32	118.05	113.95
9	B5	502	GDP	C8-N7-C5	2.29	107.36	102.99
9	A3	502	GDP	C8-N7-C5	2.28	107.33	102.99
9	B7	502	GDP	O4'-C4'-C5'	-2.28	101.88	109.37
9	B7	502	GDP	C5-C6-N1	2.26	117.95	113.95
9	B7	502	GDP	C8-N7-C5	2.26	107.30	102.99
7	B7	501	GTP	O6-C6-C5	-2.26	119.97	124.37
7	B2	501	GTP	O6-C6-C5	-2.25	119.97	124.37
7	B5	501	GTP	O6-C6-C5	-2.21	120.06	124.37
9	A3	502	GDP	O3B-PB-O3A	2.18	111.95	104.64
7	A3	501	GTP	O6-C6-C5	-2.08	120.32	124.37
9	A7	502	GDP	O3B-PB-O3A	2.07	111.58	104.64
7	A1	501	GTP	O6-C6-C5	-2.05	120.37	124.37
9	A5	502	GDP	O3B-PB-O3A	2.02	111.41	104.64

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	501	GTP	C5'-O5'-PA-O1A
7	A3	501	GTP	C5'-O5'-PA-O1A
7	A3	501	GTP	C5'-O5'-PA-O2A
7	A5	501	GTP	C5'-O5'-PA-O1A
7	A7	501	GTP	C5'-O5'-PA-O1A
7	A7	501	GTP	C5'-O5'-PA-O2A
7	B2	501	GTP	C5'-O5'-PA-O3A
7	B5	501	GTP	C5'-O5'-PA-O1A
7	B5	501	GTP	C5'-O5'-PA-O2A
7	B7	501	GTP	C5'-O5'-PA-O3A
7	B7	501	GTP	C5'-O5'-PA-O2A
9	A1	503	GDP	PA-O3A-PB-O3B
9	A1	503	GDP	C5'-O5'-PA-O1A
9	A7	502	GDP	PA-O3A-PB-O3B
9	B1	501	GDP	C5'-O5'-PA-O3A
9	B1	501	GDP	C5'-O5'-PA-O1A
9	B3	502	GDP	PA-O3A-PB-O3B
9	B3	502	GDP	C5'-O5'-PA-O1A
9	B5	502	GDP	C5'-O5'-PA-O1A
9	B7	502	GDP	PA-O3A-PB-O3B
9	B7	502	GDP	C5'-O5'-PA-O3A
9	B7	502	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B7	502	GDP	C3'-C4'-C5'-O5'
7	A7	501	GTP	C3'-C4'-C5'-O5'
7	A5	501	GTP	C3'-C4'-C5'-O5'
9	B7	502	GDP	O4'-C4'-C5'-O5'
7	A5	501	GTP	O4'-C4'-C5'-O5'
7	B5	501	GTP	C3'-C4'-C5'-O5'
9	B7	502	GDP	PA-O3A-PB-O1B
7	A7	501	GTP	O4'-C4'-C5'-O5'
7	A3	501	GTP	C4'-C5'-O5'-PA
7	A7	501	GTP	C4'-C5'-O5'-PA
7	B2	501	GTP	C4'-C5'-O5'-PA
7	B7	501	GTP	PB-O3A-PA-O5'
9	A1	503	GDP	PA-O3A-PB-O2B
7	A7	501	GTP	C5'-O5'-PA-O3A
7	A1	501	GTP	C4'-C5'-O5'-PA
7	B5	501	GTP	C4'-C5'-O5'-PA
7	B7	501	GTP	C4'-C5'-O5'-PA
7	A1	501	GTP	C5'-O5'-PA-O2A
7	A5	501	GTP	C5'-O5'-PA-O2A
7	B2	501	GTP	C5'-O5'-PA-O2A
7	A5	501	GTP	C4'-C5'-O5'-PA
7	B5	501	GTP	O4'-C4'-C5'-O5'
7	A7	501	GTP	PA-O3A-PB-O2B
9	A7	502	GDP	C3'-C4'-C5'-O5'
9	B3	502	GDP	PA-O3A-PB-O1B
7	A3	501	GTP	C3'-C4'-C5'-O5'
7	B7	501	GTP	PA-O3A-PB-O1B
9	A7	502	GDP	PA-O3A-PB-O1B
9	B5	502	GDP	PA-O3A-PB-O1B
7	B2	501	GTP	PB-O3B-PG-O3G
7	A1	501	GTP	C5'-O5'-PA-O3A
7	A3	501	GTP	C5'-O5'-PA-O3A
7	A5	501	GTP	C5'-O5'-PA-O3A
7	B5	501	GTP	C5'-O5'-PA-O3A
9	B5	502	GDP	C5'-O5'-PA-O3A
7	A1	501	GTP	C3'-C4'-C5'-O5'
9	B5	502	GDP	C3'-C4'-C5'-O5'
7	A3	501	GTP	PA-O3A-PB-O1B
7	A3	501	GTP	PA-O3A-PB-O2B
7	B5	501	GTP	PA-O3A-PB-O2B
7	B7	501	GTP	PA-O3A-PB-O2B
9	A3	502	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

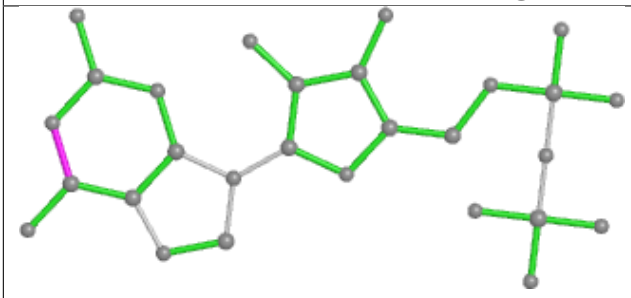
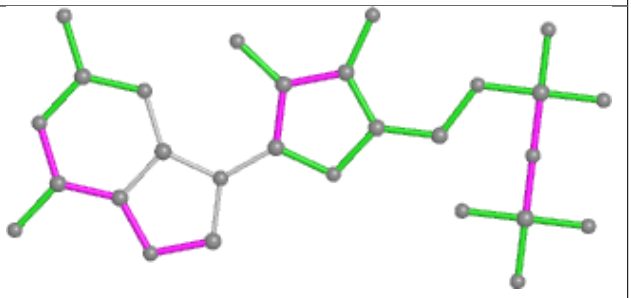
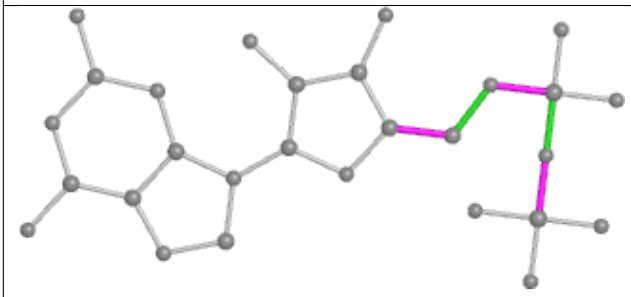
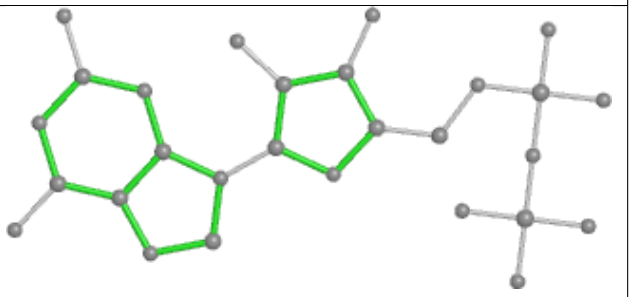
Mol	Chain	Res	Type	Atoms
9	A5	502	GDP	C5'-O5'-PA-O1A
9	A7	502	GDP	C5'-O5'-PA-O1A

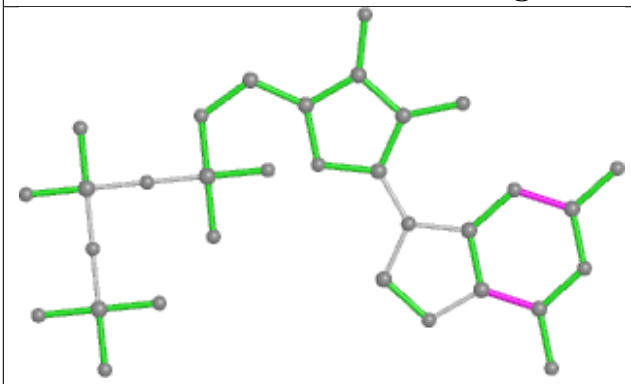
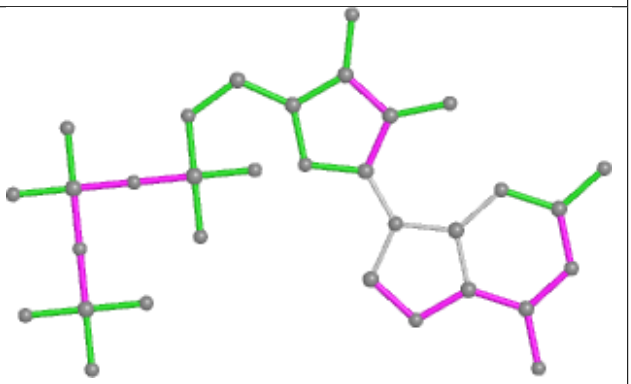
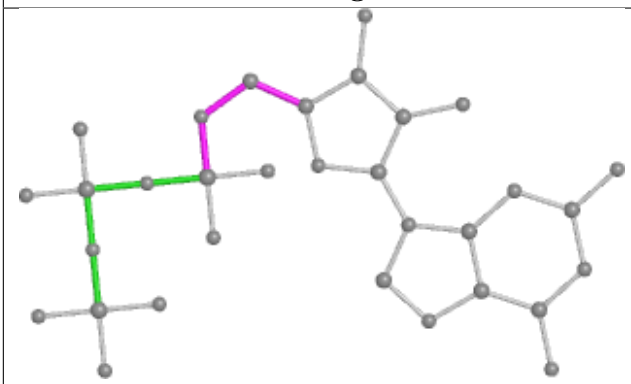
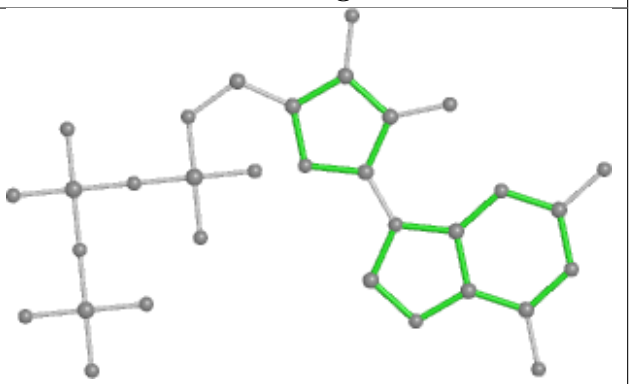
There are no ring outliers.

10 monomers are involved in 19 short contacts:

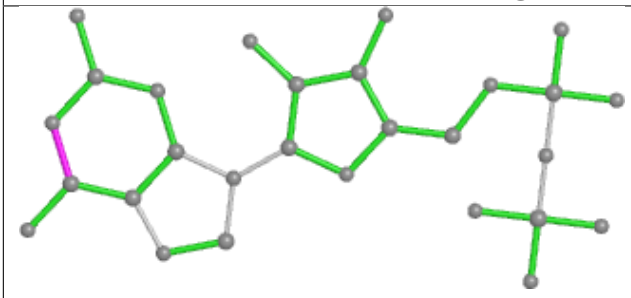
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B5	502	GDP	1	0
7	A5	501	GTP	1	0
9	A7	502	GDP	2	0
9	A3	502	GDP	2	0
9	B3	502	GDP	2	0
7	A7	501	GTP	4	0
9	B7	502	GDP	2	0
7	A3	501	GTP	1	0
7	B2	501	GTP	1	0
9	B1	501	GDP	3	0

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

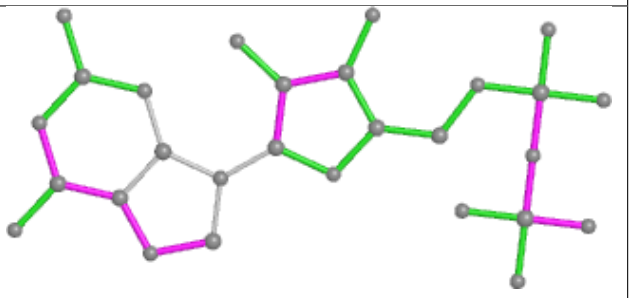
Ligand GDP B5 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP A5 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

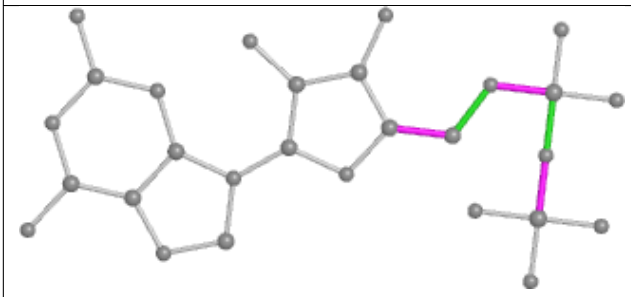
Ligand GDP A7 502



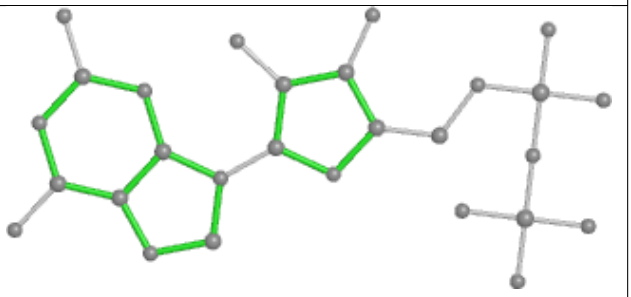
Bond lengths



Bond angles

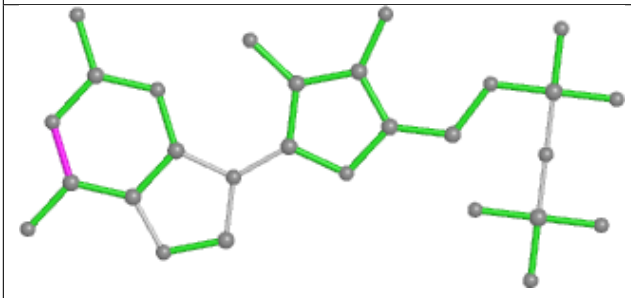


Torsions

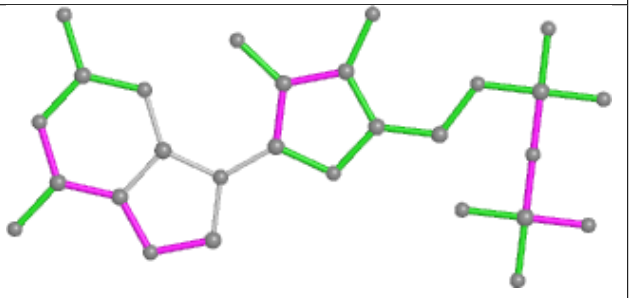


Rings

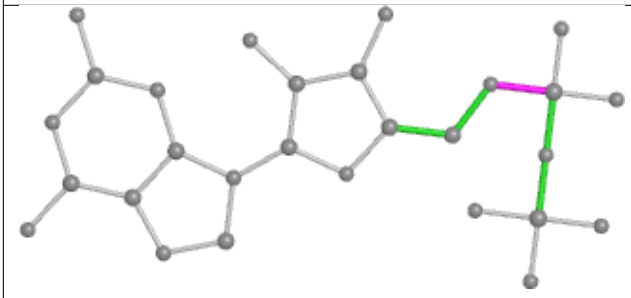
Ligand GDP A3 502



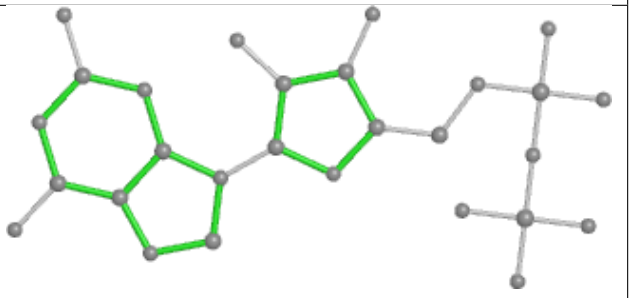
Bond lengths



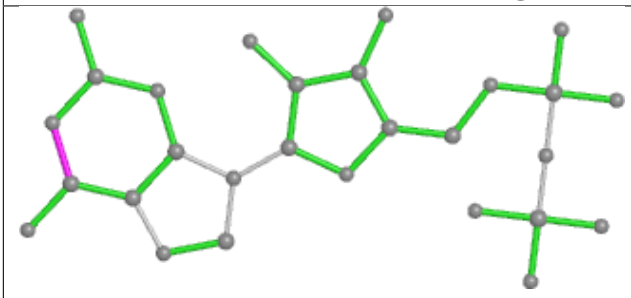
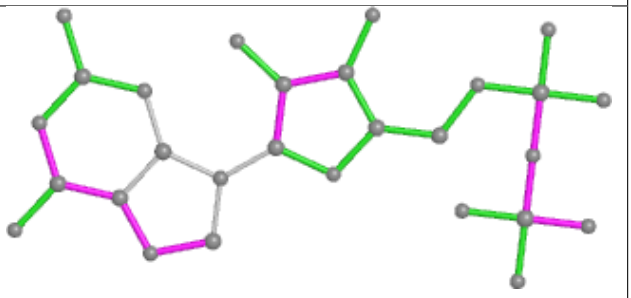
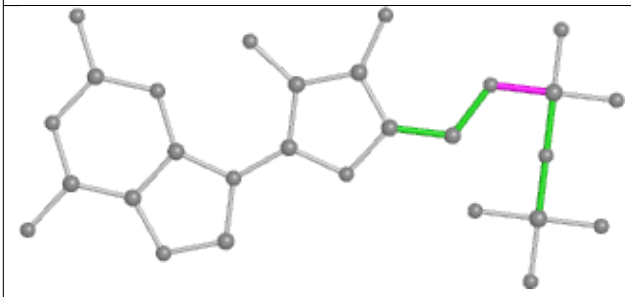
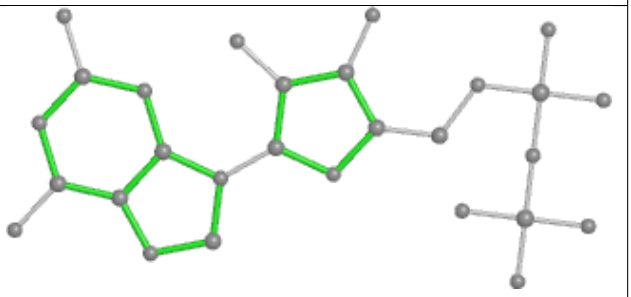
Bond angles

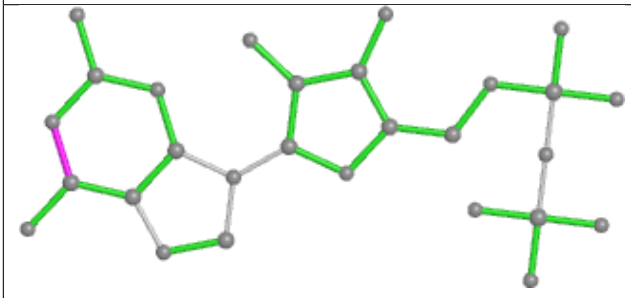
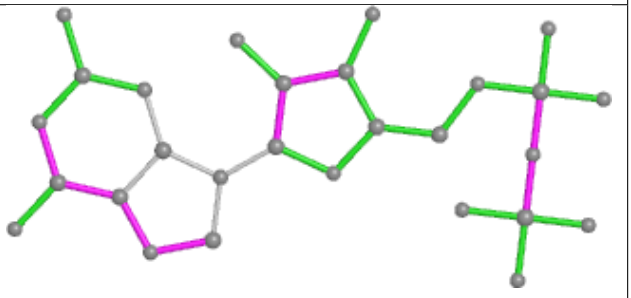
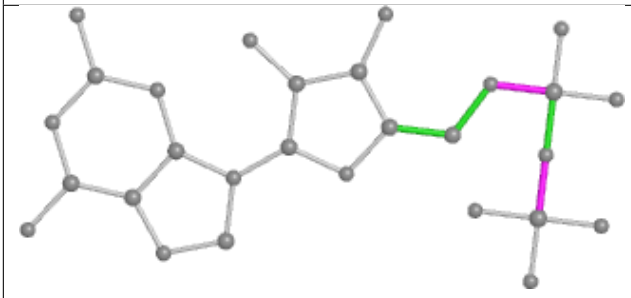
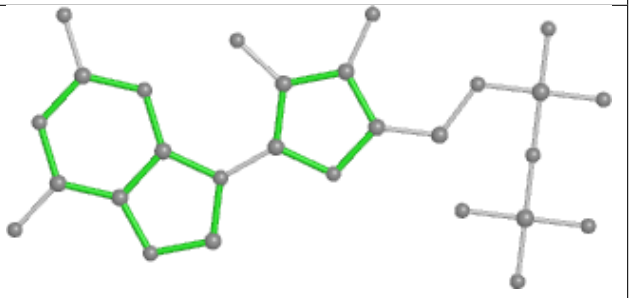


Torsions

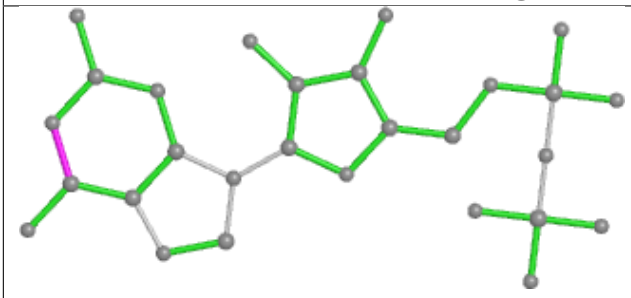


Rings

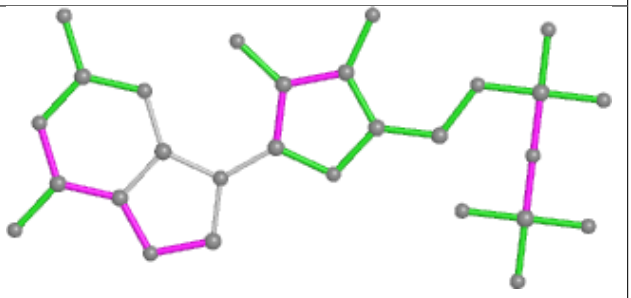
Ligand GDP A5 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP A1 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

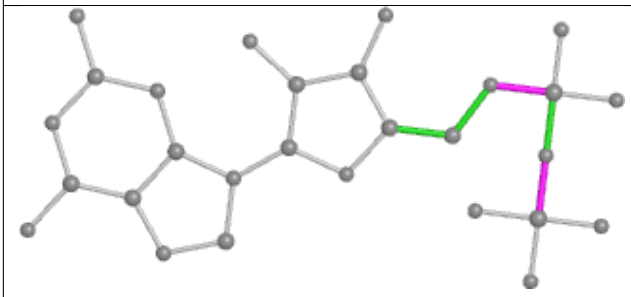
Ligand GDP B3 502



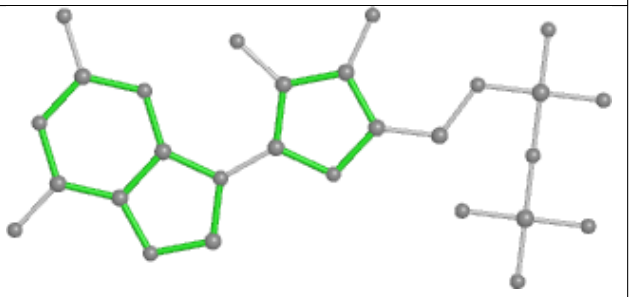
Bond lengths



Bond angles

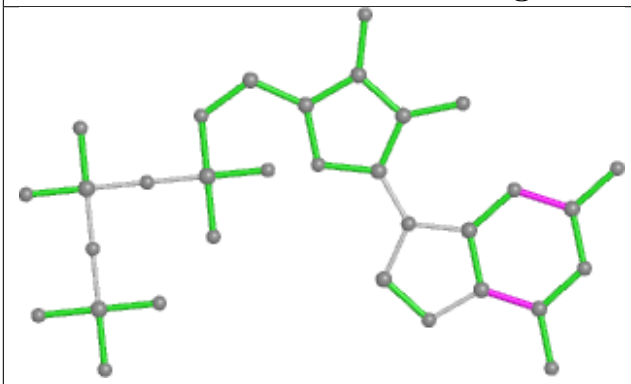


Torsions

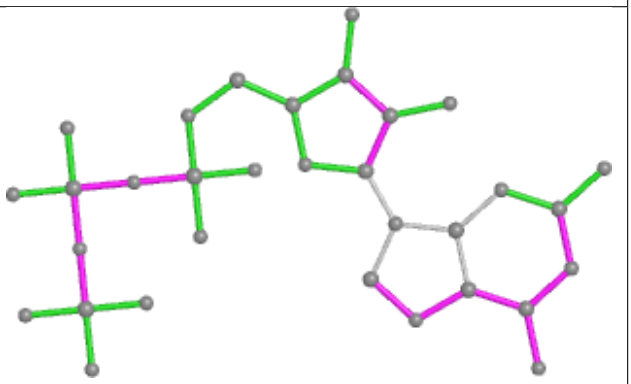


Rings

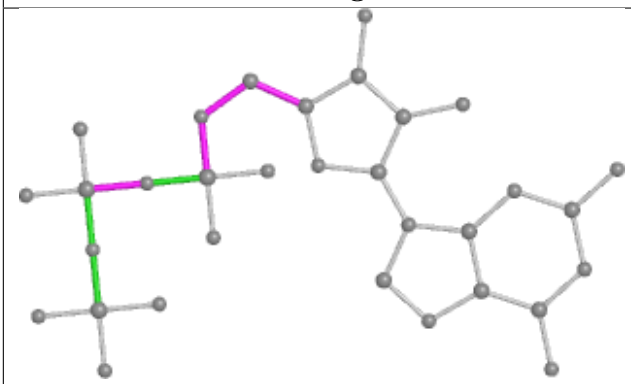
Ligand GTP A7 501



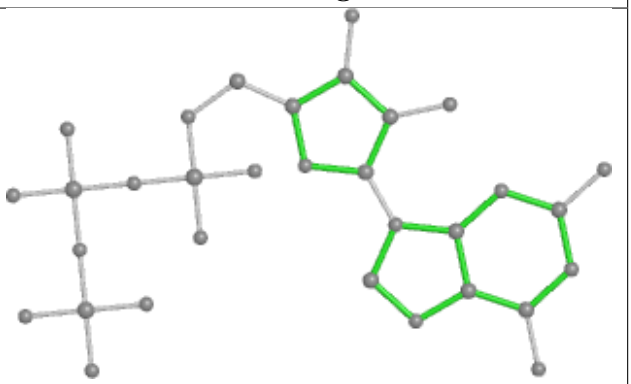
Bond lengths



Bond angles

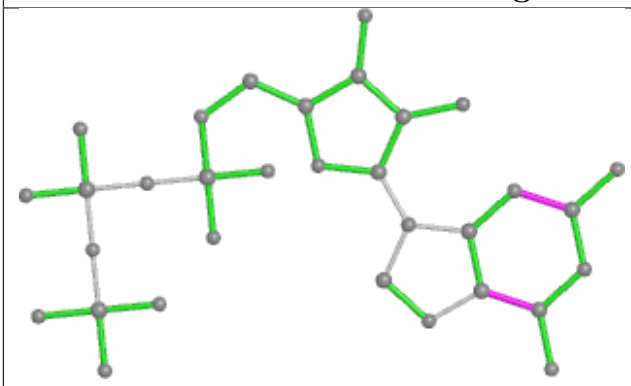


Torsions

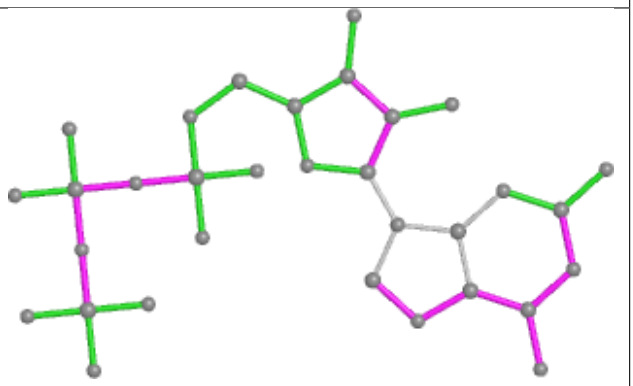


Rings

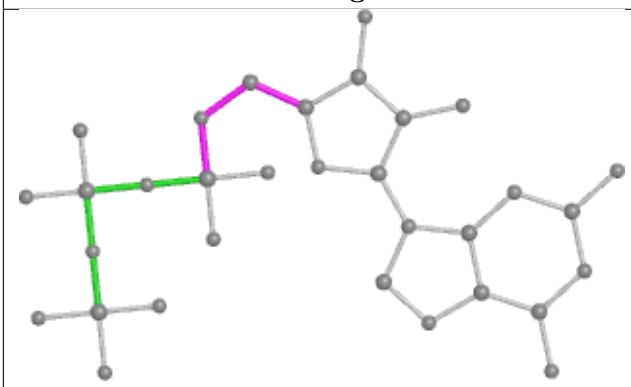
Ligand GTP A1 501



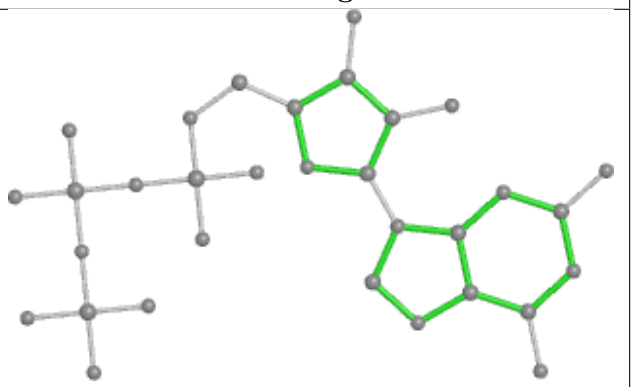
Bond lengths



Bond angles

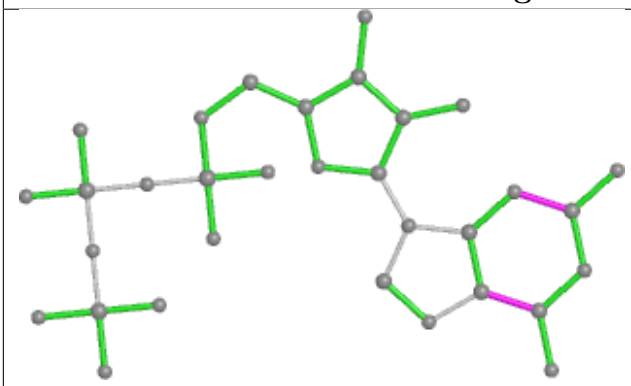


Torsions

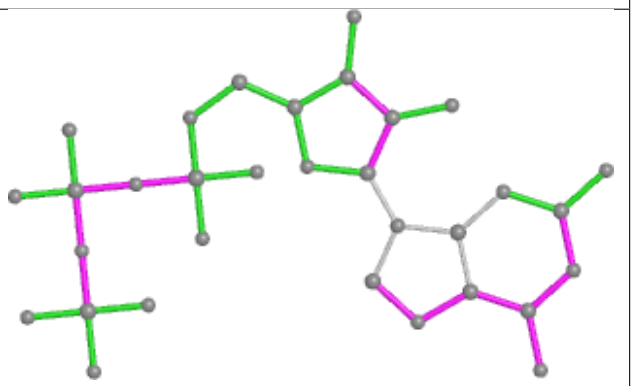


Rings

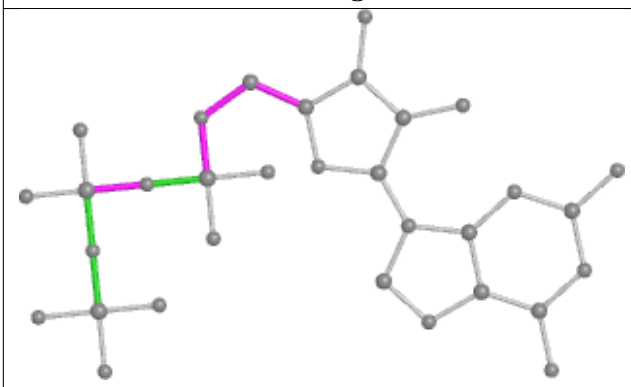
Ligand GTP B5 501



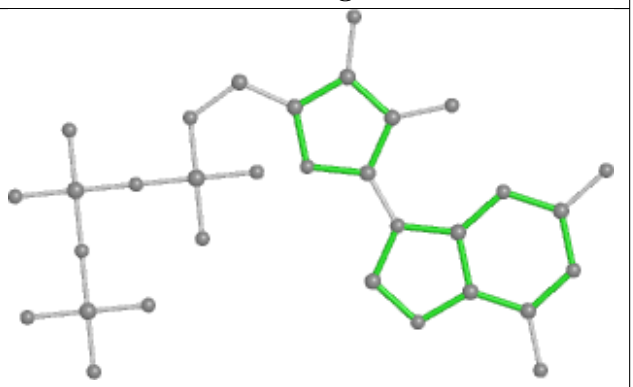
Bond lengths



Bond angles

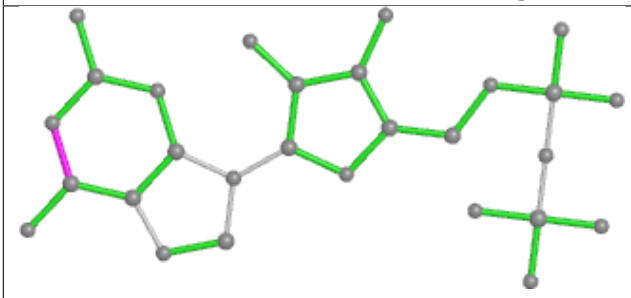


Torsions

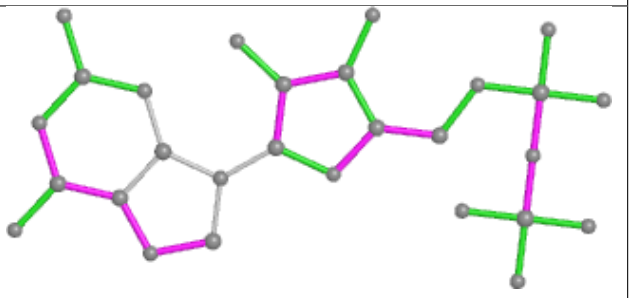


Rings

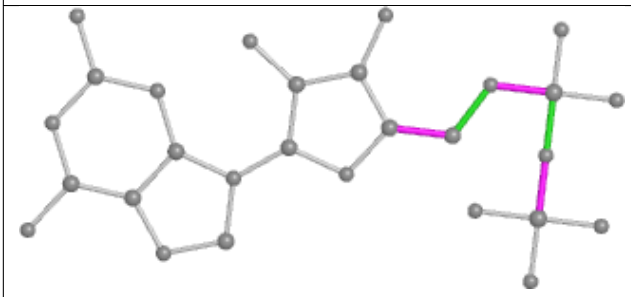
Ligand GDP B7 502



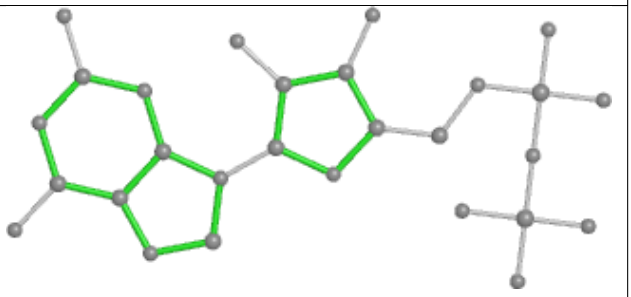
Bond lengths



Bond angles

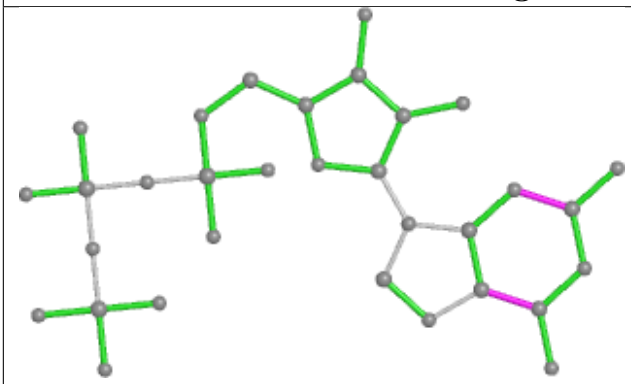


Torsions

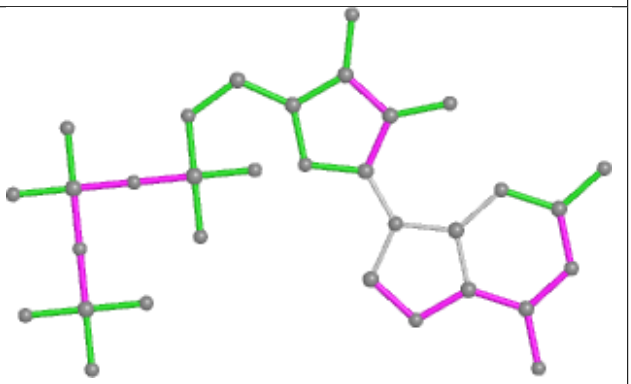


Rings

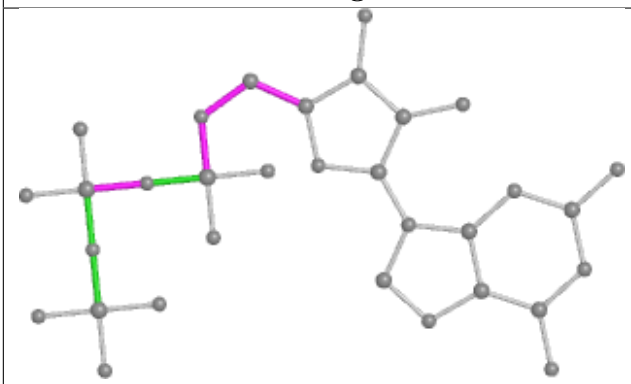
Ligand GTP A3 501



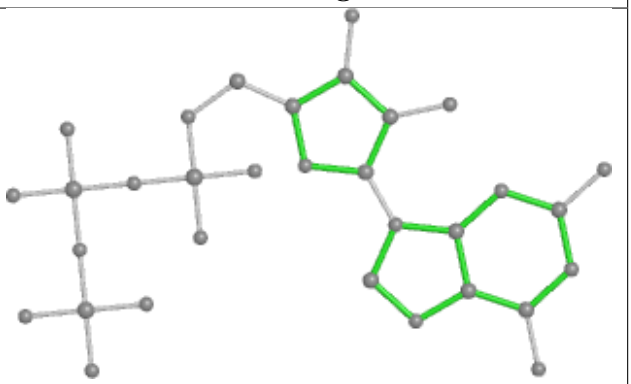
Bond lengths



Bond angles

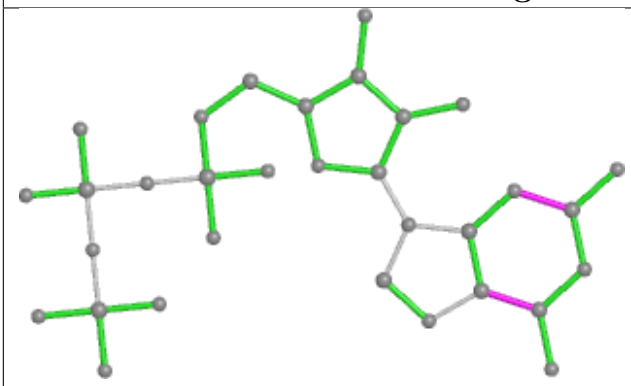


Torsions

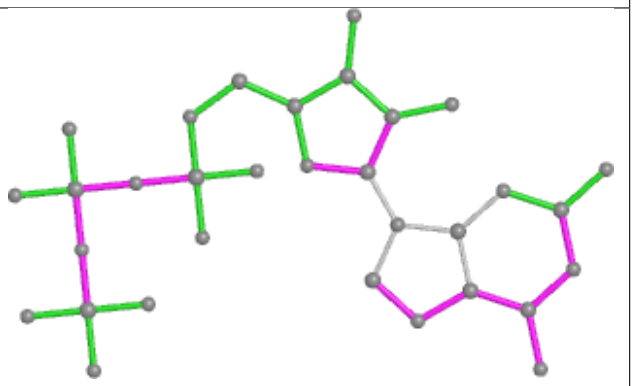


Rings

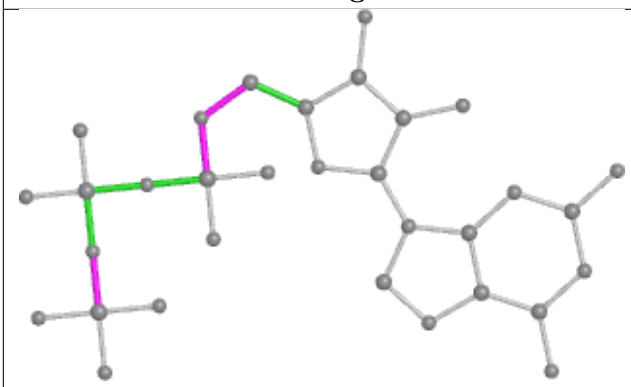
Ligand GTP B2 501



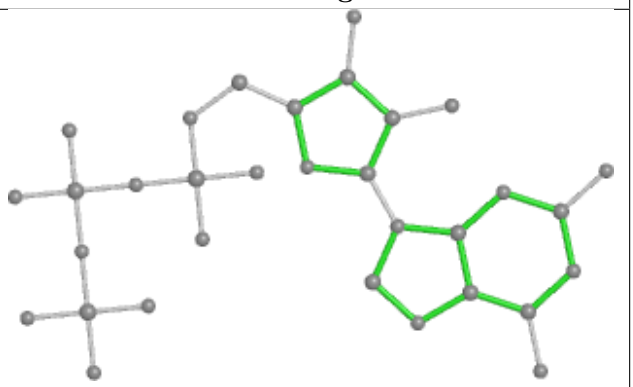
Bond lengths



Bond angles

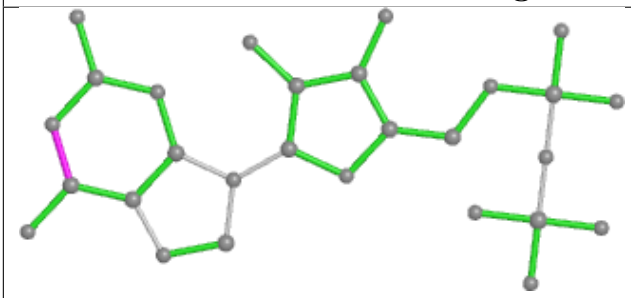


Torsions

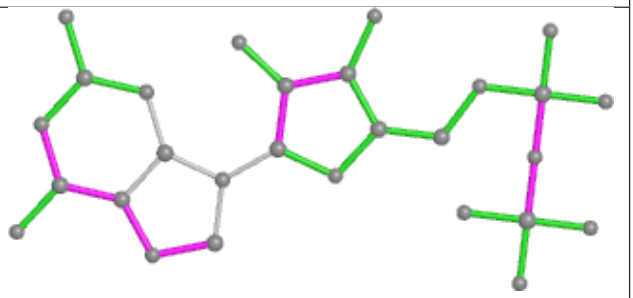


Rings

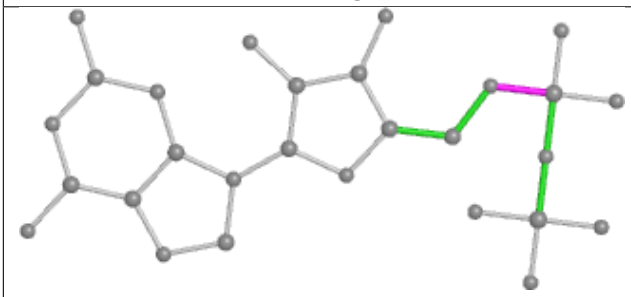
Ligand GDP B1 501



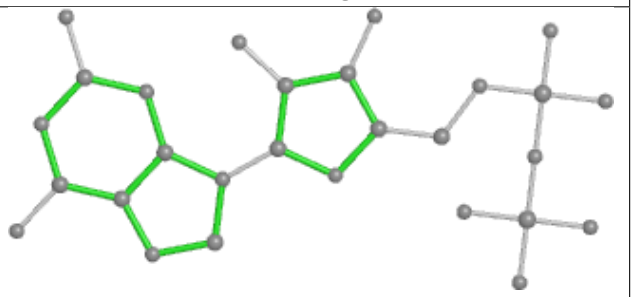
Bond lengths



Bond angles

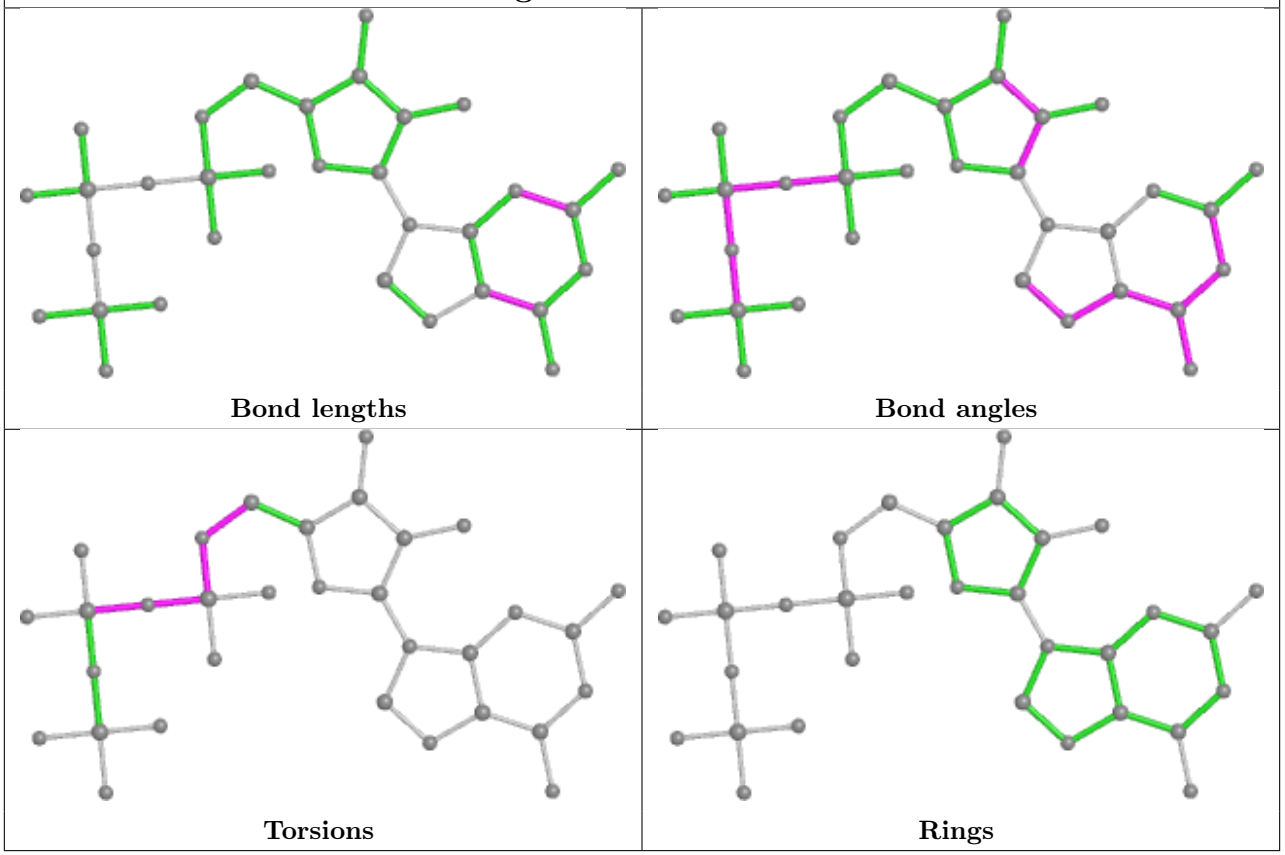


Torsions



Rings

Ligand GTP B7 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

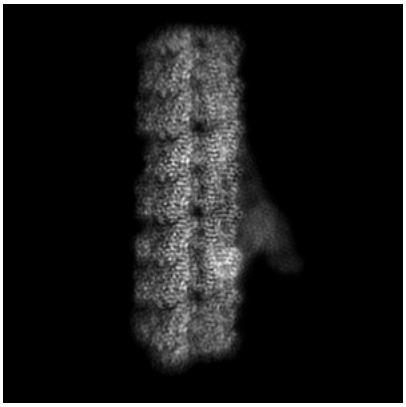
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23084. These allow visual inspection of the internal detail of the map and identification of artifacts.

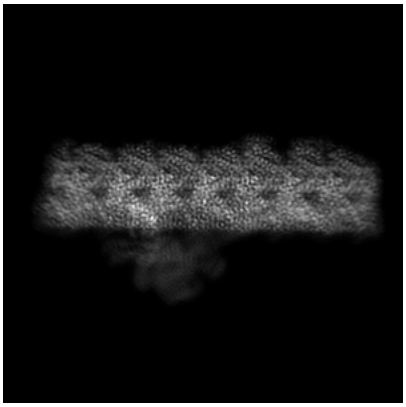
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

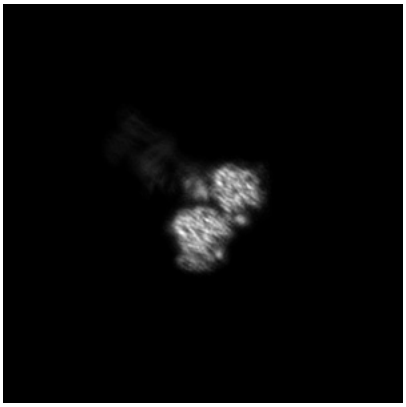
6.1.1 Primary map



X



Y

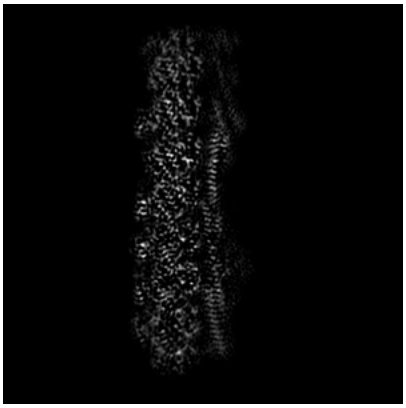


Z

The images above show the map projected in three orthogonal directions.

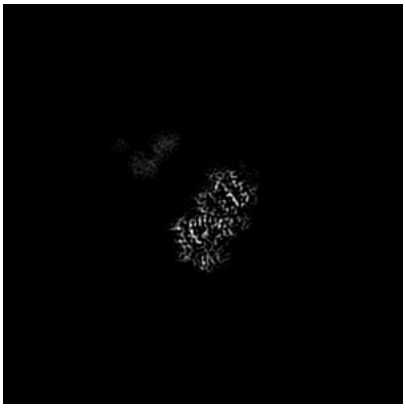
6.2 Central slices

6.2.1 Primary map



X Index: 145

Y Index: 145



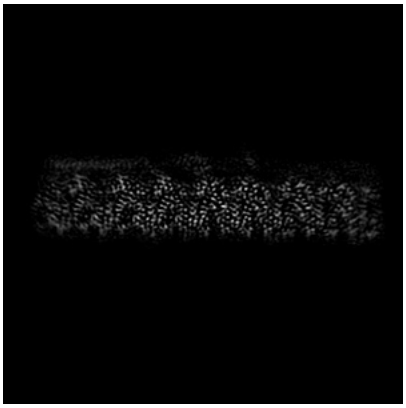
Z Index: 145

The images above show central slices of the map in three orthogonal directions.

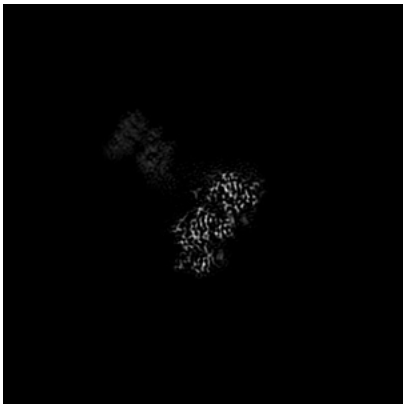
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 141



Y Index: 129

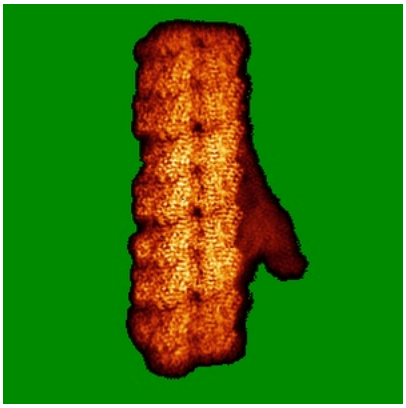


Z Index: 115

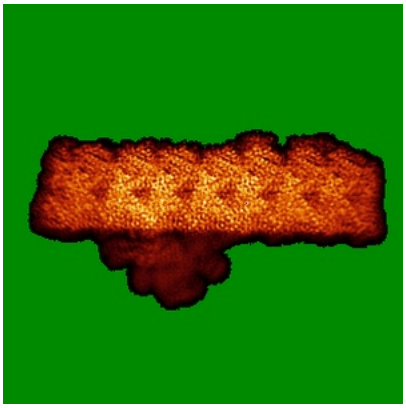
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

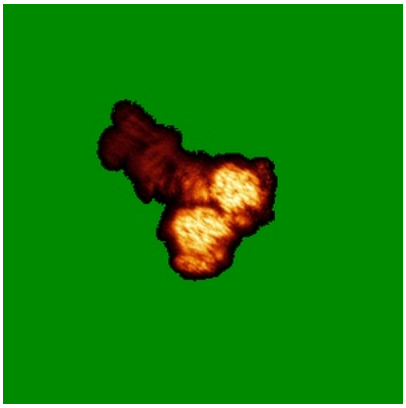
6.4.1 Primary map



X



Y

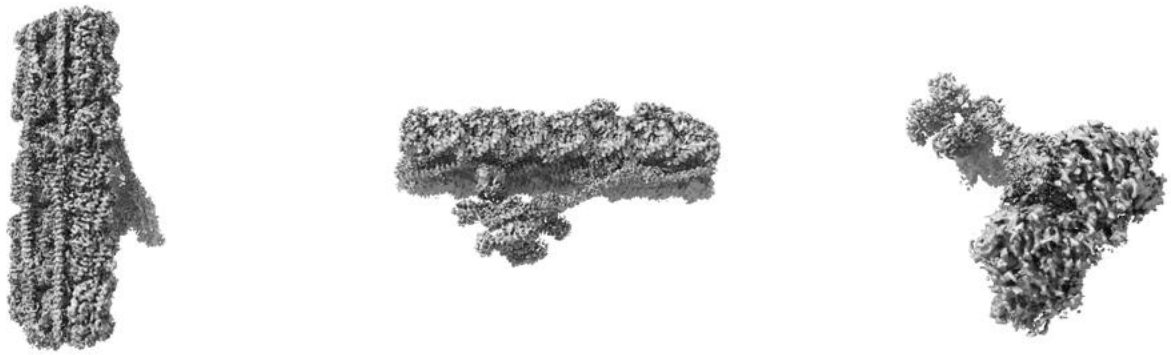


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

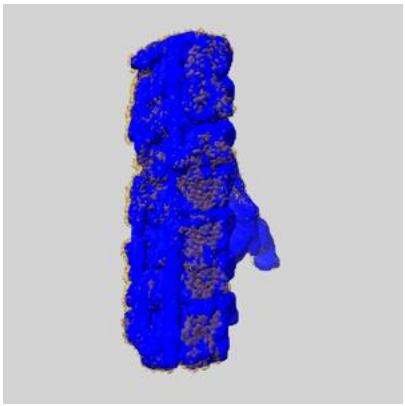
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

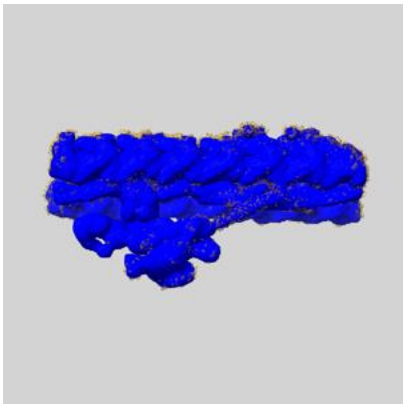
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

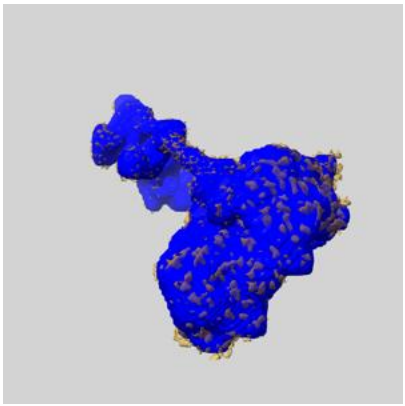
6.6.1 emd_23084_msk_1.map (i)



X



Y

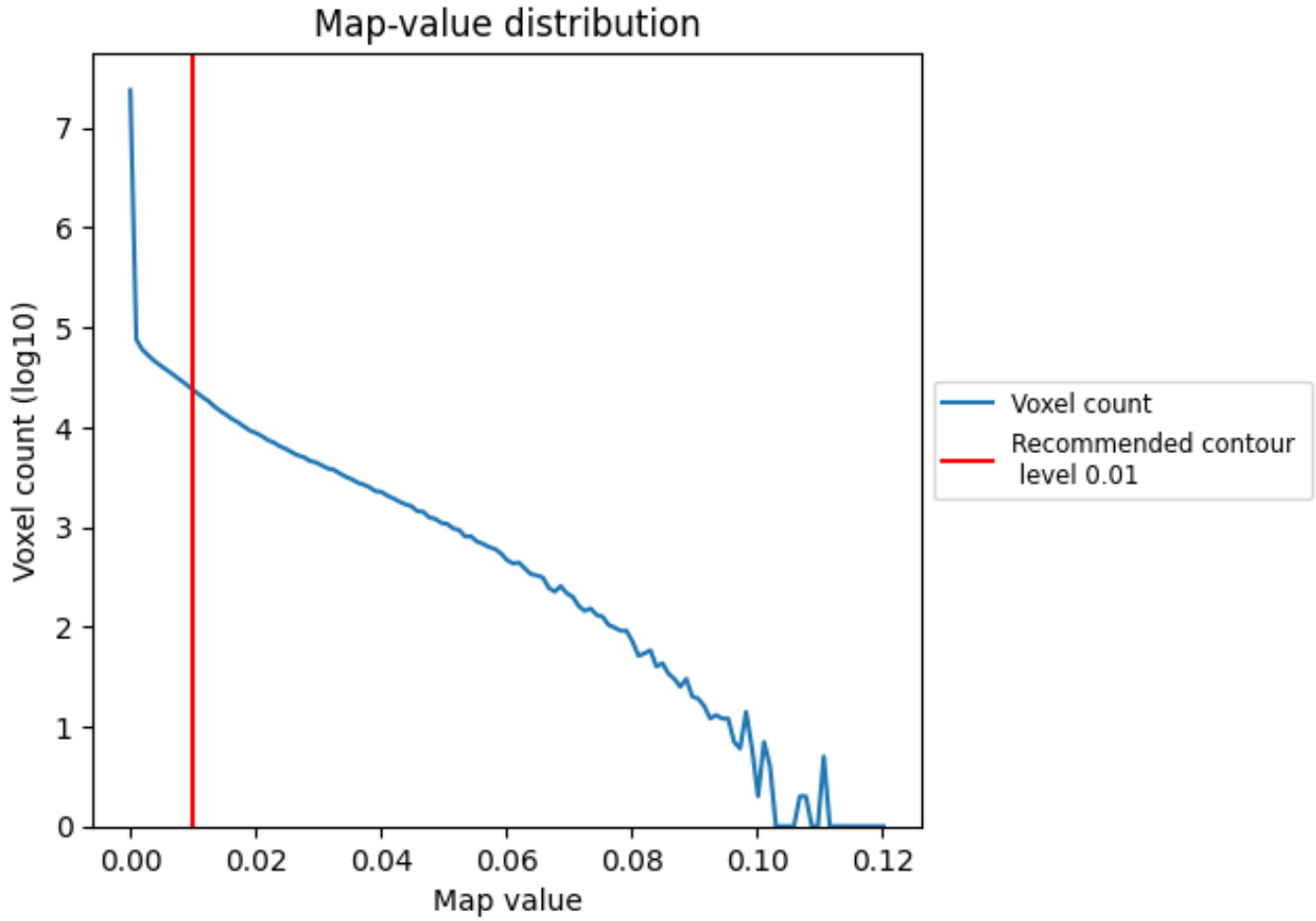


Z

7 Map analysis

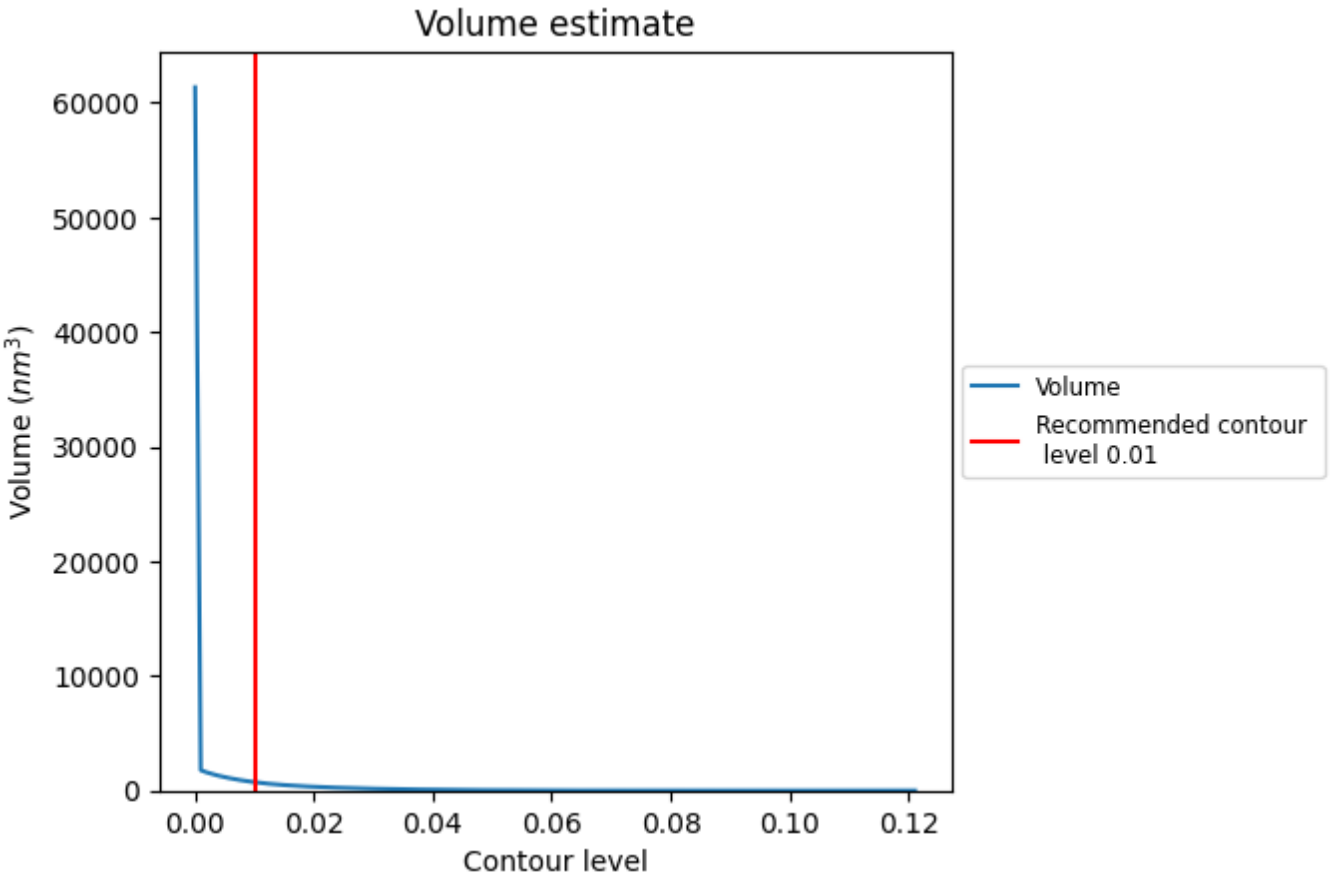
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

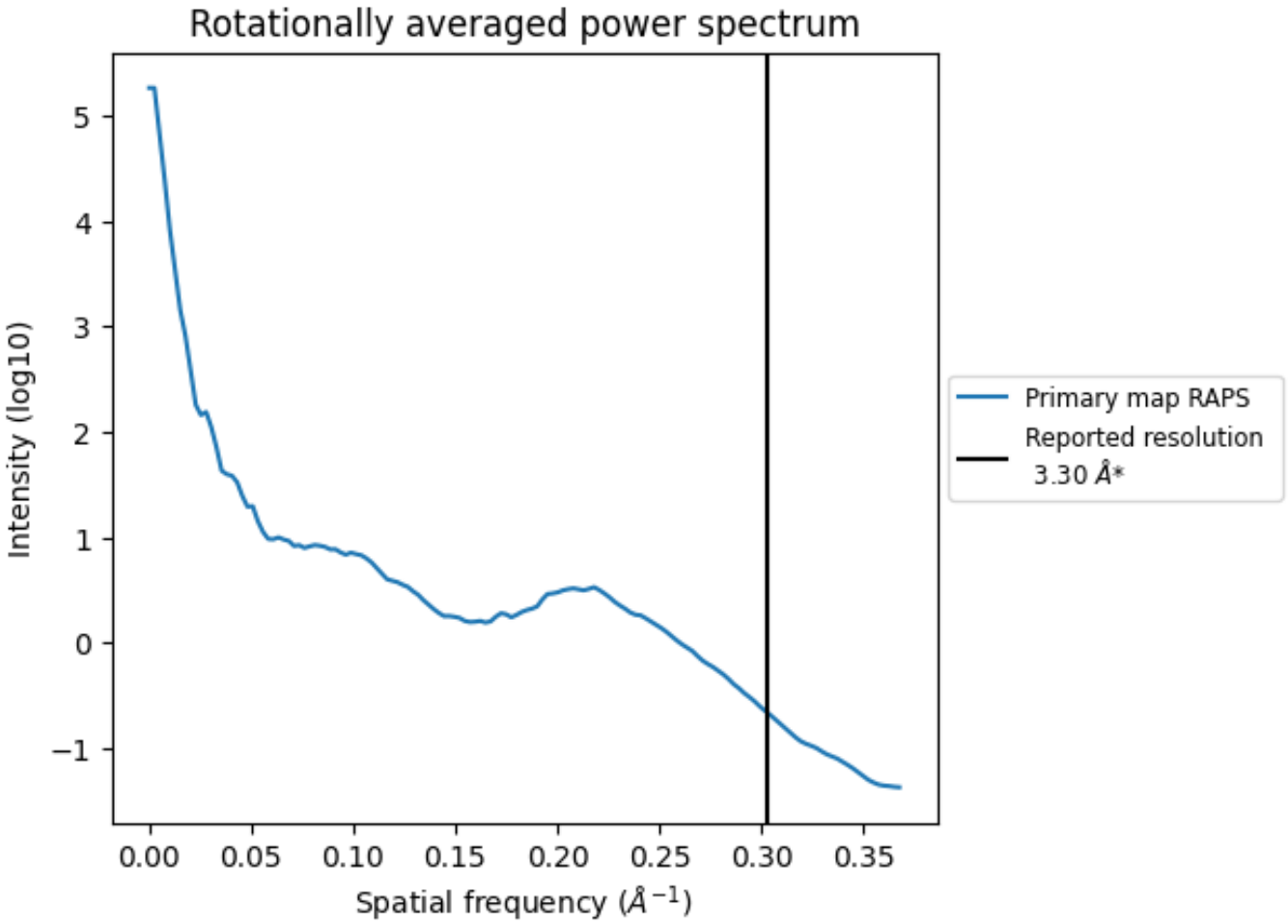
7.2 Volume estimate



The volume at the recommended contour level is 732 nm^3; this corresponds to an approximate mass of 662 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

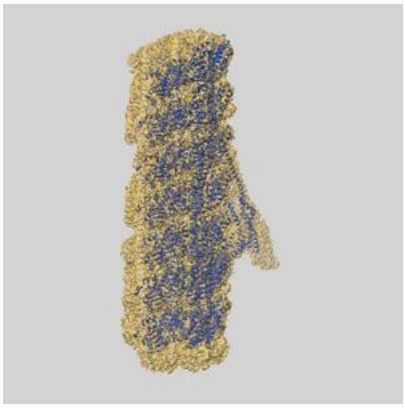
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

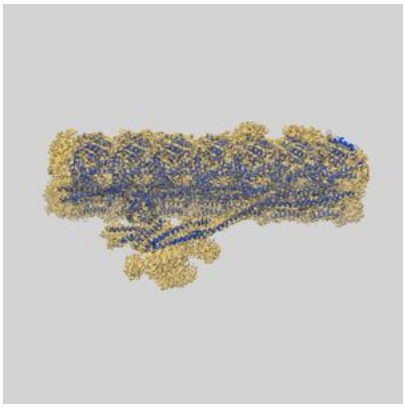
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23084 and PDB model 7KZO. Per-residue inclusion information can be found in section 3 on page 8.

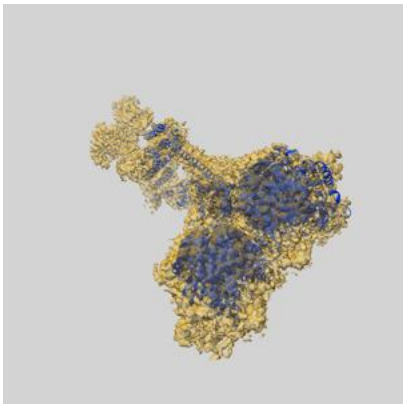
9.1 Map-model overlay



X



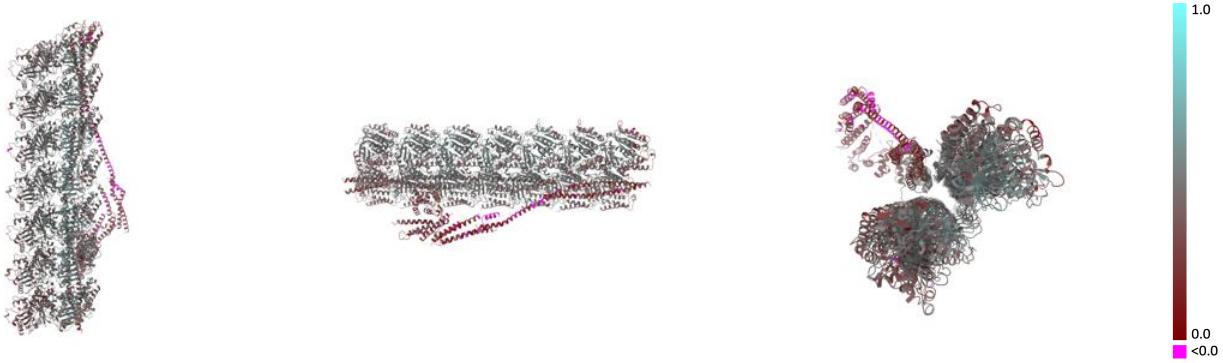
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

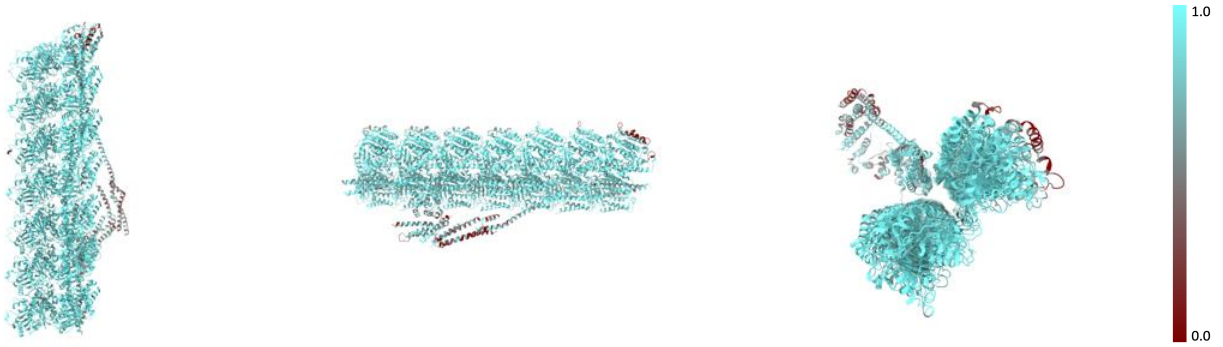
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

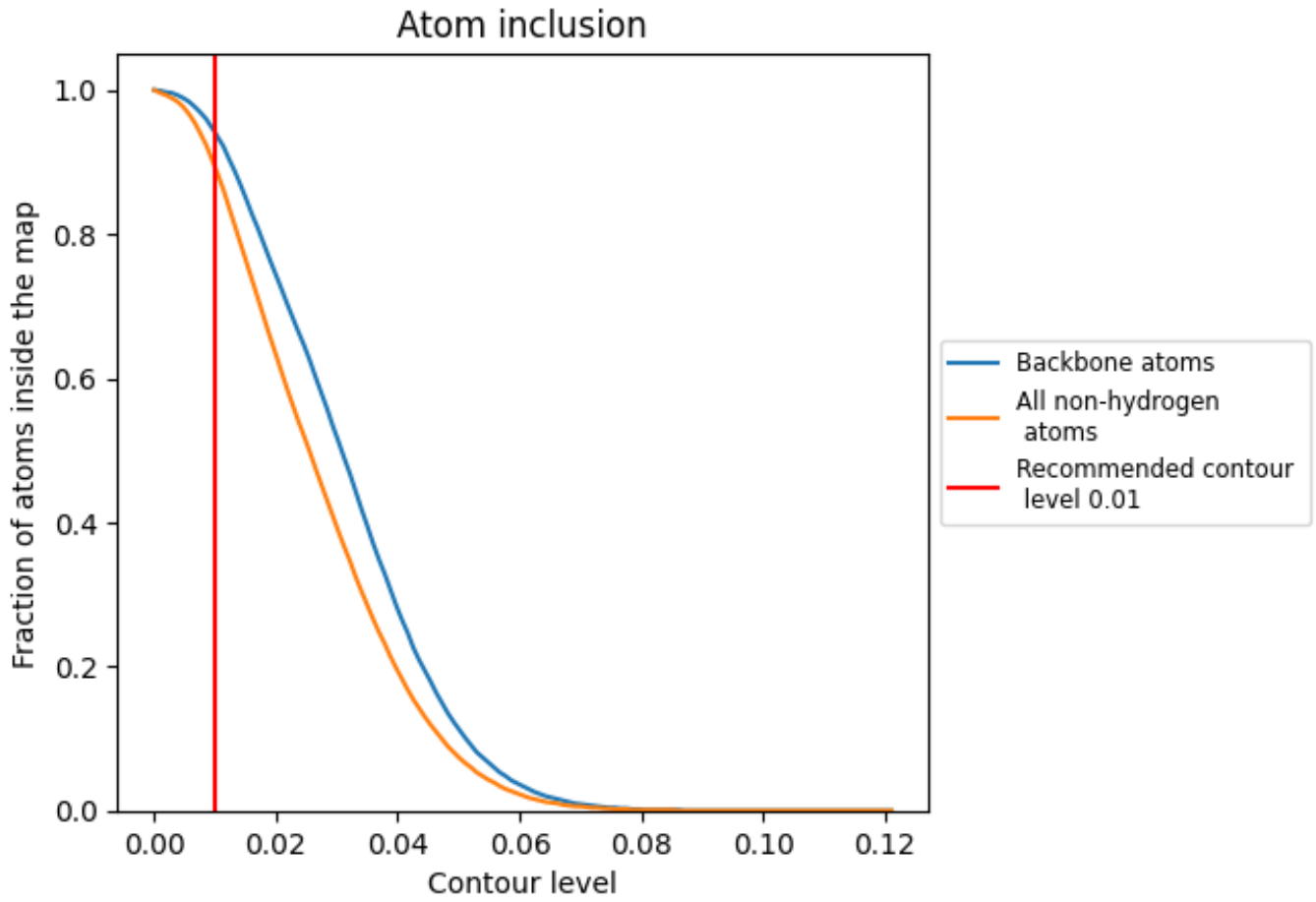
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.4310
A1	0.9070	0.3880
A2	0.9220	0.4220
A3	0.9280	0.4350
A4	0.9360	0.4490
A5	0.9310	0.4500
A6	0.9180	0.4290
A7	0.9180	0.4230
B1	0.9050	0.4540
B2	0.9220	0.4920
B3	0.9350	0.5020
B4	0.9290	0.4950
B5	0.9480	0.5050
B6	0.9200	0.4760
B7	0.8440	0.4410
C	0.6240	0.2160
X	0.6830	0.1930
X1	0.8400	0.4150
Y	0.6630	0.2040
Y1	0.8590	0.4030
Z	0.7190	0.2770