Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 03:08 AM EST

PDB ID	:	7TZC
EMDB ID	:	EMD-26205
Title	:	A drug and ATP binding site in type 1 ryanodine receptor
Authors	:	Melville, Z.; Dridi, H.; Yuan, Q.; Reiken, S.; Anetta, W.; Liu, Y.; Clarke, O.B.; Marks, A.R.
Deposited on	:	2022-02-15
Resolution	:	2.45 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:

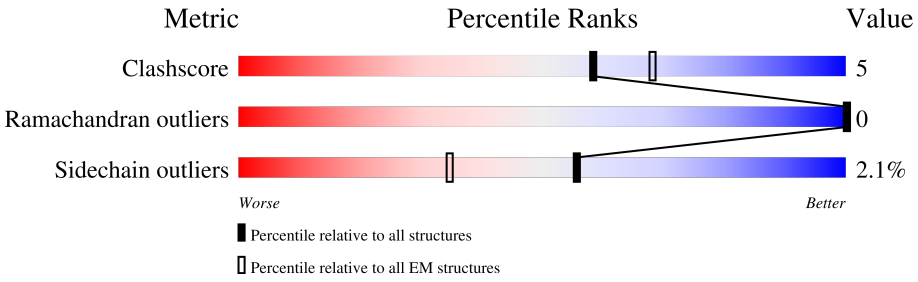
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.45 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%

Mol	Chain	Length	Quality of chain
1	C	150	77% 22% ••
1	D	150	79% 20% ••
1	E	150	79% 20% ••
1	K	150	78% 20% ••
2	F	107	86% 14%
2	H	107	85% 15%
2	J	107	88% 11% •
2	O	107	86% 13% •
3	A	5037	75% 12% 13%

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Mol	Chain	Length	Quality of chain
3	B	5037	75% 12% 13%
3	G	5037	75% 12% 13%
3	I	5037	75% 12% 13%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 149472 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	D	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	E	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	C	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P0DP23
D	-1	HIS	-	expression tag	UNP P0DP23
E	-1	HIS	-	expression tag	UNP P0DP23
C	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	J	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	O	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

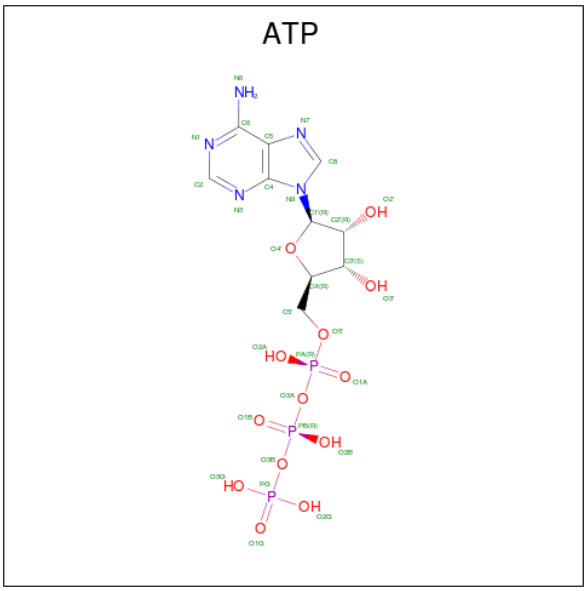
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	B	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	G	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	I	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	K	4	Total 4	Ca 4	0
4	D	4	Total 4	Ca 4	0
4	E	4	Total 4	Ca 4	0
4	C	4	Total 4	Ca 4	0
4	A	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

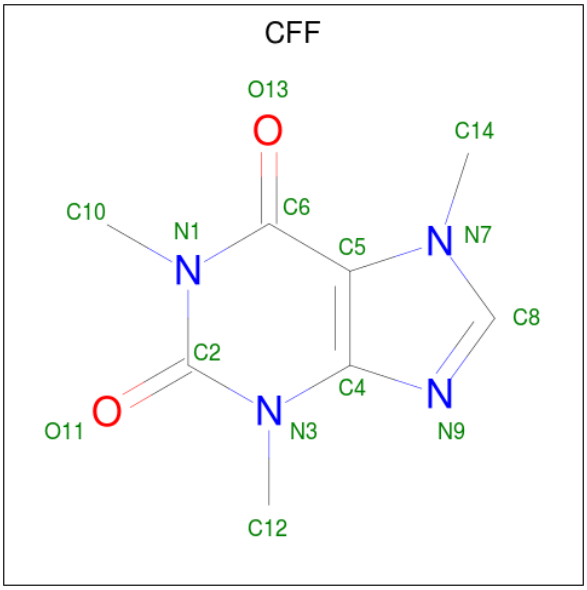


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	G	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	G	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	I	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	I	1	Total	C	N	O	P	0
			62	20	10	26	6	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

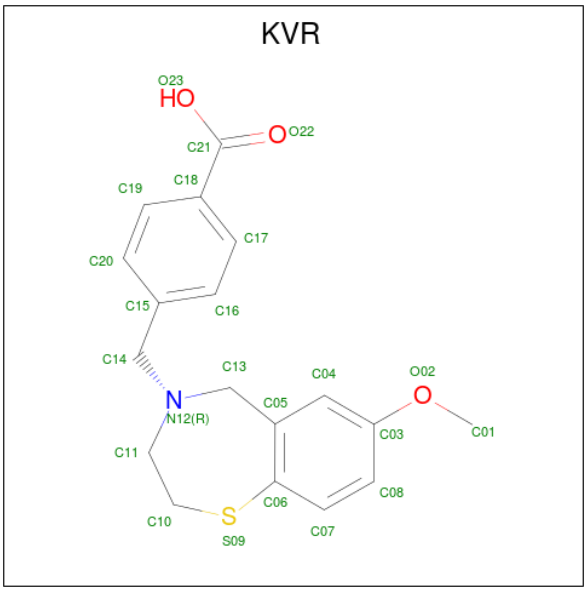
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	
6	G	1	Total	Zn	0
			1	1	
6	I	1	Total	Zn	0
			1	1	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



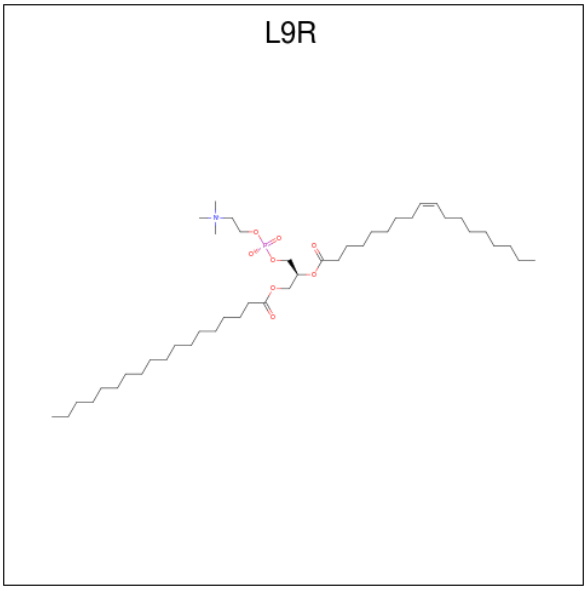
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O 14 8 4 2	0
7	B	1	Total C N O 14 8 4 2	0
7	G	1	Total C N O 14 8 4 2	0
7	I	1	Total C N O 14 8 4 2	0

- Molecule 8 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: $C_{18}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	G	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	I	1	Total	C	N	O	S	0
			23	18	1	3	1	

- Molecule 9 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: L9R) (formula: $C_{44}H_{86}NO_8P$).



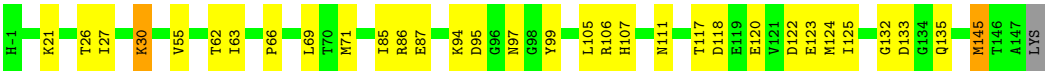
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	A	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	B	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	B	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	G	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	G	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	I	1	Total	C	N	O	P	0
			108	88	2	16	2	
9	I	1	Total	C	N	O	P	0
			108	88	2	16	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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

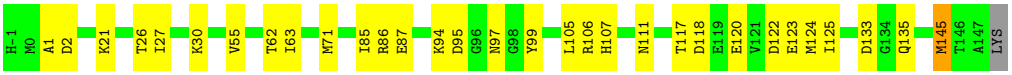
- Molecule 1: Calmodulin-1

Chain K:



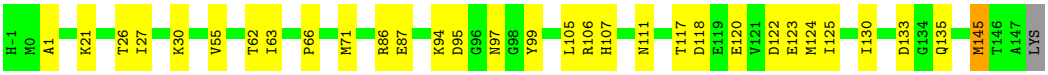
- Molecule 1: Calmodulin-1

Chain D:



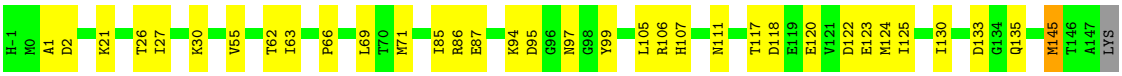
- Molecule 1: Calmodulin-1

Chain E:



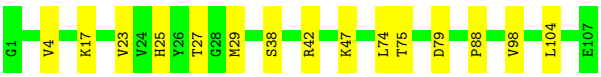
- Molecule 1: Calmodulin-1

Chain C:



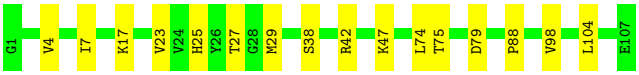
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

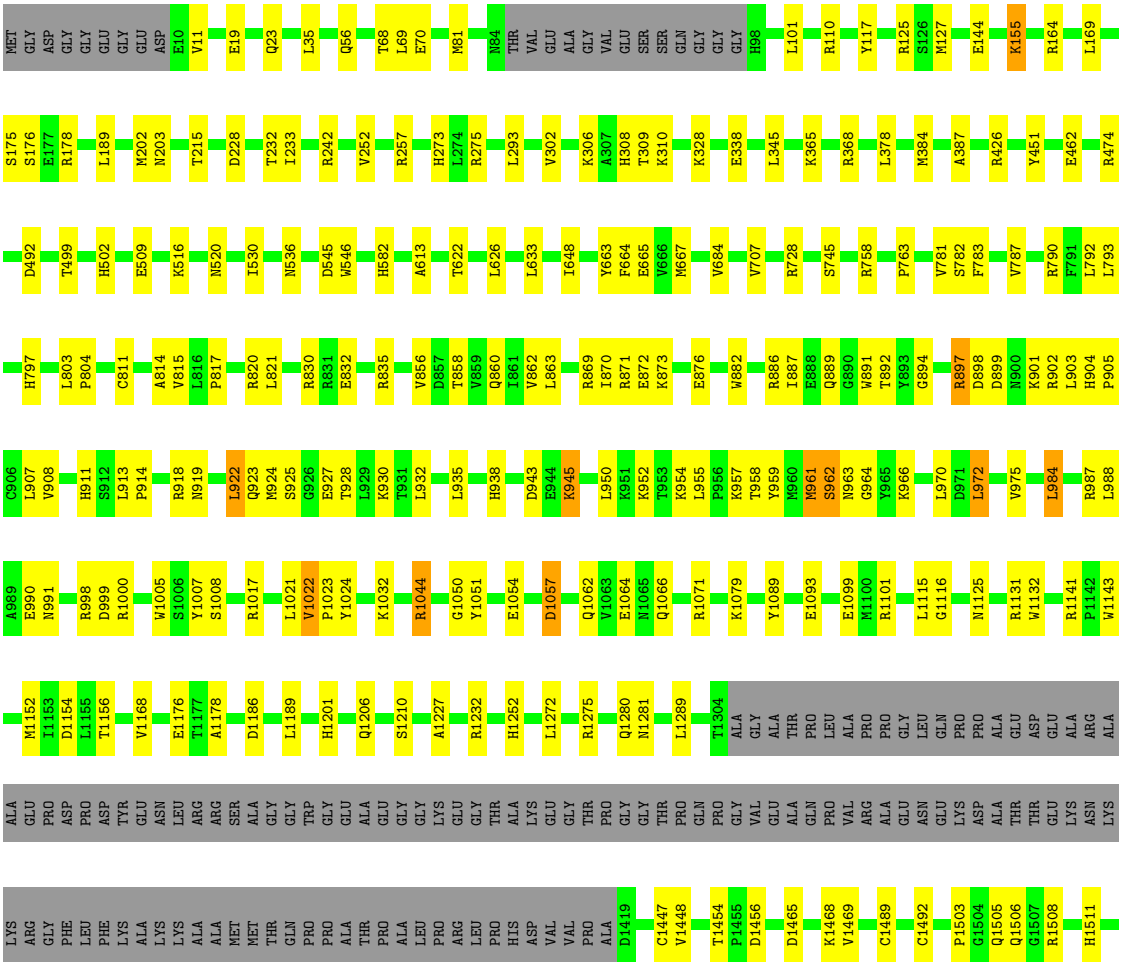
Chain J:

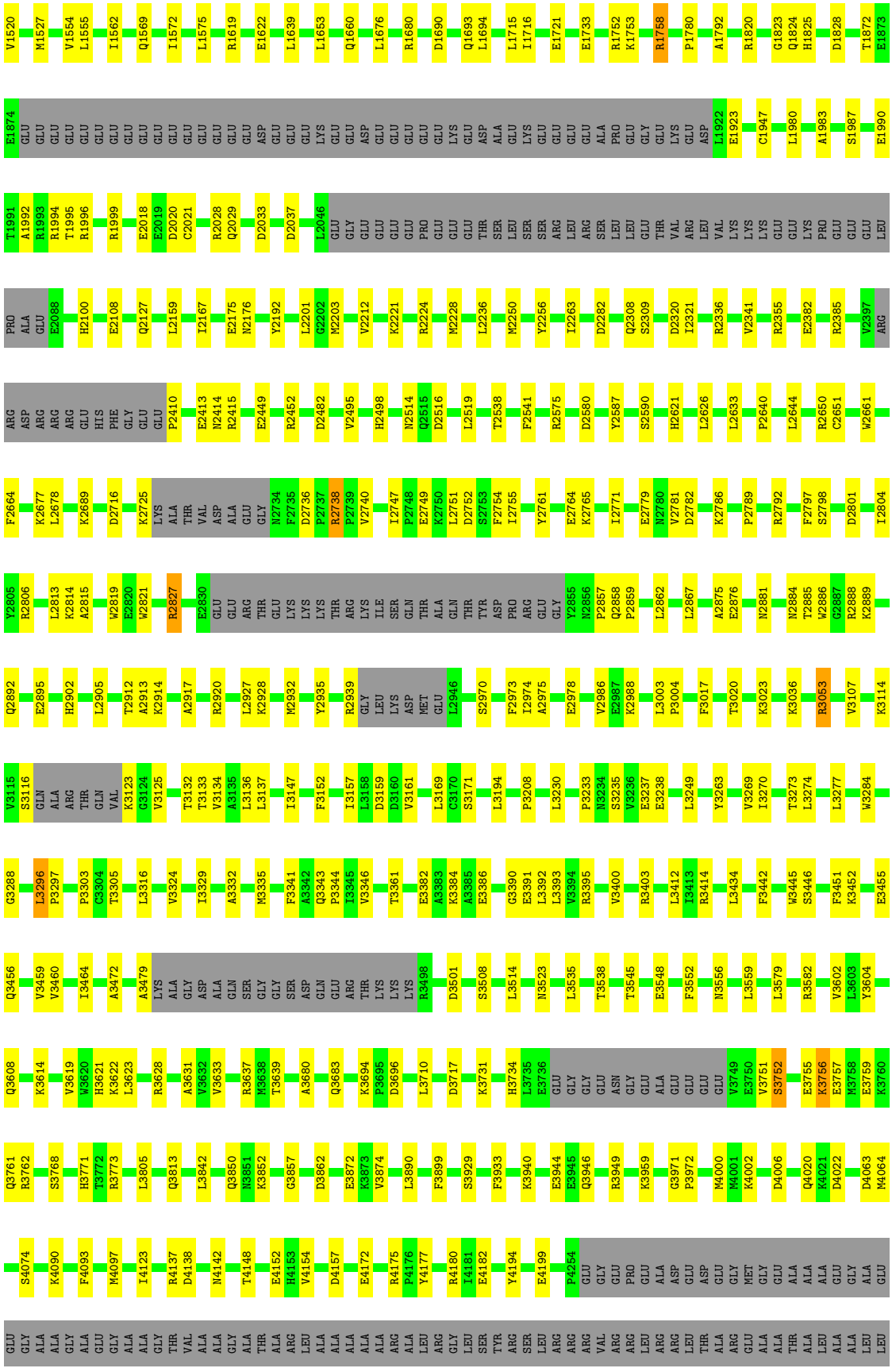
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

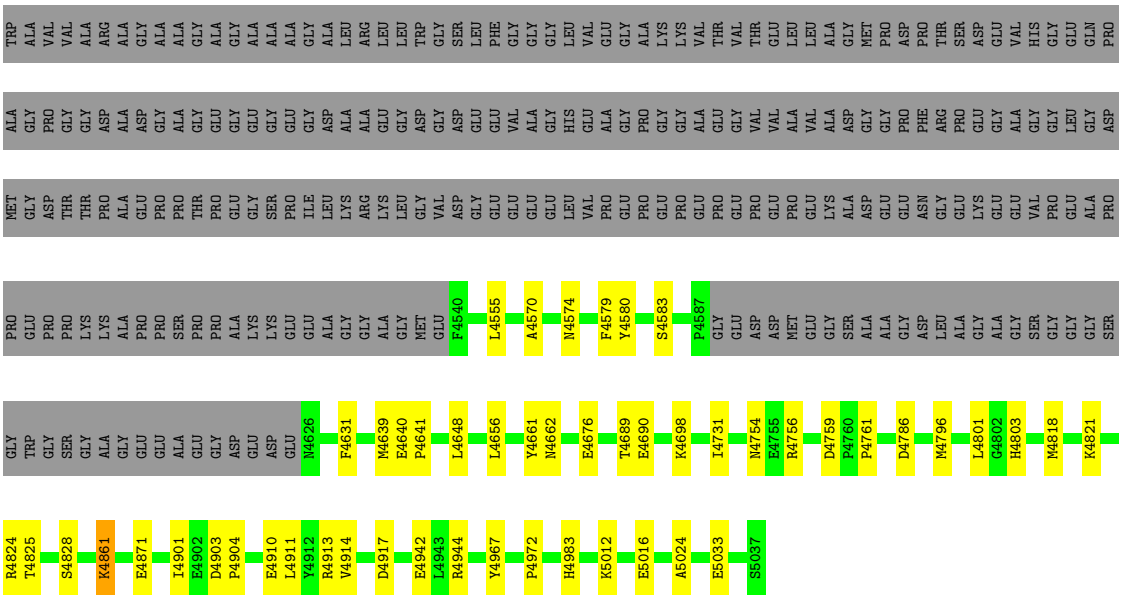
Chain O:

• Molecule 3: Ryanodine receptor 1

Chain A:

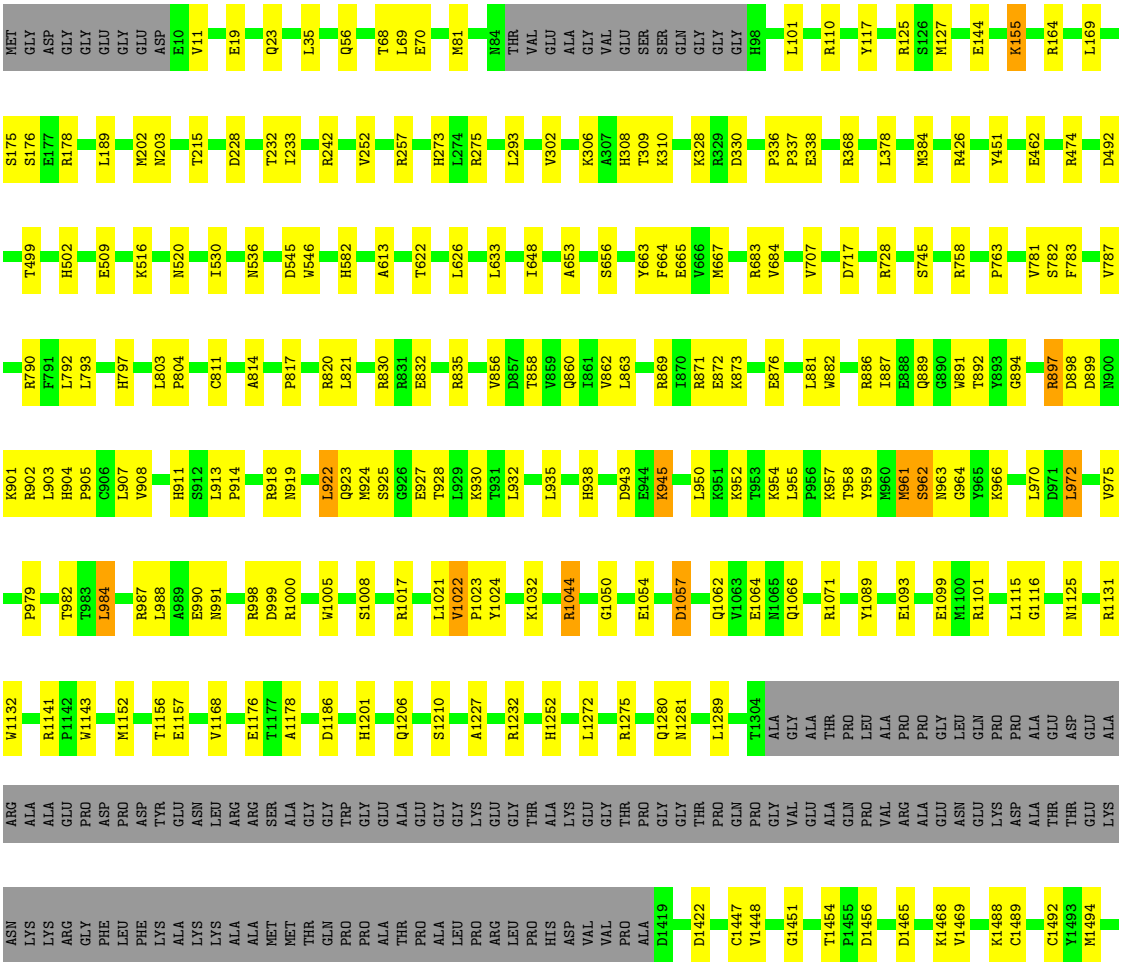


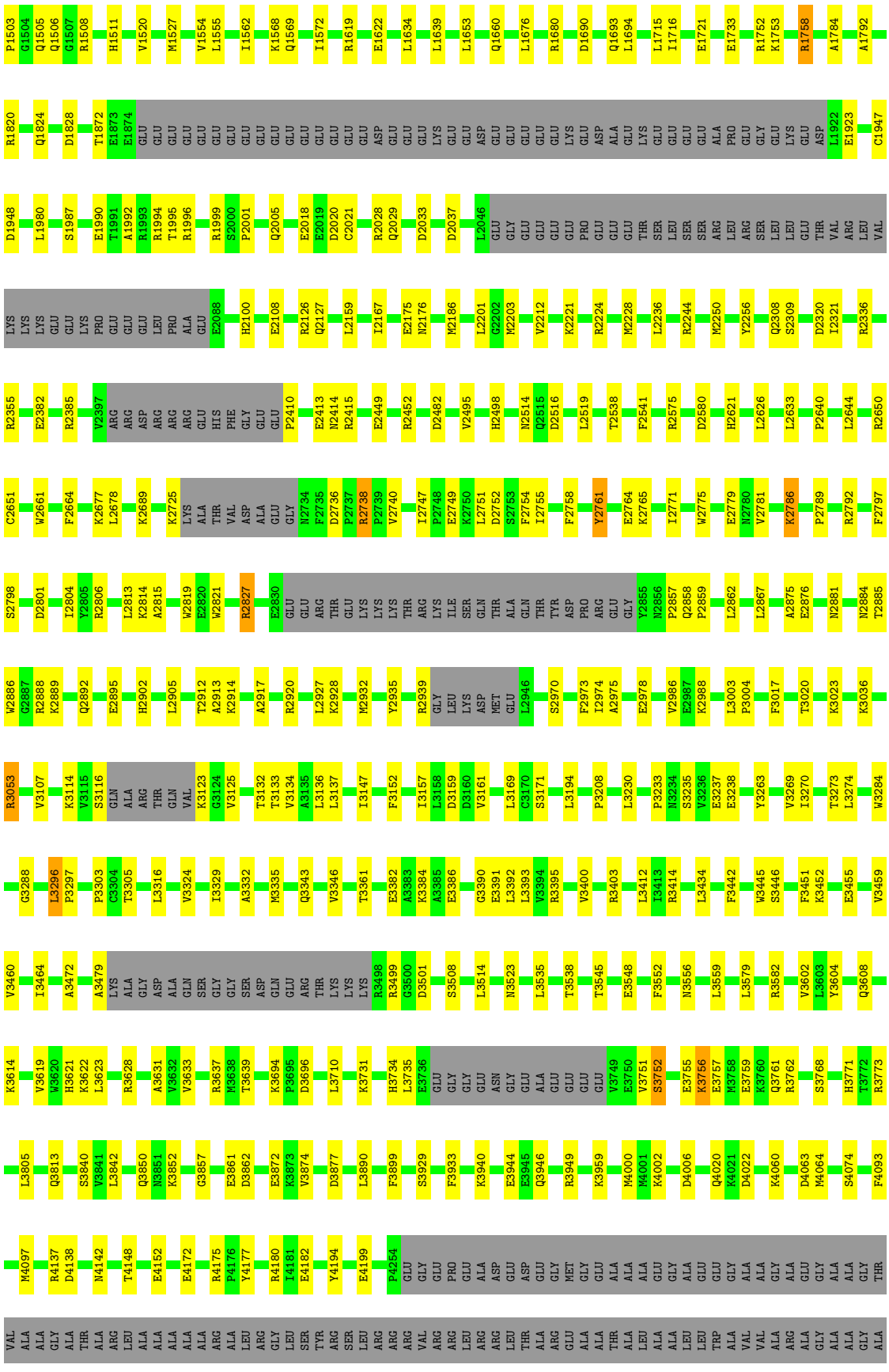


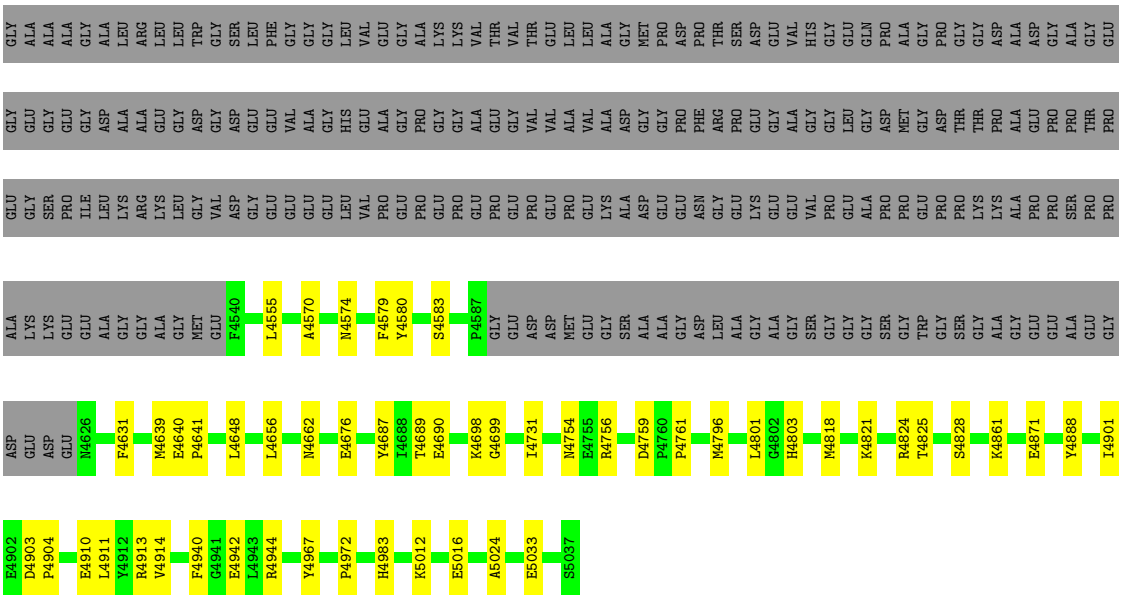


• Molecule 3: Ryanodine receptor 1

Chain B:

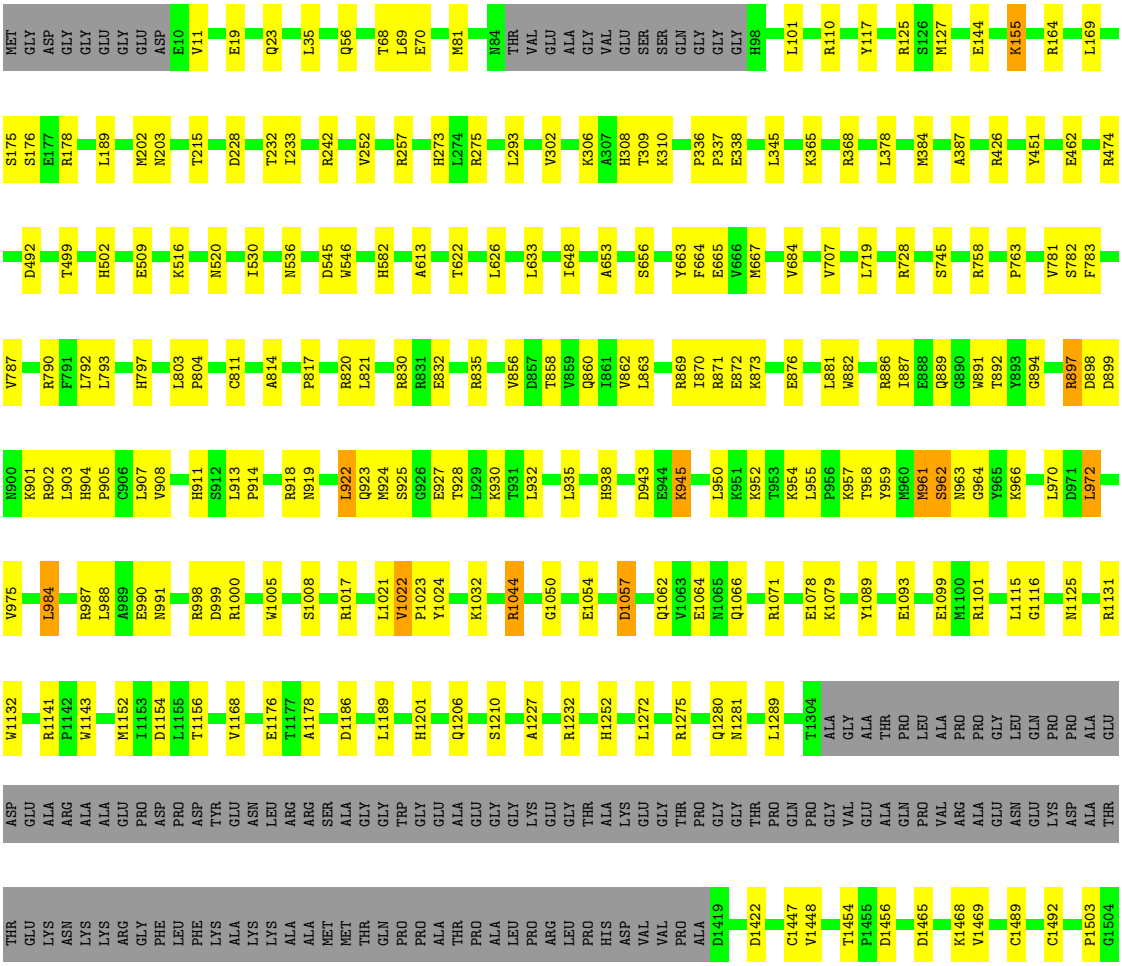


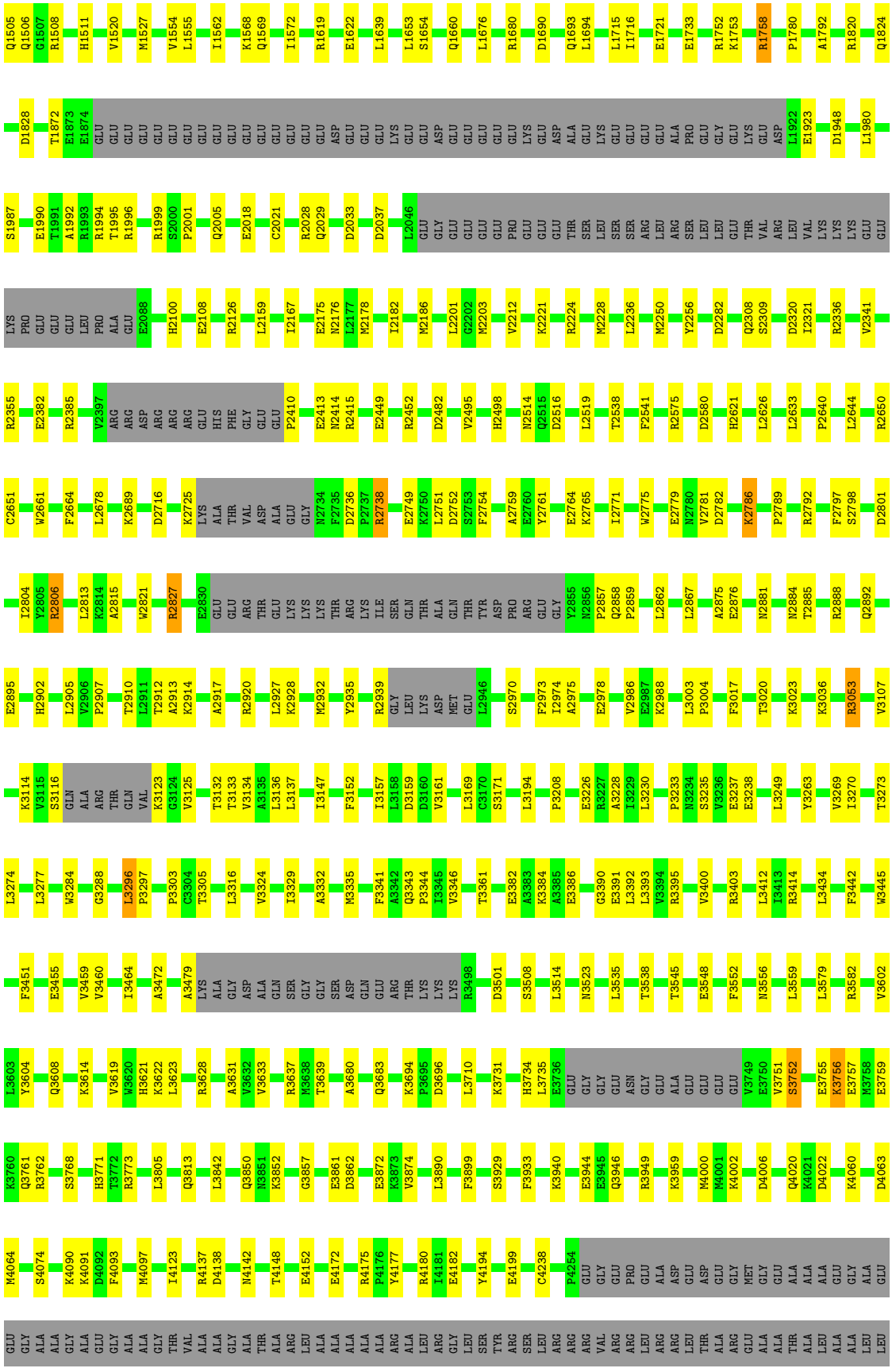

P1503 G1504 Q1505 Q1506 G1507 R1508 H1511 V1520 M1527 V1554 L1555 I1562 K1568 Q1569 I1572 R1619 E1622 L1634 L1639 L1653 Q1660 L1676 R1680 D1690 Q1693 L1694 L1715 I1716 E1721 E1733 R1752 K1753 R1758 A1784 A1792
R1820 Q1824 D1828 T1872 E1873 E1874 L1922 E1923 C1947
D1948 L1980 S1987 E1990 T1991 A1992 R1993 R1994 T1995 R1996 R1999 S2000 P2001 Q2005 E2018 E2019 D2020 C2021 R2028 Q2029 D2033 D2037 L2046
LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 H2100 E2108 R2126 Q2127 L2159 I2167 E2175 N2176 M2186 L2201 G2202 M2203 V2212 K2221 R2224 M2228 L2236 R2244 M2250 Y2256 Q2308 S2309 D2320 I2321 R2336
R2355 E2382 R2385 V2397 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 E2413 N2414 R2415 E2449 R2452 D2482 V2495 H2498 N2514 Q2515 D2516 L2519 T2538 F2541 R2575 D2580 H2621 L2626 L2633 P2640 L2644 R2650
C2651 W2661 F2664 K2677 L2678 K2689 K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 F2758 Y2761 E2764 K2765 I2771 W2775 E2779 N2780 V2781 K2786 P2789 R2792 F2797
S2798 D2801 I2804 Y2805 R2806 L2813 K2814 A2815 W2819 E2820 W2821 R2827 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 L2862 L2867 A2875 E2876 N2881 N2884 T2885
W2886 G2887 R2888 K2889 Q2892 E2895 H2902 L2905 T2912 A2913 K2914 A2917 R2920 L2927 K2928 M2932 Y2935 R2939 GLY LEU LYS ASP MET GLU L2946 S2970 F2973 I2974 A2975 E2978 V2986 E2987 K2988 L3003 P3004 F3017 T3020 K3023 K3036
R3053 V3107 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 V3125 T3132 T3133 V3134 A3135 L3136 L3137 I3147 F3152 I3157 L3158 D3159 D3160 V3161 L3169 C3170 S3171 L3194 P3208 L3230 P3233 N3234 S3235 V3236 E3237 E3238 Y3263 V3269 I3270 T3273 L3274 W3284
G3288 L3296 P3297 P3303 C3304 T3305 L3316 V3324 I3329 A3332 M3335 Q3343 V3346 T3361 E3382 A3383 K3384 A3385 E3386 G3390 E3391 L3392 L3393 V3394 R3395 V3400 R3403 L3412 I3413 R3414 L3434 F3442 W3445 S3446 F3451 K3452 E3455 V3459
V3460 I3464 A3472 A3479 LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501 S3508 L3514 N3523 L3535 T3538 T3545 E3548 F3552 N3556 L3559 L3579 R3582 V3602 L3603 Y3604 Q3608
K3614 V3619 W3620 H3621 K3622 L3623 R3628 A3631 V3632 V3633 R3637 M3638 T3639 K3694 P3695 D3696 L3710 K3731 H3734 L3735 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU V3749 E3750 V3751 S3752 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 R3762 S3768 H3771 T3772 R3773
L3805 Q3813 S3840 V3841 L3842 Q3850 N3851 K3852 G3857 E3861 D3862 E3872 K3873 V3874 D3877 L3890 F3899 S3929 F3933 K3940 E3944 E3945 Q3946 R3949 K3959 M4000 M4001 K4002 D4006 Q4020 K4021 D4022 K4060 D4063 M4064 S4074 F4093
M4097 R4137 D4138 N4142 T4148 E4152 E4172 R4175 P4176 Y4177 R4180 I4181 E4182 Y4194 E4199 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU ALA ALA GLY GLY ALA ALA ALA GLY THR
VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA ALA GLY ALA ALA ALA GLY ALA

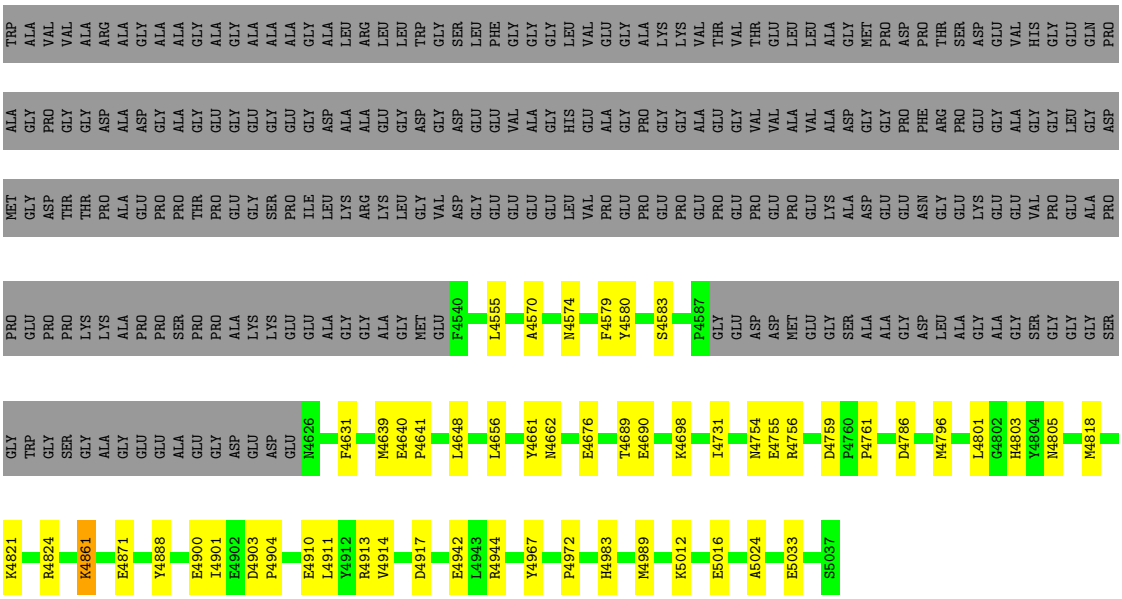


• Molecule 3: Ryanodine receptor 1

Chain G:

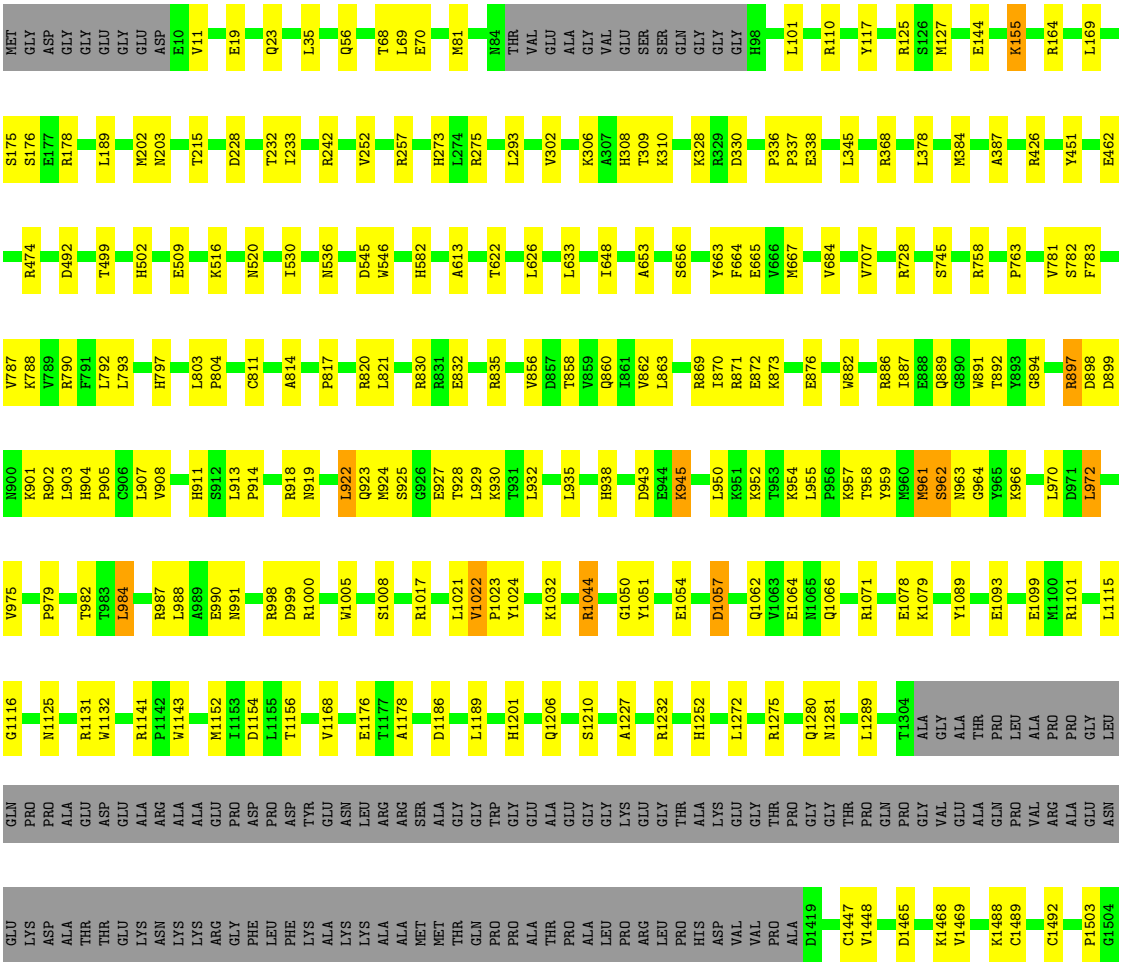


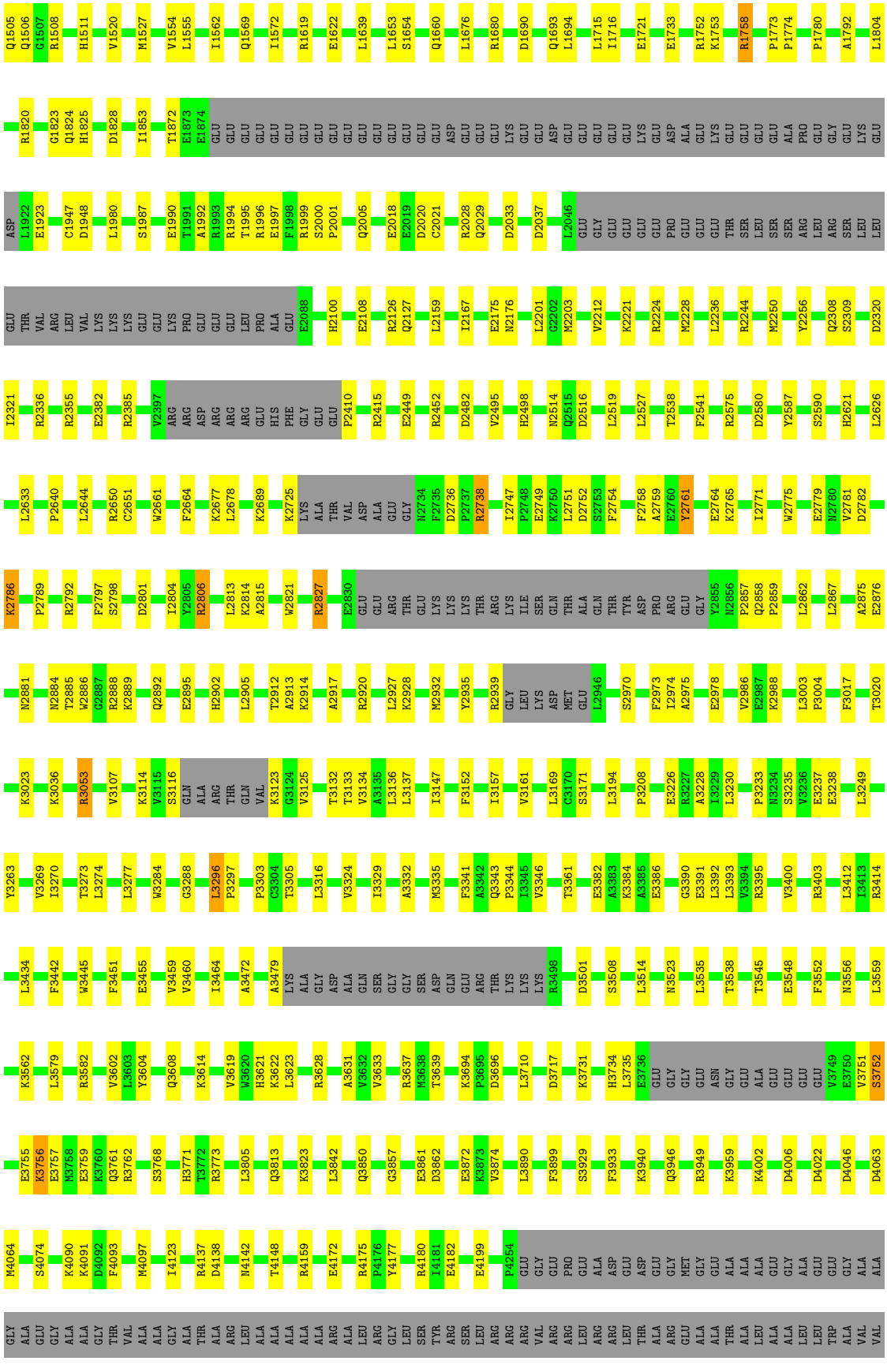


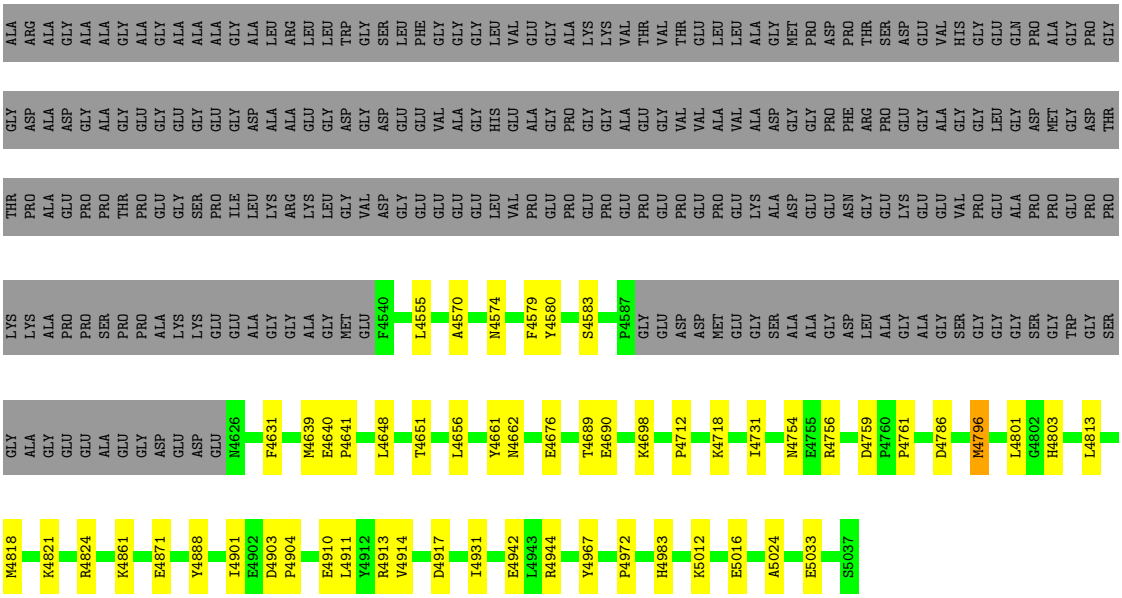


• Molecule 3: Ryanodine receptor 1

Chain I:






ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU GLY VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY THR
THR PRO ALA GLU PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU GLU ASN GLY GLU LYS GLU GLU GLY ALA GLY GLU GLU VAL PRO GLU GLN ALA PRO PRO GLU PRO PRO
LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 L4555 A4570 N4574 F4579 Y4580 S4583 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY GLY SER GLY TRP GLY SER
GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU GLU N4626 F4631 M4639 E4640 P4641 L4648 T4651 L4656 Y4661 N4662 E4676 T4689 E4690 K4698 P4712 K4718 I4731 N4754 E4755 R4756 D4759 P4760 P4761 D4786 M4796 L4801 G4802 H4803 L4813
M4818 K4821 R4824 K4861 E4871 Y4888 I4901 E4902 D4903 P4904 E4910 L4911 Y4912 R4913 V4914 D4917 I4931 E4942 L4943 R4944 Y4967 P4972 H4983 K5012 E5016 A5024 E5033 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	153840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CFF, ZN, ATP, KVR, L9R

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	C	0.24	0/1187	0.44	0/1594
1	D	0.24	0/1187	0.44	0/1594
1	E	0.24	0/1187	0.44	0/1594
1	K	0.24	0/1187	0.44	0/1594
2	F	0.32	0/850	0.52	0/1146
2	H	0.32	0/850	0.52	0/1146
2	J	0.32	0/850	0.52	0/1146
2	O	0.32	0/850	0.52	0/1146
3	A	0.25	0/35977	0.46	0/48726
3	B	0.25	0/35977	0.46	0/48726
3	G	0.25	0/35977	0.46	0/48726
3	I	0.25	0/35977	0.46	0/48726
All	All	0.25	0/152056	0.46	0/205864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1174	0	1099	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1174	0	1099	17	0
1	E	1174	0	1099	17	0
1	K	1174	0	1099	19	0
2	F	831	0	831	7	0
2	H	831	0	831	8	0
2	J	831	0	831	7	0
2	O	831	0	831	8	0
3	A	35150	0	34797	347	0
3	B	35150	0	34797	347	0
3	G	35150	0	34797	347	0
3	I	35150	0	34797	353	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	4	0	0	0	0
5	A	62	0	24	2	0
5	B	62	0	24	2	0
5	G	62	0	24	2	0
5	I	62	0	24	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	G	14	0	10	0	0
7	I	14	0	10	0	0
8	A	23	0	0	0	0
8	B	23	0	0	0	0
8	G	23	0	0	0	0
8	I	23	0	0	0	0
9	A	108	0	172	9	0
9	B	108	0	172	6	0
9	G	108	0	172	9	0
9	I	108	0	172	8	0
All	All	149472	0	147732	1461	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 5.

All (1461) 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)
3:I:4904:PRO:HB3	3:I:4913:ARG:HG2	1.57	0.86
3:G:4904:PRO:HB3	3:G:4913:ARG:HG2	1.57	0.86
3:A:4904:PRO:HB3	3:A:4913:ARG:HG2	1.57	0.84
3:B:4904:PRO:HB3	3:B:4913:ARG:HG2	1.57	0.83
3:A:2779:GLU:HG3	3:A:2792:ARG:HG2	1.66	0.78
3:G:2779:GLU:HG3	3:G:2792:ARG:HG2	1.66	0.78
3:I:2779:GLU:HG3	3:I:2792:ARG:HG2	1.66	0.77
3:B:2779:GLU:HG3	3:B:2792:ARG:HG2	1.66	0.77
3:A:1505:GLN:HG3	3:G:2771:ILE:HG12	1.67	0.77
3:B:2175:GLU:HG3	3:B:2228:MET:HB2	1.68	0.76
3:I:2175:GLU:HG3	3:I:2228:MET:HB2	1.68	0.76
1:C:106:ARG:HH22	1:C:118:ASP:HA	1.50	0.76
3:A:2175:GLU:HG3	3:A:2228:MET:HB2	1.68	0.76
3:G:2175:GLU:HG3	3:G:2228:MET:HB2	1.68	0.76
1:D:106:ARG:HH22	1:D:118:ASP:HA	1.50	0.75
1:K:106:ARG:HH22	1:K:118:ASP:HA	1.50	0.75
1:E:106:ARG:HH22	1:E:118:ASP:HA	1.50	0.75
3:G:2765:LYS:NZ	3:G:2859:PRO:O	2.22	0.73
1:K:111:ASN:O	3:A:1996:ARG:NH2	2.20	0.72
3:B:2765:LYS:NZ	3:B:2859:PRO:O	2.22	0.72
3:I:2765:LYS:NZ	3:I:2859:PRO:O	2.22	0.72
3:A:2765:LYS:NZ	3:A:2859:PRO:O	2.22	0.71
3:B:2771:ILE:HG12	3:I:1505:GLN:HG3	1.74	0.70
3:G:3114:LYS:HD3	3:G:3116:SER:H	1.58	0.69
3:B:3114:LYS:HD3	3:B:3116:SER:H	1.58	0.68
3:I:3114:LYS:HD3	3:I:3116:SER:H	1.58	0.68
3:A:1280:GLN:O	3:A:1281:ASN:ND2	2.27	0.68
3:B:876:GLU:HG2	3:B:918:ARG:HD3	1.76	0.68
3:I:858:THR:HB	3:I:930:LYS:HD2	1.76	0.68
3:A:368:ARG:HE	3:A:2308:GLN:HG3	1.59	0.68
3:A:3114:LYS:HD3	3:A:3116:SER:H	1.58	0.68
3:I:1280:GLN:O	3:I:1281:ASN:ND2	2.27	0.68
3:G:876:GLU:HG2	3:G:918:ARG:HD3	1.76	0.67
3:B:368:ARG:HE	3:B:2308:GLN:HG3	1.59	0.67
3:B:1280:GLN:O	3:B:1281:ASN:ND2	2.27	0.67
3:G:858:THR:HB	3:G:930:LYS:HD2	1.76	0.67
3:A:2771:ILE:HG12	3:B:1505:GLN:HG3	1.77	0.67
3:G:1280:GLN:O	3:G:1281:ASN:ND2	2.27	0.67
3:A:858:THR:HB	3:A:930:LYS:HD2	1.76	0.67
3:G:368:ARG:HE	3:G:2308:GLN:HG3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:876:GLU:HG2	3:I:918:ARG:HD3	1.75	0.67
3:A:2781:VAL:HA	3:A:2789:PRO:HB2	1.78	0.66
3:I:368:ARG:HE	3:I:2308:GLN:HG3	1.59	0.66
3:A:1520:VAL:HG12	3:A:1527:MET:HG2	1.78	0.66
3:G:2781:VAL:HA	3:G:2789:PRO:HB2	1.78	0.66
3:A:876:GLU:HG2	3:A:918:ARG:HD3	1.75	0.66
3:I:2781:VAL:HA	3:I:2789:PRO:HB2	1.78	0.66
3:A:3020:THR:HG23	3:A:3023:LYS:H	1.60	0.66
3:B:858:THR:HB	3:B:930:LYS:HD2	1.76	0.66
3:B:2781:VAL:HA	3:B:2789:PRO:HB2	1.78	0.66
3:B:3020:THR:HG23	3:B:3023:LYS:H	1.60	0.66
3:I:3020:THR:HG23	3:I:3023:LYS:H	1.60	0.66
1:K:133:ASP:HA	3:A:3460:VAL:HG11	1.77	0.66
3:B:2792:ARG:NH2	3:B:2798:SER:OG	2.29	0.66
3:I:961:MET:SD	3:I:961:MET:N	2.69	0.65
1:D:133:ASP:HA	3:I:3460:VAL:HG11	1.77	0.65
3:G:1520:VAL:HG12	3:G:1527:MET:HG2	1.78	0.65
3:I:2792:ARG:NH2	3:I:2798:SER:OG	2.29	0.65
3:B:1520:VAL:HG12	3:B:1527:MET:HG2	1.78	0.65
3:I:1520:VAL:HG12	3:I:1527:MET:HG2	1.78	0.65
3:A:2792:ARG:NH2	3:A:2798:SER:OG	2.29	0.65
3:B:972:LEU:HD22	3:B:1044:ARG:HB3	1.79	0.65
3:G:2792:ARG:NH2	3:G:2798:SER:OG	2.29	0.65
3:G:3020:THR:HG23	3:G:3023:LYS:H	1.60	0.65
3:A:972:LEU:HD22	3:A:1044:ARG:HB3	1.79	0.64
3:A:3329:ILE:HD11	3:A:3332:ALA:HB2	1.79	0.64
3:G:972:LEU:HD22	3:G:1044:ARG:HB3	1.79	0.64
1:D:1:ALA:HB3	3:I:3861:GLU:HG2	1.79	0.64
3:A:545:ASP:OD1	3:A:582:HIS:NE2	2.28	0.64
3:B:3329:ILE:HD11	3:B:3332:ALA:HB2	1.79	0.64
3:G:2978:GLU:OE2	3:G:3053:ARG:NH1	2.31	0.64
3:I:2978:GLU:OE2	3:I:3053:ARG:NH1	2.31	0.64
3:I:972:LEU:HD22	3:I:1044:ARG:HB3	1.79	0.63
3:B:2978:GLU:OE2	3:B:3053:ARG:NH1	2.31	0.63
3:G:961:MET:SD	3:G:961:MET:N	2.69	0.63
3:I:2018:GLU:OE1	3:I:2028:ARG:NH1	2.32	0.63
3:A:961:MET:SD	3:A:961:MET:N	2.69	0.62
3:A:2018:GLU:OE1	3:A:2028:ARG:NH1	2.32	0.62
3:G:3329:ILE:HD11	3:G:3332:ALA:HB2	1.79	0.62
3:G:2018:GLU:OE1	3:G:2028:ARG:NH1	2.32	0.62
3:A:2309:SER:OG	3:A:2321:ILE:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3017:PHE:O	3:A:3036:LYS:NZ	2.33	0.62
3:I:3329:ILE:HD11	3:I:3332:ALA:HB2	1.79	0.62
3:A:2978:GLU:OE2	3:A:3053:ARG:NH1	2.31	0.62
3:G:3017:PHE:O	3:G:3036:LYS:NZ	2.33	0.62
3:B:3445:TRP:NE1	3:B:3455:GLU:OE1	2.33	0.62
3:I:3579:LEU:HB2	3:I:3582:ARG:HG2	1.81	0.62
3:G:1116:GLY:HA3	3:G:1132:TRP:HB3	1.81	0.62
3:G:3445:TRP:NE1	3:G:3455:GLU:OE1	2.32	0.62
3:I:2902:HIS:HB3	3:I:2905:LEU:HG	1.82	0.62
3:B:2018:GLU:OE1	3:B:2028:ARG:NH1	2.32	0.62
3:G:3579:LEU:HB2	3:G:3582:ARG:HG2	1.81	0.62
3:I:3017:PHE:O	3:I:3036:LYS:NZ	2.33	0.62
3:B:2410:PRO:HB3	3:B:2415:ARG:HB3	1.82	0.61
3:B:2902:HIS:HB3	3:B:2905:LEU:HG	1.82	0.61
3:A:3445:TRP:NE1	3:A:3455:GLU:OE1	2.32	0.61
3:B:1066:GLN:HB2	3:B:1071:ARG:HE	1.65	0.61
3:B:1116:GLY:HA3	3:B:1132:TRP:HB3	1.81	0.61
3:B:3579:LEU:HB2	3:B:3582:ARG:HG2	1.81	0.61
3:I:1116:GLY:HA3	3:I:1132:TRP:HB3	1.81	0.61
3:I:2410:PRO:HB3	3:I:2415:ARG:HB3	1.82	0.61
3:I:3445:TRP:NE1	3:I:3455:GLU:OE1	2.32	0.61
3:B:961:MET:SD	3:B:961:MET:N	2.69	0.61
3:B:3017:PHE:O	3:B:3036:LYS:NZ	2.33	0.61
3:B:622:THR:HG23	3:B:626:LEU:HD12	1.83	0.61
3:G:1066:GLN:HB2	3:G:1071:ARG:HE	1.65	0.61
3:A:2902:HIS:HB3	3:A:2905:LEU:HG	1.82	0.61
3:A:2382:GLU:OE1	3:A:2385:ARG:NH1	2.31	0.61
3:A:622:THR:HG23	3:A:626:LEU:HD12	1.83	0.61
3:A:1116:GLY:HA3	3:A:1132:TRP:HB3	1.81	0.61
3:G:4583:SER:HB3	3:G:4631:PHE:HE2	1.66	0.61
3:G:545:ASP:OD1	3:G:582:HIS:NE2	2.28	0.60
3:A:1066:GLN:HB2	3:A:1071:ARG:HE	1.65	0.60
3:A:2410:PRO:HB3	3:A:2415:ARG:HB3	1.82	0.60
3:G:2902:HIS:HB3	3:G:2905:LEU:HG	1.82	0.60
3:A:228:ASP:OD2	3:B:155:LYS:NZ	2.30	0.60
3:A:3579:LEU:HB2	3:A:3582:ARG:HG2	1.81	0.60
3:G:2410:PRO:HB3	3:G:2415:ARG:HB3	1.82	0.60
3:I:622:THR:HG23	3:I:626:LEU:HD12	1.83	0.60
3:I:2309:SER:OG	3:I:2321:ILE:O	2.15	0.60
3:B:2309:SER:OG	3:B:2321:ILE:O	2.15	0.60
3:G:622:THR:HG23	3:G:626:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:897:ARG:NH2	3:G:899:ASP:OD1	2.35	0.60
3:G:1089:TYR:HD2	3:G:1152:MET:HG2	1.67	0.60
3:I:545:ASP:OD1	3:I:582:HIS:NE2	2.28	0.60
3:I:1066:GLN:HB2	3:I:1071:ARG:HE	1.65	0.60
1:E:99:TYR:HB3	1:E:135:GLN:HB3	1.84	0.60
3:A:4583:SER:HB3	3:A:4631:PHE:HE2	1.66	0.60
1:C:99:TYR:HB3	1:C:135:GLN:HB3	1.84	0.60
1:K:99:TYR:HB3	1:K:135:GLN:HB3	1.84	0.59
3:A:1089:TYR:HD2	3:A:1152:MET:HG2	1.67	0.59
3:B:633:LEU:HD13	3:B:1639:LEU:HD21	1.84	0.59
3:G:2309:SER:OG	3:G:2321:ILE:O	2.16	0.59
3:G:2382:GLU:OE1	3:G:2385:ARG:NH1	2.31	0.59
3:B:4583:SER:HB3	3:B:4631:PHE:HE2	1.66	0.59
3:G:492:ASP:OD1	3:G:546:TRP:NE1	2.33	0.59
3:I:984:LEU:HD12	3:I:987:ARG:HH12	1.68	0.59
3:A:3959:LYS:NZ	3:A:4022:ASP:OD2	2.32	0.59
3:B:545:ASP:OD1	3:B:582:HIS:NE2	2.28	0.59
3:B:830:ARG:NH2	3:B:832:GLU:OE2	2.36	0.59
3:I:830:ARG:NH2	3:I:832:GLU:OE2	2.36	0.59
3:I:4583:SER:HB3	3:I:4631:PHE:HE2	1.66	0.59
3:A:1448:VAL:HG22	3:A:1554:VAL:HG23	1.85	0.59
3:B:2382:GLU:OE1	3:B:2385:ARG:NH1	2.31	0.59
3:G:633:LEU:HD13	3:G:1639:LEU:HD21	1.84	0.59
3:G:3751:VAL:O	3:G:3756:LYS:NZ	2.35	0.59
1:K:55:VAL:HG21	1:K:71:MET:HB2	1.85	0.59
3:A:894:GLY:HA3	3:A:903:LEU:HB3	1.85	0.59
3:A:897:ARG:NH2	3:A:899:ASP:OD1	2.35	0.59
3:B:894:GLY:HA3	3:B:903:LEU:HB3	1.85	0.59
3:G:830:ARG:NH2	3:G:832:GLU:OE2	2.36	0.59
3:G:3959:LYS:NZ	3:G:4022:ASP:OD2	2.32	0.59
3:A:3751:VAL:O	3:A:3756:LYS:NZ	2.35	0.59
3:G:984:LEU:HD12	3:G:987:ARG:HH12	1.68	0.59
3:B:1089:TYR:HD2	3:B:1152:MET:HG2	1.67	0.59
3:G:1505:GLN:HG3	3:I:2771:ILE:HG12	1.84	0.59
3:B:897:ARG:NH2	3:B:899:ASP:OD1	2.35	0.59
3:B:984:LEU:HD12	3:B:987:ARG:HH12	1.68	0.59
3:I:19:GLU:HG2	3:I:68:THR:HG22	1.85	0.59
3:I:2382:GLU:OE1	3:I:2385:ARG:NH1	2.31	0.59
3:G:516:LYS:O	3:G:520:ASN:ND2	2.31	0.59
3:I:1089:TYR:HD2	3:I:1152:MET:HG2	1.67	0.59
3:B:3751:VAL:O	3:B:3756:LYS:NZ	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4138:ASP:O	3:B:4142:ASN:ND2	2.34	0.58
3:I:3751:VAL:O	3:I:3756:LYS:NZ	2.35	0.58
3:I:3959:LYS:NZ	3:I:4022:ASP:OD2	2.32	0.58
3:B:4570:ALA:O	3:B:4574:ASN:ND2	2.33	0.58
3:G:19:GLU:HG2	3:G:68:THR:HG22	1.85	0.58
3:I:897:ARG:NH2	3:I:899:ASP:OD1	2.35	0.58
3:I:1619:ARG:NH2	3:I:1622:GLU:OE1	2.37	0.58
3:B:19:GLU:HG2	3:B:68:THR:HG22	1.85	0.58
3:B:3132:THR:HG23	3:B:3136:LEU:HD23	1.85	0.58
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.86	0.58
3:G:894:GLY:HA3	3:G:903:LEU:HB3	1.85	0.58
3:G:1448:VAL:HG22	3:G:1554:VAL:HG23	1.85	0.58
1:D:99:TYR:HB3	1:D:135:GLN:HB3	1.84	0.58
3:B:1448:VAL:HG22	3:B:1554:VAL:HG23	1.85	0.58
3:I:894:GLY:HA3	3:I:903:LEU:HB3	1.85	0.58
1:C:55:VAL:HG21	1:C:71:MET:HB2	1.85	0.58
3:I:1448:VAL:HG22	3:I:1554:VAL:HG23	1.85	0.58
2:O:23:VAL:HG22	2:O:47:LYS:HG2	1.86	0.58
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.86	0.58
1:E:55:VAL:HG21	1:E:71:MET:HB2	1.85	0.58
3:A:3579:LEU:HD12	3:A:3582:ARG:HE	1.69	0.58
3:A:633:LEU:HD13	3:A:1639:LEU:HD21	1.84	0.58
3:A:830:ARG:NH2	3:A:832:GLU:OE2	2.36	0.58
3:A:955:LEU:O	3:A:966:LYS:NZ	2.31	0.58
3:A:2650:ARG:NH1	3:A:2651:CYS:SG	2.77	0.58
3:B:516:LYS:O	3:B:520:ASN:ND2	2.31	0.58
3:B:2650:ARG:NH1	3:B:2651:CYS:SG	2.77	0.58
3:G:1619:ARG:NH2	3:G:1622:GLU:OE1	2.36	0.58
3:A:19:GLU:HG2	3:A:68:THR:HG22	1.85	0.58
3:B:1619:ARG:NH2	3:B:1622:GLU:OE1	2.37	0.58
3:G:2650:ARG:NH1	3:G:2651:CYS:SG	2.77	0.58
3:G:3132:THR:HG23	3:G:3136:LEU:HD23	1.85	0.57
3:I:633:LEU:HD13	3:I:1639:LEU:HD21	1.84	0.57
3:I:2650:ARG:NH1	3:I:2651:CYS:SG	2.77	0.57
3:I:56:GLN:O	3:I:309:THR:OG1	2.19	0.57
3:I:70:GLU:OE2	3:I:110:ARG:NE	2.34	0.57
3:I:492:ASP:OD1	3:I:546:TRP:NE1	2.33	0.57
1:D:55:VAL:HG21	1:D:71:MET:HB2	1.85	0.57
3:A:984:LEU:HD12	3:A:987:ARG:HH12	1.68	0.57
3:A:3132:THR:HG23	3:A:3136:LEU:HD23	1.85	0.57
3:I:3579:LEU:HD12	3:I:3582:ARG:HE	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1619:ARG:NH2	3:A:1622:GLU:OE1	2.36	0.57
3:I:516:LYS:O	3:I:520:ASN:ND2	2.31	0.57
2:J:23:VAL:HG22	2:J:47:LYS:HG2	1.86	0.57
3:B:1987:SER:HB2	3:B:1994:ARG:HH22	1.70	0.57
3:G:110:ARG:NH2	3:G:117:TYR:OH	2.38	0.57
3:A:4689:THR:OG1	3:A:4690:GLU:OE1	2.23	0.57
3:G:3579:LEU:HD12	3:G:3582:ARG:HE	1.69	0.57
3:I:3132:THR:HG23	3:I:3136:LEU:HD23	1.85	0.57
3:B:127:MET:SD	3:B:127:MET:N	2.78	0.57
3:B:492:ASP:OD1	3:B:546:TRP:NE1	2.33	0.57
3:G:1987:SER:HB2	3:G:1994:ARG:HH22	1.70	0.57
3:A:1792:ALA:O	3:A:2176:ASN:ND2	2.38	0.57
3:G:3759:GLU:OE2	3:G:3762:ARG:NH2	2.38	0.57
3:B:426:ARG:NH2	3:B:509:GLU:OE2	2.38	0.56
3:G:1131:ARG:NH1	3:G:1178:ALA:O	2.38	0.56
3:I:3759:GLU:OE2	3:I:3762:ARG:NH2	2.38	0.56
3:G:384:MET:SD	3:G:384:MET:N	2.77	0.56
3:I:426:ARG:NH2	3:I:509:GLU:OE2	2.38	0.56
3:A:110:ARG:NH2	3:A:117:TYR:OH	2.38	0.56
3:B:1792:ALA:O	3:B:2176:ASN:ND2	2.38	0.56
3:B:2514:ASN:ND2	3:B:2516:ASP:OD1	2.38	0.56
3:B:3324:VAL:HG11	3:B:3361:THR:HG22	1.88	0.56
3:B:3579:LEU:HD12	3:B:3582:ARG:HE	1.69	0.56
3:B:3959:LYS:NZ	3:B:4022:ASP:OD2	2.32	0.56
3:G:3324:VAL:HG11	3:G:3361:THR:HG22	1.88	0.56
3:I:1131:ARG:NH1	3:I:1178:ALA:O	2.38	0.56
3:B:3270:ILE:HA	3:B:3274:LEU:HD12	1.88	0.56
3:G:426:ARG:NH2	3:G:509:GLU:OE2	2.38	0.56
3:G:2514:ASN:ND2	3:G:2516:ASP:OD1	2.39	0.56
3:I:110:ARG:NH2	3:I:117:TYR:OH	2.38	0.56
3:I:1792:ALA:O	3:I:2176:ASN:ND2	2.38	0.56
3:I:3324:VAL:HG11	3:I:3361:THR:HG22	1.88	0.56
3:A:127:MET:SD	3:A:127:MET:N	2.78	0.56
3:A:384:MET:SD	3:A:384:MET:N	2.77	0.56
3:A:3455:GLU:OE2	3:A:3508:SER:OG	2.24	0.56
3:B:1131:ARG:NH1	3:B:1178:ALA:O	2.38	0.56
3:B:3759:GLU:OE2	3:B:3762:ARG:NH2	2.38	0.56
3:B:4689:THR:OG1	3:B:4690:GLU:OE1	2.23	0.56
3:G:3270:ILE:HA	3:G:3274:LEU:HD12	1.88	0.56
3:A:3523:ASN:O	3:A:3582:ARG:NH2	2.39	0.56
3:I:1987:SER:HB2	3:I:1994:ARG:HH22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2514:ASN:ND2	3:I:2516:ASP:OD1	2.39	0.56
3:A:3759:GLU:OE2	3:A:3762:ARG:NH2	2.38	0.56
3:B:110:ARG:NH2	3:B:117:TYR:OH	2.38	0.56
3:B:302:VAL:HB	3:B:306:LYS:HE3	1.88	0.56
3:I:127:MET:SD	3:I:127:MET:N	2.78	0.56
3:I:3523:ASN:O	3:I:3582:ARG:NH2	2.39	0.56
3:A:904:HIS:HD1	3:A:905:PRO:HD2	1.71	0.56
3:G:1792:ALA:O	3:G:2176:ASN:ND2	2.38	0.56
3:G:2644:LEU:HD13	3:G:2678:LEU:HD21	1.88	0.56
3:B:667:MET:SD	3:B:790:ARG:NH2	2.80	0.56
3:G:1676:LEU:HD22	3:G:2167:ILE:HD12	1.88	0.56
3:I:4570:ALA:O	3:I:4574:ASN:ND2	2.33	0.56
3:A:1141:ARG:HB3	3:G:3479:ALA:HA	1.88	0.55
3:A:2514:ASN:ND2	3:A:2516:ASP:OD1	2.39	0.55
3:A:3270:ILE:HA	3:A:3274:LEU:HD12	1.88	0.55
3:A:3324:VAL:HG11	3:A:3361:THR:HG22	1.88	0.55
3:B:3400:VAL:HG23	3:B:3403:ARG:HH21	1.71	0.55
3:G:127:MET:SD	3:G:127:MET:N	2.78	0.55
3:G:4942:GLU:OE1	3:I:4944:ARG:NH1	2.39	0.55
3:I:904:HIS:HD1	3:I:905:PRO:HD2	1.71	0.55
3:A:302:VAL:HB	3:A:306:LYS:HE3	1.88	0.55
3:A:426:ARG:NH2	3:A:509:GLU:OE2	2.38	0.55
3:G:904:HIS:HD1	3:G:905:PRO:HD2	1.71	0.55
1:K:145:MET:SD	1:K:145:MET:N	2.80	0.55
3:A:1131:ARG:NH1	3:A:1178:ALA:O	2.38	0.55
3:G:3400:VAL:HG23	3:G:3403:ARG:HH21	1.71	0.55
3:G:3455:GLU:OE2	3:G:3508:SER:OG	2.24	0.55
3:I:1676:LEU:HD22	3:I:2167:ILE:HD12	1.88	0.55
3:I:3270:ILE:HA	3:I:3274:LEU:HD12	1.88	0.55
1:D:145:MET:SD	1:D:145:MET:N	2.80	0.55
3:A:1676:LEU:HD22	3:A:2167:ILE:HD12	1.88	0.55
3:B:904:HIS:HD1	3:B:905:PRO:HD2	1.71	0.55
3:B:2159:LEU:HD13	3:B:2203:MET:HG3	1.88	0.55
3:B:3169:LEU:HD12	3:B:3194:LEU:HD11	1.89	0.55
3:G:817:PRO:O	3:G:820:ARG:NH2	2.40	0.55
3:I:667:MET:SD	3:I:790:ARG:NH2	2.80	0.55
3:I:2827:ARG:NH2	3:I:2935:TYR:OH	2.40	0.55
2:J:75:THR:HG23	2:J:98:VAL:HG22	1.89	0.55
1:C:145:MET:SD	1:C:145:MET:N	2.80	0.55
3:B:56:GLN:O	3:B:309:THR:OG1	2.19	0.55
3:B:2827:ARG:NH2	3:B:2935:TYR:OH	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1057:ASP:OD1	3:G:1057:ASP:N	2.31	0.55
3:I:2159:LEU:HD13	3:I:2203:MET:HG3	1.88	0.55
3:I:2644:LEU:HD13	3:I:2678:LEU:HD21	1.88	0.55
3:I:4901:ILE:HG13	3:I:4913:ARG:NH2	2.21	0.55
2:O:75:THR:HG23	2:O:98:VAL:HG22	1.89	0.55
3:A:667:MET:SD	3:A:790:ARG:NH2	2.80	0.55
3:A:3169:LEU:HD12	3:A:3194:LEU:HD11	1.89	0.55
3:A:4944:ARG:NH1	3:B:4942:GLU:OE1	2.39	0.55
3:B:2765:LYS:HZ3	3:B:2857:PRO:HB2	1.71	0.55
3:G:4689:THR:OG1	3:G:4690:GLU:OE1	2.23	0.55
2:F:75:THR:HG23	2:F:98:VAL:HG22	1.89	0.55
3:A:1987:SER:HB2	3:A:1994:ARG:HH22	1.70	0.55
3:B:3523:ASN:O	3:B:3582:ARG:NH2	2.39	0.55
3:B:3696:ASP:OD2	3:B:3773:ARG:NE	2.38	0.55
3:G:4901:ILE:HG13	3:G:4913:ARG:NH2	2.21	0.55
3:I:4689:THR:OG1	3:I:4690:GLU:OE1	2.23	0.55
1:E:145:MET:N	1:E:145:MET:SD	2.80	0.55
3:A:817:PRO:O	3:A:820:ARG:NH2	2.40	0.55
3:A:2827:ARG:NH2	3:A:2935:TYR:OH	2.40	0.55
3:G:302:VAL:HB	3:G:306:LYS:HE3	1.88	0.55
3:G:2827:ARG:NH2	3:G:2935:TYR:OH	2.40	0.55
3:I:3169:LEU:HD12	3:I:3194:LEU:HD11	1.89	0.55
3:A:2159:LEU:HD13	3:A:2203:MET:HG3	1.88	0.55
3:B:4137:ARG:NH2	3:B:4199:GLU:OE2	2.40	0.55
3:G:3523:ASN:O	3:G:3582:ARG:NH2	2.39	0.55
3:G:3696:ASP:OD2	3:G:3773:ARG:NE	2.38	0.55
3:G:4137:ARG:NH2	3:G:4199:GLU:OE2	2.40	0.55
3:I:384:MET:SD	3:I:384:MET:N	2.77	0.55
3:I:4676:GLU:OE2	3:I:4698:LYS:NZ	2.40	0.55
3:B:4944:ARG:NH1	3:I:4942:GLU:OE1	2.41	0.55
3:G:2159:LEU:HD13	3:G:2203:MET:HG3	1.88	0.55
3:G:2519:LEU:HD13	3:G:2575:ARG:HG3	1.89	0.55
3:I:302:VAL:HB	3:I:306:LYS:HE3	1.88	0.55
2:H:75:THR:HG23	2:H:98:VAL:HG22	1.89	0.55
3:A:1062:GLN:NE2	3:A:1064:GLU:OE1	2.37	0.54
3:A:3400:VAL:HG23	3:A:3403:ARG:HH21	1.71	0.54
3:G:667:MET:SD	3:G:790:ARG:NH2	2.80	0.54
3:G:3169:LEU:HD12	3:G:3194:LEU:HD11	1.89	0.54
3:I:2892:GLN:NE2	3:I:2895:GLU:OE2	2.40	0.54
3:I:3400:VAL:HG23	3:I:3403:ARG:HH21	1.71	0.54
3:A:2892:GLN:NE2	3:A:2895:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4570:ALA:O	3:A:4574:ASN:ND2	2.33	0.54
3:A:4676:GLU:OE2	3:A:4698:LYS:NZ	2.40	0.54
3:B:4901:ILE:HG13	3:B:4913:ARG:NH2	2.21	0.54
3:I:924:MET:HG3	5:I:5106:ATP:HN61	1.72	0.54
3:A:2644:LEU:HD13	3:A:2678:LEU:HD21	1.88	0.54
3:B:1676:LEU:HD22	3:B:2167:ILE:HD12	1.88	0.54
3:B:1680:ARG:HH12	2:O:88:PRO:HB2	1.73	0.54
3:B:2644:LEU:HD13	3:B:2678:LEU:HD21	1.88	0.54
3:B:3455:GLU:OE2	3:B:3508:SER:OG	2.24	0.54
3:G:2892:GLN:NE2	3:G:2895:GLU:OE2	2.40	0.54
1:E:95:ASP:OD2	1:E:97:ASN:ND2	2.41	0.54
3:A:70:GLU:OE2	3:A:110:ARG:NE	2.34	0.54
3:A:155:LYS:NZ	3:G:228:ASP:OD2	2.31	0.54
3:A:530:ILE:HG22	3:A:536:ASN:HB3	1.90	0.54
3:A:4137:ARG:NH2	3:A:4199:GLU:OE2	2.40	0.54
3:A:4901:ILE:HG13	3:A:4913:ARG:NH2	2.21	0.54
3:B:530:ILE:HG22	3:B:536:ASN:HB3	1.90	0.54
3:B:4676:GLU:OE2	3:B:4698:LYS:NZ	2.40	0.54
3:G:1062:GLN:NE2	3:G:1064:GLU:OE1	2.37	0.54
3:G:1252:HIS:O	3:G:1275:ARG:NH1	2.41	0.54
3:I:23:GLN:NE2	3:I:203:ASN:OD1	2.41	0.54
3:I:1252:HIS:O	3:I:1275:ARG:NH1	2.41	0.54
3:I:2519:LEU:HD13	3:I:2575:ARG:HG3	1.89	0.54
3:B:23:GLN:NE2	3:B:203:ASN:OD1	2.41	0.54
3:B:1252:HIS:O	3:B:1275:ARG:NH1	2.41	0.54
3:A:492:ASP:OD1	3:A:546:TRP:NE1	2.33	0.54
3:B:2892:GLN:NE2	3:B:2895:GLU:OE2	2.40	0.54
3:G:23:GLN:NE2	3:G:203:ASN:OD1	2.40	0.54
3:I:3233:PRO:HB2	3:I:3238:GLU:HB2	1.90	0.54
3:B:3335:MET:SD	3:B:3403:ARG:NH1	2.81	0.54
3:G:56:GLN:O	3:G:309:THR:OG1	2.19	0.54
3:G:70:GLU:OE2	3:G:110:ARG:NE	2.34	0.54
3:G:530:ILE:HG22	3:G:536:ASN:HB3	1.90	0.54
3:G:4570:ALA:O	3:G:4574:ASN:ND2	2.33	0.54
3:I:817:PRO:O	3:I:820:ARG:NH2	2.40	0.54
3:I:3335:MET:SD	3:I:3403:ARG:NH1	2.81	0.54
3:I:4137:ARG:NH2	3:I:4199:GLU:OE2	2.40	0.54
3:G:924:MET:HG3	5:G:5106:ATP:HN61	1.72	0.54
3:G:3335:MET:SD	3:G:3403:ARG:NH1	2.81	0.54
3:I:530:ILE:HG22	3:I:536:ASN:HB3	1.90	0.54
3:B:817:PRO:O	3:B:820:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:913:LEU:HD12	3:B:914:PRO:HD2	1.89	0.54
1:C:95:ASP:OD2	1:C:97:ASN:ND2	2.41	0.54
3:A:2519:LEU:HD13	3:A:2575:ARG:HG3	1.89	0.54
3:A:4942:GLU:OE1	3:G:4944:ARG:NH1	2.41	0.54
3:B:924:MET:HG3	5:B:5305:ATP:HN61	1.72	0.54
3:B:2519:LEU:HD13	3:B:2575:ARG:HG3	1.89	0.54
3:B:3233:PRO:HB2	3:B:3238:GLU:HB2	1.90	0.54
3:G:293:LEU:HD13	3:G:378:LEU:HD12	1.90	0.54
3:G:4676:GLU:OE2	3:G:4698:LYS:NZ	2.40	0.54
3:I:2970:SER:HA	3:I:2973:PHE:CE2	2.43	0.54
3:I:3455:GLU:OE2	3:I:3508:SER:OG	2.24	0.54
3:A:23:GLN:NE2	3:A:203:ASN:OD1	2.40	0.53
3:G:2970:SER:HA	3:G:2973:PHE:CE2	2.44	0.53
3:A:293:LEU:HD13	3:A:378:LEU:HD12	1.90	0.53
3:B:1454:THR:OG1	3:B:1456:ASP:OD1	2.20	0.53
3:A:1252:HIS:O	3:A:1275:ARG:NH1	2.41	0.53
3:I:293:LEU:HD13	3:I:378:LEU:HD12	1.90	0.53
1:K:95:ASP:OD2	1:K:97:ASN:ND2	2.41	0.53
3:A:3335:MET:SD	3:A:3403:ARG:NH1	2.81	0.53
3:A:3940:LYS:O	3:A:4002:LYS:NZ	2.39	0.53
3:I:913:LEU:HD12	3:I:914:PRO:HD2	1.89	0.53
1:K:27:ILE:HB	1:K:63:ILE:HB	1.91	0.53
1:D:95:ASP:OD2	1:D:97:ASN:ND2	2.41	0.53
3:A:924:MET:HG3	5:A:5305:ATP:HN61	1.72	0.53
3:G:745:SER:HB2	3:G:758:ARG:HB2	1.91	0.53
3:I:1062:GLN:NE2	3:I:1064:GLU:OE1	2.37	0.53
3:A:3157:ILE:HA	3:A:3161:VAL:HB	1.91	0.53
3:G:3233:PRO:HB2	3:G:3238:GLU:HB2	1.90	0.53
3:A:913:LEU:HD12	3:A:914:PRO:HD2	1.89	0.53
3:G:3850:GLN:NE2	3:G:3872:GLU:OE1	2.36	0.53
3:G:3940:LYS:O	3:G:4002:LYS:NZ	2.39	0.53
1:D:27:ILE:HB	1:D:63:ILE:HB	1.90	0.53
3:A:3628:ARG:NH1	3:A:3857:GLY:O	2.42	0.53
3:G:913:LEU:HD12	3:G:914:PRO:HD2	1.89	0.53
3:A:2970:SER:HA	3:A:2973:PHE:CE2	2.43	0.53
3:B:228:ASP:OD2	3:I:155:LYS:NZ	2.34	0.53
3:G:975:VAL:HG12	3:G:1044:ARG:HH11	1.74	0.53
3:G:4138:ASP:O	3:G:4142:ASN:ND2	2.34	0.53
3:I:215:THR:HG22	3:I:273:HIS:HA	1.90	0.53
3:I:975:VAL:HG12	3:I:1044:ARG:HH11	1.74	0.53
3:B:1062:GLN:NE2	3:B:1064:GLU:OE1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3850:GLN:NE2	3:B:3872:GLU:OE1	2.36	0.53
3:G:3157:ILE:HA	3:G:3161:VAL:HB	1.91	0.53
3:B:2754:PHE:HE2	3:B:2813:LEU:HD11	1.74	0.52
3:A:215:THR:HG22	3:A:273:HIS:HA	1.90	0.52
3:B:2970:SER:HA	3:B:2973:PHE:CE2	2.43	0.52
3:B:3628:ARG:NH1	3:B:3857:GLY:O	2.42	0.52
3:G:1093:GLU:HB3	3:G:1201:HIS:HB3	1.92	0.52
3:G:3296:LEU:HG	3:G:3297:PRO:HD3	1.92	0.52
3:I:745:SER:HB2	3:I:758:ARG:HB2	1.91	0.52
3:I:4759:ASP:O	3:I:4761:PRO:HD3	2.09	0.52
1:C:1:ALA:HB3	3:B:3861:GLU:HG2	1.90	0.52
3:A:4759:ASP:O	3:A:4761:PRO:HD3	2.09	0.52
3:B:3157:ILE:HA	3:B:3161:VAL:HB	1.91	0.52
3:G:2754:PHE:HE2	3:G:2813:LEU:HD11	1.74	0.52
1:E:27:ILE:HB	1:E:63:ILE:HB	1.90	0.52
3:A:3296:LEU:HG	3:A:3297:PRO:HD3	1.92	0.52
3:B:70:GLU:OE2	3:B:110:ARG:NE	2.34	0.52
3:B:215:THR:HG22	3:B:273:HIS:HA	1.90	0.52
3:B:293:LEU:HD13	3:B:378:LEU:HD12	1.90	0.52
3:B:499:THR:HG23	3:B:502:HIS:H	1.74	0.52
3:B:1422:ASP:OD2	3:B:1568:LYS:NZ	2.37	0.52
3:A:3233:PRO:HB2	3:A:3238:GLU:HB2	1.90	0.52
3:I:1093:GLU:HB3	3:I:1201:HIS:HB3	1.92	0.52
3:I:3628:ARG:NH1	3:I:3857:GLY:O	2.42	0.52
1:C:27:ILE:HB	1:C:63:ILE:HB	1.90	0.52
3:A:499:THR:HG23	3:A:502:HIS:H	1.74	0.52
3:I:3813:GLN:NE2	3:I:3890:LEU:O	2.43	0.52
3:A:745:SER:HB2	3:A:758:ARG:HB2	1.91	0.52
3:A:1093:GLU:HB3	3:A:1201:HIS:HB3	1.92	0.52
3:B:2986:VAL:HG22	3:B:2988:LYS:H	1.75	0.52
3:B:3296:LEU:HG	3:B:3297:PRO:HD3	1.92	0.52
3:B:919:ASN:HA	3:B:922:LEU:HB2	1.92	0.52
3:G:215:THR:HG22	3:G:273:HIS:HA	1.90	0.52
3:G:499:THR:HG23	3:G:502:HIS:H	1.74	0.52
3:I:2986:VAL:HG22	3:I:2988:LYS:H	1.75	0.52
3:I:3157:ILE:HA	3:I:3161:VAL:HB	1.91	0.52
3:I:961:MET:HE2	3:I:964:GLY:H	1.75	0.52
3:B:975:VAL:HG12	3:B:1044:ARG:HH11	1.74	0.52
3:B:1156:THR:OG1	3:B:1157:GLU:OE1	2.28	0.52
3:B:3288:GLY:HA2	3:B:3303:PRO:HB3	1.91	0.52
3:G:3288:GLY:HA2	3:G:3303:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:919:ASN:HA	3:G:922:LEU:HB2	1.92	0.51
3:I:3296:LEU:HG	3:I:3297:PRO:HD3	1.92	0.51
3:I:3940:LYS:O	3:I:4002:LYS:NZ	2.39	0.51
3:A:975:VAL:HG12	3:A:1044:ARG:HH11	1.74	0.51
3:A:3696:ASP:OD2	3:A:3773:ARG:NE	2.38	0.51
3:B:1093:GLU:HB3	3:B:1201:HIS:HB3	1.92	0.51
3:G:961:MET:HE2	3:G:964:GLY:H	1.75	0.51
3:I:919:ASN:HA	3:I:922:LEU:HB2	1.92	0.51
3:B:955:LEU:O	3:B:966:LYS:NZ	2.31	0.51
3:G:3813:GLN:NE2	3:G:3890:LEU:O	2.43	0.51
3:G:4759:ASP:O	3:G:4761:PRO:HD3	2.09	0.51
3:A:961:MET:HE2	3:A:964:GLY:H	1.75	0.51
3:B:4759:ASP:O	3:B:4761:PRO:HD3	2.09	0.51
3:G:891:TRP:HA	3:G:902:ARG:HB3	1.93	0.51
3:I:3414:ARG:HE	3:I:3472:ALA:HB3	1.75	0.51
3:I:3850:GLN:NE2	3:I:3872:GLU:OE1	2.36	0.51
3:A:3288:GLY:HA2	3:A:3303:PRO:HB3	1.91	0.51
3:B:745:SER:HB2	3:B:758:ARG:HB2	1.91	0.51
3:B:3414:ARG:HE	3:B:3472:ALA:HB3	1.75	0.51
3:I:891:TRP:HA	3:I:902:ARG:HB3	1.93	0.51
3:I:3696:ASP:OD2	3:I:3773:ARG:NE	2.38	0.51
3:A:56:GLN:O	3:A:309:THR:OG1	2.19	0.51
3:A:891:TRP:HA	3:A:902:ARG:HB3	1.93	0.51
3:A:3850:GLN:NE2	3:A:3872:GLU:OE1	2.36	0.51
3:B:35:LEU:HD11	3:B:189:LEU:HD13	1.93	0.51
3:G:176:SER:OG	3:G:178:ARG:NH1	2.38	0.51
3:I:2754:PHE:HE2	3:I:2813:LEU:HD11	1.74	0.51
3:A:2754:PHE:HE2	3:A:2813:LEU:HD11	1.74	0.51
3:B:384:MET:SD	3:B:384:MET:N	2.77	0.51
3:I:499:THR:HG23	3:I:502:HIS:H	1.74	0.51
3:A:3414:ARG:HE	3:A:3472:ALA:HB3	1.75	0.51
3:I:3132:THR:HA	3:I:3136:LEU:HB3	1.93	0.51
3:B:3479:ALA:HA	3:I:1141:ARG:HB3	1.93	0.51
3:G:3552:PHE:O	3:G:3556:ASN:ND2	2.35	0.51
3:I:1992:ALA:HA	3:I:1995:THR:HG22	1.93	0.51
3:A:35:LEU:HD11	3:A:189:LEU:HD13	1.93	0.51
3:A:1272:LEU:HD22	3:A:1289:LEU:HD11	1.93	0.51
3:B:3208:PRO:HB2	3:B:3237:GLU:HG3	1.93	0.51
3:I:228:ASP:OD1	3:I:228:ASP:N	2.44	0.51
3:I:955:LEU:O	3:I:966:LYS:NZ	2.31	0.51
1:C:130:ILE:O	3:B:3499:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1057:ASP:OD1	3:A:1057:ASP:N	2.31	0.50
3:B:3813:GLN:NE2	3:B:3890:LEU:O	2.43	0.50
3:G:1272:LEU:HD22	3:G:1289:LEU:HD11	1.93	0.50
3:I:35:LEU:HD11	3:I:189:LEU:HD13	1.93	0.50
3:I:2736:ASP:OD1	3:I:2736:ASP:N	2.44	0.50
3:I:3288:GLY:HA2	3:I:3303:PRO:HB3	1.91	0.50
3:G:3414:ARG:HE	3:G:3472:ALA:HB3	1.75	0.50
1:C:86:ARG:NH2	1:C:87:GLU:OE2	2.45	0.50
3:A:919:ASN:HA	3:A:922:LEU:HB2	1.92	0.50
3:B:891:TRP:HA	3:B:902:ARG:HB3	1.93	0.50
3:G:1289:LEU:HD12	3:G:1562:ILE:HD11	1.93	0.50
3:I:4138:ASP:O	3:I:4142:ASN:ND2	2.34	0.50
3:B:1272:LEU:HD22	3:B:1289:LEU:HD11	1.93	0.50
3:G:35:LEU:HD11	3:G:189:LEU:HD13	1.93	0.50
3:G:155:LYS:NZ	3:I:228:ASP:OD2	2.34	0.50
3:G:2986:VAL:HG22	3:G:2988:LYS:H	1.75	0.50
3:G:3132:THR:HA	3:G:3136:LEU:HB3	1.93	0.50
3:I:1272:LEU:HD22	3:I:1289:LEU:HD11	1.93	0.50
2:F:88:PRO:HB2	3:A:1680:ARG:HH12	1.76	0.50
3:A:835:ARG:NH2	3:A:1210:SER:O	2.38	0.50
3:I:892:THR:HA	3:I:961:MET:HB3	1.94	0.50
3:A:892:THR:HA	3:A:961:MET:HB3	1.94	0.50
1:D:86:ARG:NH2	1:D:87:GLU:OE2	2.45	0.50
3:A:2986:VAL:HG22	3:A:2988:LYS:H	1.75	0.50
3:G:3628:ARG:NH1	3:G:3857:GLY:O	2.42	0.50
3:A:4138:ASP:O	3:A:4142:ASN:ND2	2.34	0.50
3:G:4172:GLU:OE1	3:G:4175:ARG:NH1	2.45	0.50
3:A:1992:ALA:HA	3:A:1995:THR:HG22	1.93	0.50
3:G:955:LEU:O	3:G:966:LYS:NZ	2.31	0.50
3:B:1733:GLU:HG2	3:B:2201:LEU:HD23	1.94	0.49
3:B:3132:THR:HA	3:B:3136:LEU:HB3	1.93	0.49
3:B:4172:GLU:OE1	3:B:4175:ARG:NH1	2.45	0.49
3:G:892:THR:HA	3:G:961:MET:HB3	1.94	0.49
3:G:1992:ALA:HA	3:G:1995:THR:HG22	1.93	0.49
3:G:3208:PRO:HB2	3:G:3237:GLU:HG3	1.93	0.49
3:A:1232:ARG:NH2	3:A:1828:ASP:O	2.45	0.49
3:A:4172:GLU:OE1	3:A:4175:ARG:NH1	2.45	0.49
3:I:4801:LEU:HD22	9:I:5101:L9R:H13A	1.92	0.49
1:K:86:ARG:NH2	1:K:87:GLU:OE2	2.45	0.49
1:E:111:ASN:O	3:G:1996:ARG:NH2	2.34	0.49
3:A:1289:LEU:HD12	3:A:1562:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1733:GLU:HG2	3:A:2201:LEU:HD23	1.94	0.49
1:E:66:PRO:HG3	3:G:2186:MET:HB3	1.94	0.49
3:A:1469:VAL:HG13	3:A:1492:CYS:HB3	1.95	0.49
3:B:892:THR:HA	3:B:961:MET:HB3	1.94	0.49
3:G:889:GLN:HB3	3:G:902:ARG:HH21	1.78	0.49
3:G:3133:THR:HG23	3:G:3134:VAL:HG23	1.94	0.49
3:I:1980:LEU:HD11	3:I:1994:ARG:HB3	1.94	0.49
3:A:3132:THR:HA	3:A:3136:LEU:HB3	1.93	0.49
3:A:4972:PRO:HB3	3:B:5024:ALA:HB3	1.94	0.49
3:B:228:ASP:OD1	3:B:228:ASP:N	2.44	0.49
3:B:1289:LEU:HD12	3:B:1562:ILE:HD11	1.93	0.49
3:G:4182:GLU:OE1	3:G:4983:HIS:NE2	2.46	0.49
3:I:3133:THR:HG23	3:I:3134:VAL:HG23	1.94	0.49
3:I:4172:GLU:OE1	3:I:4175:ARG:NH1	2.45	0.49
3:I:4182:GLU:OE1	3:I:4983:HIS:NE2	2.46	0.49
1:E:86:ARG:NH2	1:E:87:GLU:OE2	2.45	0.49
3:B:1992:ALA:HA	3:B:1995:THR:HG22	1.93	0.49
3:G:1232:ARG:NH2	3:G:1828:ASP:O	2.45	0.49
3:I:1289:LEU:HD12	3:I:1562:ILE:HD11	1.93	0.49
3:I:3208:PRO:HB2	3:I:3237:GLU:HG3	1.93	0.49
3:A:3208:PRO:HB2	3:A:3237:GLU:HG3	1.93	0.49
3:B:2884:ASN:OD1	3:B:2885:THR:N	2.46	0.49
3:A:4182:GLU:OE1	3:A:4983:HIS:NE2	2.46	0.49
3:A:4801:LEU:HD22	9:A:5308:L9R:H13A	1.93	0.49
3:B:1980:LEU:HD11	3:B:1994:ARG:HB3	1.94	0.49
3:B:3633:VAL:HG12	3:B:3637:ARG:HE	1.78	0.49
3:I:1733:GLU:HG2	3:I:2201:LEU:HD23	1.95	0.49
3:I:3459:VAL:HG13	3:I:3464:ILE:HB	1.95	0.49
3:A:3132:THR:HG22	3:A:3137:LEU:HD13	1.95	0.49
3:A:3133:THR:HG23	3:A:3134:VAL:HG23	1.94	0.49
3:A:5012:LYS:NZ	3:A:5016:GLU:OE2	2.41	0.49
3:B:4182:GLU:OE1	3:B:4983:HIS:NE2	2.46	0.49
3:I:2884:ASN:OD1	3:I:2885:THR:N	2.46	0.49
3:A:3633:VAL:HG12	3:A:3637:ARG:HE	1.78	0.49
3:B:1784:ALA:HA	2:O:55:VAL:HA	1.95	0.49
3:G:3633:VAL:HG12	3:G:3637:ARG:HE	1.78	0.49
3:I:3132:THR:HG22	3:I:3137:LEU:HD13	1.95	0.49
3:A:1447:CYS:HB3	3:A:1555:LEU:HB3	1.95	0.48
3:A:2867:LEU:HB2	3:A:2928:LYS:HZ3	1.78	0.48
3:B:3459:VAL:HG13	3:B:3464:ILE:HB	1.95	0.48
3:G:228:ASP:OD1	3:G:228:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1980:LEU:HD11	3:G:1994:ARG:HB3	1.94	0.48
3:G:2884:ASN:OD1	3:G:2885:THR:N	2.46	0.48
3:A:3459:VAL:HG13	3:A:3464:ILE:HB	1.95	0.48
3:B:889:GLN:HB3	3:B:902:ARG:HH21	1.78	0.48
3:B:961:MET:HE1	3:B:964:GLY:H	1.78	0.48
3:B:990:GLU:HG3	3:B:1024:TYR:HB3	1.94	0.48
3:G:1733:GLU:HG2	3:G:2201:LEU:HD23	1.95	0.48
3:G:3514:LEU:HD21	3:G:3602:VAL:HG13	1.95	0.48
3:I:1680:ARG:HH12	2:J:88:PRO:HB2	1.77	0.48
3:I:4983:HIS:O	5:I:5102:ATP:N6	2.46	0.48
1:C:117:THR:OG1	1:C:120:GLU:OE1	2.31	0.48
3:A:4983:HIS:O	5:A:5301:ATP:N6	2.46	0.48
3:B:1232:ARG:NH2	3:B:1828:ASP:O	2.45	0.48
3:B:3514:LEU:HD21	3:B:3602:VAL:HG13	1.95	0.48
3:G:919:ASN:HA	3:G:922:LEU:HD23	1.96	0.48
3:G:990:GLU:HG3	3:G:1024:TYR:HB3	1.94	0.48
3:G:3459:VAL:HG13	3:G:3464:ILE:HB	1.95	0.48
3:G:4731:ILE:O	3:I:4074:SER:OG	2.31	0.48
3:I:2725:LYS:HE2	3:I:2738:ARG:HH22	1.79	0.48
3:A:889:GLN:HB3	3:A:902:ARG:HH21	1.78	0.48
3:B:3940:LYS:O	3:B:4002:LYS:NZ	2.39	0.48
3:G:3545:THR:HG22	3:G:3548:GLU:HG3	1.95	0.48
3:G:3757:GLU:OE2	3:G:3761:GLN:NE2	2.46	0.48
3:I:919:ASN:HA	3:I:922:LEU:HD23	1.96	0.48
3:I:3633:VAL:HG12	3:I:3637:ARG:HE	1.78	0.48
3:A:228:ASP:OD1	3:A:228:ASP:N	2.44	0.48
3:A:516:LYS:O	3:A:520:ASN:ND2	2.31	0.48
3:B:1447:CYS:HB3	3:B:1555:LEU:HB3	1.95	0.48
3:B:1469:VAL:HG13	3:B:1492:CYS:HB3	1.95	0.48
3:B:2725:LYS:HE2	3:B:2738:ARG:HH22	1.78	0.48
3:B:3133:THR:HG23	3:B:3134:VAL:HG23	1.94	0.48
3:G:2736:ASP:O	3:G:2738:ARG:NH1	2.47	0.48
3:I:990:GLU:HG3	3:I:1024:TYR:HB3	1.94	0.48
3:I:1447:CYS:HB3	3:I:1555:LEU:HB3	1.95	0.48
3:I:3552:PHE:O	3:I:3556:ASN:ND2	2.35	0.48
9:I:5108:L9R:H6A	9:I:5108:L9R:H4A	1.47	0.48
3:A:1101:ARG:NH1	3:A:1115:LEU:O	2.46	0.48
3:B:1101:ARG:NH1	3:B:1115:LEU:O	2.46	0.48
3:G:684:VAL:HG22	3:G:781:VAL:HG12	1.96	0.48
3:G:1780:PRO:HG2	2:H:42:ARG:HD3	1.96	0.48
3:G:2736:ASP:OD1	3:G:2736:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3132:THR:HG22	3:G:3137:LEU:HD13	1.94	0.48
3:G:3316:LEU:HD21	3:G:3346:VAL:HG23	1.96	0.48
3:I:1469:VAL:HG13	3:I:1492:CYS:HB3	1.95	0.48
1:D:2:ASP:OD2	3:I:2244:ARG:NH1	2.46	0.48
3:A:919:ASN:HA	3:A:922:LEU:HD23	1.96	0.48
3:A:2884:ASN:OD1	3:A:2885:THR:N	2.46	0.48
3:A:4074:SER:OG	3:B:4731:ILE:O	2.31	0.48
3:B:925:SER:O	3:B:928:THR:OG1	2.32	0.48
3:G:1469:VAL:HG13	3:G:1492:CYS:HB3	1.95	0.48
3:I:728:ARG:NH2	3:I:1489:CYS:SG	2.87	0.48
3:A:3316:LEU:HD21	3:A:3346:VAL:HG23	1.96	0.48
3:B:2867:LEU:HB2	3:B:2928:LYS:HZ3	1.78	0.48
3:B:3132:THR:HG22	3:B:3137:LEU:HD13	1.95	0.48
3:B:4983:HIS:O	5:B:5301:ATP:N6	2.46	0.48
3:G:2725:LYS:HE2	3:G:2738:ARG:HH22	1.79	0.48
3:I:2867:LEU:HB2	3:I:2928:LYS:HZ3	1.79	0.48
3:I:3757:GLU:OE2	3:I:3761:GLN:NE2	2.46	0.48
1:E:133:ASP:HA	3:G:3460:VAL:HG11	1.95	0.48
3:A:990:GLU:HG3	3:A:1024:TYR:HB3	1.94	0.48
3:A:3545:THR:HG22	3:A:3548:GLU:HG3	1.95	0.48
3:A:4731:ILE:O	3:G:4074:SER:OG	2.31	0.48
3:B:4555:LEU:HD21	3:B:4656:LEU:HD22	1.96	0.48
3:G:925:SER:O	3:G:928:THR:OG1	2.32	0.48
3:G:1447:CYS:HB3	3:G:1555:LEU:HB3	1.95	0.48
3:I:3545:THR:HG22	3:I:3548:GLU:HG3	1.95	0.48
3:I:4555:LEU:HD21	3:I:4656:LEU:HD22	1.96	0.48
3:A:793:LEU:HD12	3:A:821:LEU:HD21	1.96	0.48
3:A:3757:GLU:OE2	3:A:3761:GLN:NE2	2.46	0.48
3:B:728:ARG:NH2	3:B:1489:CYS:SG	2.87	0.48
3:B:793:LEU:HD12	3:B:821:LEU:HD21	1.96	0.48
3:B:3768:SER:HA	3:B:3771:HIS:CD2	2.49	0.48
3:G:3768:SER:HA	3:G:3771:HIS:CD2	2.49	0.48
3:I:1078:GLU:OE2	3:I:1654:SER:OG	2.26	0.48
3:A:1503:PRO:HA	3:A:1508:ARG:HH22	1.79	0.47
3:A:1980:LEU:HD11	3:A:1994:ARG:HB3	1.94	0.47
3:A:2725:LYS:HE2	3:A:2738:ARG:HH22	1.79	0.47
3:A:2736:ASP:O	3:A:2738:ARG:NH1	2.47	0.47
3:B:919:ASN:HA	3:B:922:LEU:HD23	1.96	0.47
3:B:2736:ASP:O	3:B:2738:ARG:NH1	2.47	0.47
3:B:3757:GLU:OE2	3:B:3761:GLN:NE2	2.46	0.47
3:G:728:ARG:NH2	3:G:1489:CYS:SG	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3946:GLN:OE1	3:G:3949:ARG:NH2	2.39	0.47
3:A:728:ARG:NH2	3:A:1489:CYS:SG	2.87	0.47
3:A:3263:TYR:HD1	3:A:3270:ILE:HD12	1.79	0.47
3:A:3768:SER:HA	3:A:3771:HIS:CD2	2.49	0.47
3:A:3813:GLN:NE2	3:A:3890:LEU:O	2.43	0.47
3:B:1503:PRO:HA	3:B:1508:ARG:HH22	1.79	0.47
3:B:3263:TYR:HD1	3:B:3270:ILE:HD12	1.79	0.47
3:B:3545:THR:HG22	3:B:3548:GLU:HG3	1.95	0.47
3:G:2867:LEU:HB2	3:G:2928:LYS:HZ3	1.80	0.47
3:G:4983:HIS:O	5:G:5102:ATP:N6	2.46	0.47
3:I:889:GLN:HB3	3:I:902:ARG:HH21	1.78	0.47
3:I:1503:PRO:HA	3:I:1508:ARG:HH22	1.79	0.47
3:I:3514:LEU:HD21	3:I:3602:VAL:HG13	1.95	0.47
3:A:176:SER:OG	3:A:178:ARG:NH1	2.38	0.47
3:A:935:LEU:HD23	3:A:987:ARG:HH11	1.80	0.47
3:I:2029:GLN:NE2	3:I:2033:ASP:OD1	2.48	0.47
3:I:2736:ASP:O	3:I:2738:ARG:NH1	2.47	0.47
3:I:3768:SER:HA	3:I:3771:HIS:CD2	2.49	0.47
3:B:3552:PHE:O	3:B:3556:ASN:ND2	2.35	0.47
3:B:4006:ASP:OD1	3:B:4006:ASP:N	2.46	0.47
3:A:1569:GLN:HB2	3:A:1572:ILE:HD12	1.97	0.47
9:A:5308:L9R:H44	9:A:5308:L9R:H47A	1.52	0.47
3:I:793:LEU:HD12	3:I:821:LEU:HD21	1.96	0.47
3:I:925:SER:O	3:I:928:THR:OG1	2.32	0.47
3:B:935:LEU:HD23	3:B:987:ARG:HH11	1.80	0.47
3:B:4972:PRO:HB3	3:I:5024:ALA:HB3	1.96	0.47
3:G:793:LEU:HD12	3:G:821:LEU:HD21	1.96	0.47
3:G:835:ARG:NH2	3:G:1210:SER:O	2.38	0.47
3:G:3535:LEU:O	3:G:3538:THR:OG1	2.31	0.47
3:G:4006:ASP:OD1	3:G:4006:ASP:N	2.46	0.47
3:A:144:GLU:OE1	3:G:2452:ARG:NH1	2.47	0.47
3:A:2815:ALA:HB1	3:A:2881:ASN:HD22	1.80	0.47
3:A:3479:ALA:HA	3:B:1141:ARG:HB3	1.96	0.47
3:A:3514:LEU:HD21	3:A:3602:VAL:HG13	1.95	0.47
3:B:684:VAL:HG22	3:B:781:VAL:HG12	1.95	0.47
3:B:2020:ASP:OD1	3:B:2020:ASP:N	2.47	0.47
3:B:2029:GLN:NE2	3:B:2033:ASP:OD1	2.47	0.47
3:B:2815:ALA:HB1	3:B:2881:ASN:HD22	1.80	0.47
3:G:943:ASP:HB2	3:G:1050:GLY:HA3	1.97	0.47
3:G:1569:GLN:HB2	3:G:1572:ILE:HD12	1.97	0.47
3:G:2029:GLN:NE2	3:G:2033:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4148:THR:HG21	3:G:4180:ARG:HH21	1.80	0.47
3:I:684:VAL:HG22	3:I:781:VAL:HG12	1.96	0.47
3:I:1101:ARG:NH1	3:I:1115:LEU:O	2.46	0.47
3:I:3343:GLN:O	3:I:3346:VAL:HG12	2.15	0.47
3:A:684:VAL:HG22	3:A:781:VAL:HG12	1.96	0.47
3:A:1454:THR:OG1	3:A:1456:ASP:OD1	2.20	0.47
3:A:2029:GLN:NE2	3:A:2033:ASP:OD1	2.48	0.47
3:A:4006:ASP:N	3:A:4006:ASP:OD1	2.46	0.47
3:B:2626:LEU:HD22	3:B:2640:PRO:HB3	1.97	0.47
3:G:935:LEU:HD23	3:G:987:ARG:HH11	1.80	0.47
3:I:1232:ARG:NH2	3:I:1828:ASP:O	2.45	0.47
3:I:3316:LEU:HD21	3:I:3346:VAL:HG23	1.96	0.47
9:I:5101:L9R:H4A	9:I:5101:L9R:H7B	1.45	0.47
3:A:2538:THR:HG23	3:A:2541:PHE:H	1.80	0.47
3:A:3343:GLN:O	3:A:3346:VAL:HG12	2.15	0.47
9:A:5308:L9R:H7B	9:A:5308:L9R:H4A	1.45	0.47
3:B:872:GLU:HA	3:B:922:LEU:HD11	1.97	0.47
3:B:3343:GLN:O	3:B:3346:VAL:HG12	2.15	0.47
3:B:3862:ASP:OD1	3:B:3862:ASP:N	2.48	0.47
3:G:144:GLU:HG3	3:G:175:SER:HB3	1.96	0.47
3:G:1653:LEU:O	3:G:1660:GLN:NE2	2.48	0.47
3:G:2626:LEU:HD22	3:G:2640:PRO:HB3	1.97	0.47
3:I:2626:LEU:HD22	3:I:2640:PRO:HB3	1.97	0.47
3:I:2815:ALA:HB1	3:I:2881:ASN:HD22	1.80	0.47
3:I:3263:TYR:HD1	3:I:3270:ILE:HD12	1.79	0.47
1:E:94:LYS:HE3	1:E:107:HIS:HB3	1.97	0.47
3:A:872:GLU:HA	3:A:922:LEU:HD11	1.97	0.47
3:A:2626:LEU:HD22	3:A:2640:PRO:HB3	1.97	0.47
3:A:3862:ASP:OD1	3:A:3862:ASP:N	2.48	0.47
3:B:176:SER:OG	3:B:178:ARG:NH1	2.38	0.47
3:I:835:ARG:NH2	3:I:1210:SER:O	2.38	0.47
3:I:935:LEU:HD23	3:I:987:ARG:HH11	1.80	0.47
3:I:943:ASP:HB2	3:I:1050:GLY:HA3	1.97	0.47
3:I:1569:GLN:HB2	3:I:1572:ILE:HD12	1.97	0.47
3:A:2452:ARG:NH1	3:B:144:GLU:OE1	2.49	0.46
3:B:835:ARG:NH2	3:B:1210:SER:O	2.38	0.46
3:G:943:ASP:OD2	3:G:945:LYS:NZ	2.47	0.46
3:G:2538:THR:HG23	3:G:2541:PHE:H	1.80	0.46
3:G:3343:GLN:O	3:G:3346:VAL:HG12	2.15	0.46
1:D:94:LYS:HE3	1:D:107:HIS:HB3	1.97	0.46
1:C:94:LYS:HE3	1:C:107:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:943:ASP:HB2	3:A:1050:GLY:HA3	1.97	0.46
3:B:1569:GLN:HB2	3:B:1572:ILE:HD12	1.97	0.46
3:B:3944:GLU:OE1	3:B:3946:GLN:N	2.47	0.46
3:G:1503:PRO:HA	3:G:1508:ARG:HH22	1.79	0.46
3:G:3263:TYR:HD1	3:G:3270:ILE:HD12	1.79	0.46
3:G:3412:LEU:HD11	3:G:3434:LEU:HD21	1.98	0.46
3:G:5024:ALA:HB3	3:I:4972:PRO:HB3	1.96	0.46
3:I:2538:THR:HG23	3:I:2541:PHE:H	1.80	0.46
3:A:3412:LEU:HD11	3:A:3434:LEU:HD21	1.98	0.46
3:B:4074:SER:OG	3:I:4731:ILE:O	2.33	0.46
3:G:1101:ARG:NH1	3:G:1115:LEU:O	2.46	0.46
3:G:4555:LEU:HD21	3:G:4656:LEU:HD22	1.96	0.46
3:B:3316:LEU:HD21	3:B:3346:VAL:HG23	1.96	0.46
3:G:4801:LEU:HD22	9:G:5101:L9R:H13A	1.97	0.46
3:I:144:GLU:HG3	3:I:175:SER:HB3	1.96	0.46
3:A:144:GLU:HG3	3:A:175:SER:HB3	1.96	0.46
3:A:1465:ASP:OD1	3:A:1468:LYS:HG2	2.16	0.46
3:B:1653:LEU:O	3:B:1660:GLN:NE2	2.48	0.46
3:B:3412:LEU:HD11	3:B:3434:LEU:HD21	1.97	0.46
3:G:1996:ARG:HH21	3:G:1999:ARG:HE	1.64	0.46
3:G:2815:ALA:HB1	3:G:2881:ASN:HD22	1.80	0.46
3:G:3604:TYR:O	3:G:3608:GLN:HG2	2.16	0.46
3:I:2020:ASP:OD1	3:I:2020:ASP:N	2.47	0.46
3:I:3946:GLN:OE1	3:I:3949:ARG:NH2	2.39	0.46
3:I:4006:ASP:OD1	3:I:4006:ASP:N	2.46	0.46
3:I:4148:THR:HG21	3:I:4180:ARG:HH21	1.80	0.46
1:K:94:LYS:HE3	1:K:107:HIS:HB3	1.97	0.46
3:A:3552:PHE:O	3:A:3556:ASN:ND2	2.35	0.46
3:A:4148:THR:HG21	3:A:4180:ARG:HH21	1.80	0.46
3:A:4555:LEU:HD21	3:A:4656:LEU:HD22	1.96	0.46
3:B:4801:LEU:HD22	9:B:5308:L9R:H13A	1.97	0.46
3:G:275:ARG:NH1	3:G:338:GLU:OE2	2.49	0.46
3:I:1465:ASP:OD1	3:I:1468:LYS:HG2	2.16	0.46
3:B:2736:ASP:OD1	3:B:2736:ASP:N	2.44	0.46
3:G:886:ARG:HB3	3:G:891:TRP:CG	2.51	0.46
3:G:3842:LEU:HB2	3:G:3929:SER:HB2	1.98	0.46
3:I:663:TYR:CD2	3:I:804:PRO:HB3	2.51	0.46
3:I:1653:LEU:O	3:I:1660:GLN:NE2	2.48	0.46
1:K:117:THR:OG1	1:K:120:GLU:OE1	2.31	0.46
3:A:803:LEU:HD12	3:A:804:PRO:HD2	1.98	0.46
3:A:2309:SER:OG	3:A:2320:ASP:OD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:943:ASP:HB2	3:B:1050:GLY:HA3	1.97	0.46
3:B:2538:THR:HG23	3:B:2541:PHE:H	1.80	0.46
3:B:3840:SER:OG	3:B:3877:ASP:OD1	2.29	0.46
9:I:5108:L9R:H32A	9:I:5108:L9R:H35A	1.75	0.46
3:A:886:ARG:HB3	3:A:891:TRP:CG	2.51	0.46
3:I:2917:ALA:HA	3:I:2920:ARG:HB3	1.98	0.46
1:K:122:ASP:HA	1:K:125:ILE:HG22	1.99	0.45
1:E:117:THR:OG1	1:E:120:GLU:OE1	2.31	0.45
3:B:1024:TYR:CZ	3:B:1032:LYS:HG3	2.51	0.45
3:B:2309:SER:OG	3:B:2320:ASP:OD1	2.34	0.45
3:B:2355:ARG:NH2	3:B:2449:GLU:OE2	2.49	0.45
3:B:3604:TYR:O	3:B:3608:GLN:HG2	2.16	0.45
3:B:4754:ASN:HB3	3:B:4756:ARG:HH21	1.81	0.45
1:K:132:GLY:O	3:A:3456:GLN:NE2	2.43	0.45
3:A:1996:ARG:HH21	3:A:1999:ARG:HE	1.64	0.45
3:A:2917:ALA:HA	3:A:2920:ARG:HB3	1.98	0.45
3:A:3604:TYR:O	3:A:3608:GLN:HG2	2.16	0.45
3:B:144:GLU:HG3	3:B:175:SER:HB3	1.96	0.45
3:B:950:LEU:HD13	3:B:970:LEU:HG	1.99	0.45
3:B:4579:PHE:CD1	3:B:4639:MET:HE1	2.51	0.45
3:G:663:TYR:CD2	3:G:804:PRO:HB3	2.51	0.45
9:G:5108:L9R:H6A	9:G:5108:L9R:H4A	1.46	0.45
3:I:943:ASP:OD2	3:I:945:LYS:NZ	2.47	0.45
1:C:2:ASP:OD2	3:B:2244:ARG:NH1	2.49	0.45
3:A:4000:MET:SD	3:A:4020:GLN:NE2	2.73	0.45
3:G:336:PRO:HA	3:G:337:PRO:HD3	1.88	0.45
3:G:803:LEU:HD12	3:G:804:PRO:HD2	1.98	0.45
3:I:872:GLU:HA	3:I:922:LEU:HD11	1.97	0.45
3:I:3412:LEU:HD11	3:I:3434:LEU:HD21	1.97	0.45
3:I:5012:LYS:NZ	3:I:5016:GLU:OE2	2.41	0.45
3:A:233:ILE:O	3:A:257:ARG:NH1	2.49	0.45
3:B:4148:THR:HG21	3:B:4180:ARG:HH21	1.80	0.45
3:B:5012:LYS:NZ	3:B:5016:GLU:OE2	2.41	0.45
9:B:5307:L9R:H6A	9:B:5307:L9R:H4A	1.46	0.45
3:G:1024:TYR:CZ	3:G:1032:LYS:HG3	2.51	0.45
3:G:3862:ASP:OD1	3:G:3862:ASP:N	2.48	0.45
3:I:886:ARG:HB3	3:I:891:TRP:CG	2.51	0.45
3:A:663:TYR:CD2	3:A:804:PRO:HB3	2.51	0.45
3:B:758:ARG:HG2	3:B:763:PRO:HA	1.99	0.45
3:B:2917:ALA:HA	3:B:2920:ARG:HB3	1.99	0.45
3:G:2309:SER:OG	3:G:2320:ASP:OD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:665:GLU:HB2	3:I:792:LEU:HB2	1.98	0.45
3:I:2309:SER:OG	3:I:2320:ASP:OD1	2.34	0.45
3:I:3604:TYR:O	3:I:3608:GLN:HG2	2.16	0.45
3:A:2974:ILE:HG13	3:A:2975:ALA:N	2.32	0.45
3:A:4754:ASN:HB3	3:A:4756:ARG:HH21	1.81	0.45
9:A:5307:L9R:H32A	9:A:5307:L9R:H35A	1.75	0.45
3:B:2974:ILE:HG13	3:B:2975:ALA:N	2.32	0.45
3:G:872:GLU:HA	3:G:922:LEU:HD11	1.97	0.45
3:G:2917:ALA:HA	3:G:2920:ARG:HB3	1.99	0.45
9:G:5101:L9R:H4A	9:G:5101:L9R:H7B	1.45	0.45
3:I:2881:ASN:HA	3:I:2884:ASN:ND2	2.32	0.45
3:I:4754:ASN:HB3	3:I:4756:ARG:HH21	1.81	0.45
3:A:665:GLU:HB2	3:A:792:LEU:HB2	1.98	0.45
3:A:950:LEU:HD13	3:A:970:LEU:HG	1.99	0.45
3:A:1008:SER:HB3	3:A:1017:ARG:HB3	1.99	0.45
3:B:665:GLU:HB2	3:B:792:LEU:HB2	1.98	0.45
3:B:803:LEU:HD12	3:B:804:PRO:HD2	1.98	0.45
3:B:1099:GLU:OE2	3:B:1125:ASN:ND2	2.50	0.45
3:B:3842:LEU:HB2	3:B:3929:SER:HB2	1.98	0.45
3:G:1465:ASP:OD1	3:G:1468:LYS:HG2	2.16	0.45
3:I:1996:ARG:HH21	3:I:1999:ARG:HE	1.64	0.45
3:I:2677:LYS:HE2	3:I:2677:LYS:HB3	1.81	0.45
3:A:758:ARG:HG2	3:A:763:PRO:HA	1.99	0.45
3:A:2736:ASP:OD1	3:A:2736:ASP:N	2.44	0.45
3:A:3731:LYS:HA	3:A:3734:HIS:HE1	1.82	0.45
3:B:1008:SER:HB3	3:B:1017:ARG:HB3	1.99	0.45
3:B:3752:SER:OG	3:B:3755:GLU:OE1	2.35	0.45
3:G:2881:ASN:HA	3:G:2884:ASN:ND2	2.32	0.45
3:G:2974:ILE:HG13	3:G:2975:ALA:N	2.32	0.45
3:G:3731:LYS:HA	3:G:3734:HIS:CE1	2.52	0.45
3:I:803:LEU:HD12	3:I:804:PRO:HD2	1.98	0.45
3:I:3731:LYS:HA	3:I:3734:HIS:CE1	2.52	0.45
3:I:3842:LEU:HB2	3:I:3929:SER:HB2	1.98	0.45
1:E:122:ASP:HA	1:E:125:ILE:HG22	1.99	0.45
3:A:648:ILE:HG23	3:A:814:ALA:HB3	1.99	0.45
3:A:3731:LYS:HA	3:A:3734:HIS:CE1	2.52	0.45
3:B:663:TYR:CD2	3:B:804:PRO:HB3	2.51	0.45
3:B:2912:THR:OG1	3:B:2913:ALA:N	2.50	0.45
3:G:4648:LEU:HD12	3:G:4803:HIS:HE1	1.82	0.45
3:I:2355:ARG:NH2	3:I:2449:GLU:OE2	2.50	0.45
3:I:2974:ILE:HG13	3:I:2975:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:856:VAL:H	3:A:991:ASN:ND2	2.15	0.45
3:A:3842:LEU:HB2	3:A:3929:SER:HB2	1.98	0.45
3:A:4152:GLU:OE1	3:A:4194:TYR:OH	2.28	0.45
9:A:5308:L9R:H3A	9:B:5307:L9R:H33A	1.99	0.45
3:B:648:ILE:HG23	3:B:814:ALA:HB3	1.99	0.45
3:B:1465:ASP:OD1	3:B:1468:LYS:HG2	2.16	0.45
3:B:2452:ARG:NH1	3:I:144:GLU:OE1	2.50	0.45
3:G:2912:THR:OG1	3:G:2913:ALA:N	2.50	0.45
3:I:856:VAL:H	3:I:991:ASN:ND2	2.15	0.45
3:I:1024:TYR:CZ	3:I:1032:LYS:HG3	2.51	0.45
3:I:4661:TYR:OH	3:I:4786:ASP:OD2	2.33	0.45
2:O:4:VAL:HG22	2:O:74:LEU:HD22	1.99	0.45
3:A:275:ARG:NH1	3:A:338:GLU:OE2	2.49	0.44
3:B:275:ARG:NH1	3:B:338:GLU:OE2	2.49	0.44
3:G:613:ALA:HB2	3:G:1676:LEU:HD12	1.99	0.44
3:G:3731:LYS:HA	3:G:3734:HIS:HE1	1.82	0.44
3:I:3872:GLU:HG3	3:I:3874:VAL:H	1.83	0.44
2:J:4:VAL:HG22	2:J:74:LEU:HD22	2.00	0.44
3:A:1024:TYR:CZ	3:A:1032:LYS:HG3	2.51	0.44
3:A:3332:ALA:HB3	3:A:3403:ARG:NH1	2.32	0.44
3:A:4640:GLU:HB3	3:A:4641:PRO:HD3	2.00	0.44
9:A:5307:L9R:H33A	9:G:5101:L9R:H3A	2.00	0.44
3:B:886:ARG:HB3	3:B:891:TRP:CG	2.51	0.44
3:B:1996:ARG:HH21	3:B:1999:ARG:HE	1.64	0.44
3:B:3731:LYS:HA	3:B:3734:HIS:HE1	1.82	0.44
3:I:275:ARG:NH1	3:I:338:GLU:OE2	2.49	0.44
3:A:2020:ASP:OD1	3:A:2020:ASP:N	2.47	0.44
3:A:2821:TRP:HD1	3:A:2939:ARG:HA	1.82	0.44
3:A:3805:LEU:HB3	3:A:3890:LEU:HB3	1.99	0.44
3:B:943:ASP:OD2	3:B:945:LYS:NZ	2.47	0.44
3:B:2821:TRP:HD1	3:B:2939:ARG:HA	1.82	0.44
3:G:1680:ARG:HH12	2:H:88:PRO:HB2	1.82	0.44
3:G:2355:ARG:NH2	3:G:2449:GLU:OE2	2.49	0.44
3:G:2875:ALA:HB2	3:G:2927:LEU:HD22	2.00	0.44
3:G:3332:ALA:HB3	3:G:3403:ARG:NH1	2.32	0.44
3:G:3872:GLU:HG3	3:G:3874:VAL:H	1.82	0.44
3:I:2912:THR:OG1	3:I:2913:ALA:N	2.50	0.44
1:D:122:ASP:HA	1:D:125:ILE:HG22	1.99	0.44
3:A:2881:ASN:HA	3:A:2884:ASN:ND2	2.32	0.44
3:A:2912:THR:OG1	3:A:2913:ALA:N	2.50	0.44
3:B:2633:LEU:O	3:B:2689:LYS:NZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:952:LYS:HD3	3:G:970:LEU:HA	2.00	0.44
3:G:1008:SER:HB3	3:G:1017:ARG:HB3	1.99	0.44
9:G:5108:L9R:H33A	9:I:5101:L9R:H3A	1.99	0.44
3:I:176:SER:OG	3:I:178:ARG:NH1	2.38	0.44
3:I:758:ARG:HG2	3:I:763:PRO:HA	1.99	0.44
3:I:952:LYS:HD3	3:I:970:LEU:HA	2.00	0.44
3:A:923:GLN:O	3:A:927:GLU:HG2	2.18	0.44
3:A:2355:ARG:NH2	3:A:2449:GLU:OE2	2.50	0.44
3:A:3946:GLN:OE1	3:A:3949:ARG:NH2	2.39	0.44
3:B:856:VAL:H	3:B:991:ASN:ND2	2.15	0.44
3:B:4000:MET:SD	3:B:4020:GLN:NE2	2.73	0.44
3:B:4640:GLU:HB3	3:B:4641:PRO:HD3	2.00	0.44
9:B:5308:L9R:H3A	9:I:5108:L9R:H33A	1.99	0.44
3:G:4177:TYR:CE1	3:G:4199:GLU:HG3	2.53	0.44
3:I:2821:TRP:HD1	3:I:2939:ARG:HA	1.83	0.44
3:I:3442:PHE:CG	3:I:3514:LEU:HD22	2.53	0.44
3:I:3805:LEU:HB3	3:I:3890:LEU:HB3	1.99	0.44
3:I:4640:GLU:HB3	3:I:4641:PRO:HD3	2.00	0.44
3:I:4648:LEU:HD12	3:I:4803:HIS:HE1	1.82	0.44
1:K:85:ILE:H	1:K:85:ILE:HG13	1.57	0.44
3:A:613:ALA:HB2	3:A:1676:LEU:HD12	2.00	0.44
3:A:783:PHE:HB2	3:A:787:VAL:HG21	1.99	0.44
3:A:1694:LEU:HB3	3:A:1715:LEU:HD12	2.00	0.44
3:A:3872:GLU:HG3	3:A:3874:VAL:H	1.82	0.44
3:B:69:LEU:HD13	3:B:101:LEU:HD11	1.99	0.44
3:B:932:LEU:HD21	3:B:988:LEU:HD11	2.00	0.44
3:B:3332:ALA:HB3	3:B:3403:ARG:NH1	2.32	0.44
3:B:4177:TYR:CE1	3:B:4199:GLU:HG3	2.53	0.44
3:G:69:LEU:HD13	3:G:101:LEU:HD11	1.99	0.44
3:G:758:ARG:HG2	3:G:763:PRO:HA	1.99	0.44
3:G:2108:GLU:O	3:G:3694:LYS:NZ	2.51	0.44
3:G:2633:LEU:O	3:G:2689:LYS:NZ	2.51	0.44
3:G:4648:LEU:HD12	3:G:4803:HIS:CE1	2.53	0.44
3:I:1008:SER:HB3	3:I:1017:ARG:HB3	1.99	0.44
3:I:3731:LYS:HA	3:I:3734:HIS:HE1	1.82	0.44
3:I:4177:TYR:CE1	3:I:4199:GLU:HG3	2.53	0.44
1:C:111:ASN:O	3:B:1996:ARG:NH2	2.36	0.44
3:A:4648:LEU:HD12	3:A:4803:HIS:CE1	2.53	0.44
3:B:783:PHE:HB2	3:B:787:VAL:HG21	1.99	0.44
3:B:1820:ARG:O	3:B:1824:GLN:HG2	2.18	0.44
3:B:3731:LYS:HA	3:B:3734:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4000:MET:SD	3:G:4020:GLN:NE2	2.73	0.44
3:G:4754:ASN:HB3	3:G:4756:ARG:HH21	1.81	0.44
3:G:4818:MET:HA	3:G:4824:ARG:HH11	1.83	0.44
9:G:5101:L9R:H23	9:G:5101:L9R:H20	1.32	0.44
3:I:950:LEU:HD13	3:I:970:LEU:HG	1.99	0.44
2:H:4:VAL:HG22	2:H:74:LEU:HD22	2.00	0.44
3:B:923:GLN:O	3:B:927:GLU:HG2	2.18	0.44
3:B:3872:GLU:HG3	3:B:3874:VAL:H	1.82	0.44
3:G:648:ILE:HG23	3:G:814:ALA:HB3	1.99	0.44
3:G:856:VAL:H	3:G:991:ASN:ND2	2.15	0.44
3:G:950:LEU:HD13	3:G:970:LEU:HG	1.99	0.44
3:G:3752:SER:OG	3:G:3755:GLU:OE1	2.34	0.44
3:I:2633:LEU:O	3:I:2689:LYS:NZ	2.51	0.44
3:I:2875:ALA:HB2	3:I:2927:LEU:HD22	2.00	0.44
1:C:122:ASP:HA	1:C:125:ILE:HG22	1.98	0.44
3:A:664:PHE:HB3	3:A:811:CYS:SG	2.58	0.44
3:A:943:ASP:OD2	3:A:945:LYS:NZ	2.47	0.44
3:A:4648:LEU:HD12	3:A:4803:HIS:HE1	1.82	0.44
3:A:4818:MET:HA	3:A:4824:ARG:HH11	1.83	0.44
3:A:5024:ALA:HB3	3:G:4972:PRO:HB3	1.98	0.44
3:B:1716:ILE:O	3:B:1721:GLU:N	2.51	0.44
3:B:2765:LYS:HA	3:B:2765:LYS:HD3	1.78	0.44
3:B:4648:LEU:HD12	3:B:4803:HIS:HE1	1.82	0.44
3:G:2821:TRP:HD1	3:G:2939:ARG:HA	1.82	0.44
3:G:4579:PHE:CD1	3:G:4639:MET:HE1	2.53	0.44
3:G:4640:GLU:HB3	3:G:4641:PRO:HD3	2.00	0.44
3:I:664:PHE:HB3	3:I:811:CYS:SG	2.58	0.44
3:I:783:PHE:HB2	3:I:787:VAL:HG21	1.99	0.44
3:I:3230:LEU:H	3:I:3230:LEU:HD23	1.83	0.44
1:C:85:ILE:H	1:C:85:ILE:HG13	1.57	0.43
3:A:932:LEU:HD21	3:A:988:LEU:HD11	2.00	0.43
3:A:1653:LEU:O	3:A:1660:GLN:NE2	2.48	0.43
3:A:2633:LEU:O	3:A:2689:LYS:NZ	2.51	0.43
3:A:2875:ALA:HB2	3:A:2927:LEU:HD22	2.00	0.43
3:A:3446:SER:O	3:A:3452:LYS:NZ	2.42	0.43
3:A:3752:SER:OG	3:A:3755:GLU:OE1	2.34	0.43
3:A:4177:TYR:CE1	3:A:4199:GLU:HG3	2.53	0.43
3:G:923:GLN:O	3:G:927:GLU:HG2	2.18	0.43
3:G:1141:ARG:HB3	3:I:3479:ALA:HA	2.00	0.43
3:G:4861:LYS:H	3:G:4861:LYS:HG3	1.53	0.43
3:I:2765:LYS:HD3	3:I:2765:LYS:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3621:HIS:ND1	3:I:3623:LEU:HD23	2.33	0.43
3:I:3862:ASP:OD1	3:I:3862:ASP:N	2.48	0.43
3:A:815:VAL:O	3:A:1007:TYR:OH	2.27	0.43
3:A:1820:ARG:O	3:A:1824:GLN:HG2	2.18	0.43
3:A:3442:PHE:CG	3:A:3514:LEU:HD22	2.53	0.43
3:A:3556:ASN:HB3	3:A:3559:LEU:HD13	2.00	0.43
3:A:4579:PHE:CD1	3:A:4639:MET:HE1	2.52	0.43
3:B:952:LYS:HD3	3:B:970:LEU:HA	2.00	0.43
3:B:3805:LEU:HB3	3:B:3890:LEU:HB3	1.99	0.43
3:G:664:PHE:HB3	3:G:811:CYS:SG	2.58	0.43
3:G:1454:THR:OG1	3:G:1456:ASP:OD1	2.20	0.43
3:G:2580:ASP:OD1	3:G:2621:HIS:HB2	2.19	0.43
3:I:451:TYR:CZ	3:I:474:ARG:HD2	2.53	0.43
3:I:1780:PRO:HG2	2:J:42:ARG:HD3	1.99	0.43
2:F:4:VAL:HG22	2:F:74:LEU:HD22	2.00	0.43
3:A:3123:LYS:HG3	3:A:3125:VAL:H	1.83	0.43
3:B:233:ILE:O	3:B:257:ARG:NH1	2.49	0.43
3:B:451:TYR:CZ	3:B:474:ARG:HD2	2.53	0.43
3:B:664:PHE:HB3	3:B:811:CYS:SG	2.58	0.43
3:B:2881:ASN:HA	3:B:2884:ASN:ND2	2.32	0.43
3:B:3852:LYS:HE3	3:B:3852:LYS:HB3	1.89	0.43
3:G:3123:LYS:HG3	3:G:3125:VAL:H	1.83	0.43
3:I:1694:LEU:HB3	3:I:1715:LEU:HD12	2.00	0.43
3:I:3332:ALA:HB3	3:I:3403:ARG:NH1	2.32	0.43
3:I:3535:LEU:O	3:I:3538:THR:OG1	2.31	0.43
3:B:1022:VAL:HG22	3:B:1023:PRO:HD2	2.01	0.43
3:B:2764:GLU:HG3	3:B:2857:PRO:HB3	2.01	0.43
3:B:3446:SER:O	3:B:3452:LYS:NZ	2.42	0.43
3:G:1099:GLU:OE2	3:G:1125:ASN:ND2	2.50	0.43
3:G:3805:LEU:HB3	3:G:3890:LEU:HB3	1.99	0.43
3:I:1168:VAL:HG11	3:I:1176:GLU:HG2	2.00	0.43
3:I:2888:ARG:O	3:I:2892:GLN:HG2	2.18	0.43
3:I:3752:SER:OG	3:I:3755:GLU:OE1	2.35	0.43
9:I:5101:L9R:H47A	9:I:5101:L9R:H44	1.53	0.43
3:A:2580:ASP:OD1	3:A:2621:HIS:HB2	2.19	0.43
3:A:2764:GLU:HG3	3:A:2857:PRO:HB3	2.01	0.43
3:A:3159:ASP:OD1	3:A:3159:ASP:N	2.52	0.43
3:A:3621:HIS:ND1	3:A:3623:LEU:HD23	2.33	0.43
3:A:3852:LYS:HE3	3:A:3852:LYS:HB3	1.89	0.43
3:A:4967:TYR:OH	3:A:5033:GLU:OE2	2.29	0.43
3:B:1168:VAL:HG11	3:B:1176:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1694:LEU:HB3	3:B:1715:LEU:HD12	2.00	0.43
3:B:2677:LYS:HB3	3:B:2677:LYS:HE2	1.81	0.43
3:G:665:GLU:HB2	3:G:792:LEU:HB2	1.98	0.43
3:I:328:LYS:HE3	3:I:328:LYS:HB3	1.80	0.43
3:I:2580:ASP:OD1	3:I:2621:HIS:HB2	2.19	0.43
2:J:25:HIS:CD2	2:J:104:LEU:HD11	2.54	0.43
2:F:42:ARG:HD3	3:A:1780:PRO:HG2	2.01	0.43
1:D:117:THR:OG1	1:D:120:GLU:OE1	2.31	0.43
3:A:365:LYS:HB3	3:A:365:LYS:HE3	1.80	0.43
3:A:1099:GLU:OE2	3:A:1125:ASN:ND2	2.50	0.43
3:A:2765:LYS:HZ3	3:A:2857:PRO:HB2	1.84	0.43
3:A:3230:LEU:HD23	3:A:3230:LEU:H	1.83	0.43
3:B:11:VAL:HG11	3:B:164:ARG:HD3	2.01	0.43
3:G:783:PHE:HB2	3:G:787:VAL:HG21	1.99	0.43
3:I:169:LEU:HD22	3:I:202:MET:HG3	2.00	0.43
3:I:613:ALA:HB2	3:I:1676:LEU:HD12	1.99	0.43
3:I:923:GLN:O	3:I:927:GLU:HG2	2.18	0.43
3:I:1022:VAL:HG22	3:I:1023:PRO:HD2	2.01	0.43
3:I:1206:GLN:HA	3:I:1227:ALA:O	2.18	0.43
3:I:1773:PRO:HA	3:I:1774:PRO:HD3	1.90	0.43
3:I:4818:MET:HA	3:I:4824:ARG:HH11	1.83	0.43
2:O:25:HIS:CD2	2:O:104:LEU:HD11	2.54	0.43
3:A:69:LEU:HD13	3:A:101:LEU:HD11	1.99	0.43
3:A:451:TYR:CZ	3:A:474:ARG:HD2	2.53	0.43
3:A:2236:LEU:HD13	3:A:2250:MET:HE1	2.01	0.43
3:A:2888:ARG:O	3:A:2892:GLN:HG2	2.18	0.43
3:B:613:ALA:HB2	3:B:1676:LEU:HD12	1.99	0.43
3:B:2580:ASP:OD1	3:B:2621:HIS:HB2	2.19	0.43
3:B:3442:PHE:CG	3:B:3514:LEU:HD22	2.53	0.43
3:B:3556:ASN:HB3	3:B:3559:LEU:HD13	2.00	0.43
3:G:11:VAL:HG11	3:G:164:ARG:HD3	2.01	0.43
3:I:69:LEU:HD13	3:I:101:LEU:HD11	1.99	0.43
3:I:648:ILE:HG23	3:I:814:ALA:HB3	1.99	0.43
3:I:932:LEU:HD21	3:I:988:LEU:HD11	2.00	0.43
3:I:1057:ASP:OD1	3:I:1057:ASP:N	2.31	0.43
3:I:1753:LYS:HB3	3:I:1758:ARG:HA	2.01	0.43
3:I:2108:GLU:O	3:I:3694:LYS:NZ	2.51	0.43
3:I:4648:LEU:HD12	3:I:4803:HIS:CE1	2.53	0.43
3:A:11:VAL:HG11	3:A:164:ARG:HD3	2.01	0.43
3:A:1022:VAL:HG22	3:A:1023:PRO:HD2	2.01	0.43
3:A:1168:VAL:HG11	3:A:1176:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4661:TYR:OH	3:A:4786:ASP:OD2	2.33	0.43
3:B:2875:ALA:HB2	3:B:2927:LEU:HD22	2.00	0.43
3:B:3621:HIS:ND1	3:B:3623:LEU:HD23	2.33	0.43
3:I:11:VAL:HG11	3:I:164:ARG:HD3	2.01	0.43
3:I:232:THR:HG21	3:I:252:VAL:HG21	2.01	0.43
3:A:952:LYS:HD3	3:A:970:LEU:HA	2.00	0.43
3:A:1206:GLN:HA	3:A:1227:ALA:O	2.18	0.43
3:A:2587:TYR:O	3:A:2590:SER:OG	2.31	0.43
3:A:3391:GLU:HG3	3:A:3395:ARG:HE	1.84	0.43
3:A:3392:LEU:HD13	3:A:3395:ARG:HD2	2.01	0.43
3:A:3944:GLU:OE1	3:A:3946:GLN:N	2.47	0.43
9:A:5307:L9R:H6A	9:A:5307:L9R:H4A	1.46	0.43
3:B:169:LEU:HD22	3:B:202:MET:HG3	2.00	0.43
3:B:2108:GLU:O	3:B:3694:LYS:NZ	2.51	0.43
3:B:3123:LYS:HG3	3:B:3125:VAL:H	1.83	0.43
3:B:4648:LEU:HD12	3:B:4803:HIS:CE1	2.53	0.43
3:G:2888:ARG:O	3:G:2892:GLN:HG2	2.18	0.43
3:G:3442:PHE:CG	3:G:3514:LEU:HD22	2.53	0.43
3:G:3556:ASN:HB3	3:G:3559:LEU:HD13	1.99	0.43
3:I:233:ILE:O	3:I:257:ARG:NH1	2.49	0.43
3:I:2801:ASP:HA	3:I:2804:ILE:HG12	2.01	0.43
3:I:4579:PHE:CD1	3:I:4639:MET:HE1	2.54	0.43
2:O:17:LYS:HE3	2:O:17:LYS:HB3	1.84	0.43
3:A:925:SER:O	3:A:928:THR:OG1	2.32	0.43
3:B:2021:CYS:O	3:B:2028:ARG:NH2	2.52	0.43
3:G:451:TYR:CZ	3:G:474:ARG:HD2	2.53	0.43
3:G:1022:VAL:HG22	3:G:1023:PRO:HD2	2.01	0.43
3:G:3230:LEU:H	3:G:3230:LEU:HD23	1.82	0.43
3:G:3269:VAL:HA	3:G:3273:THR:HB	2.01	0.43
3:G:3391:GLU:HG3	3:G:3395:ARG:HE	1.84	0.43
3:G:3621:HIS:ND1	3:G:3623:LEU:HD23	2.33	0.43
3:I:2765:LYS:HZ3	3:I:2857:PRO:HB2	1.84	0.43
1:C:133:ASP:HA	3:B:3460:VAL:HG11	2.01	0.42
3:A:3628:ARG:HG3	3:A:3631:ALA:HB3	2.01	0.42
3:B:2236:LEU:HD13	3:B:2250:MET:HE1	2.01	0.42
3:B:3384:LYS:HD2	3:B:3386:GLU:HB3	2.01	0.42
3:B:3392:LEU:HD13	3:B:3395:ARG:HD2	2.01	0.42
3:B:4818:MET:HA	3:B:4824:ARG:HH11	1.83	0.42
3:G:1168:VAL:HG11	3:G:1176:GLU:HG2	2.00	0.42
3:I:1154:ASP:OD1	3:I:1156:THR:OG1	2.37	0.42
3:I:1948:ASP:OD1	3:I:2126:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:HIS:CD2	2:F:104:LEU:HD11	2.54	0.42
3:A:1716:ILE:O	3:A:1721:GLU:N	2.51	0.42
3:A:2661:TRP:HB3	3:A:2664:PHE:HB2	2.01	0.42
3:B:3230:LEU:H	3:B:3230:LEU:HD23	1.83	0.42
3:B:4910:GLU:O	3:B:4914:VAL:HG13	2.19	0.42
3:G:365:LYS:HE3	3:G:365:LYS:HB3	1.81	0.42
3:G:932:LEU:HD21	3:G:988:LEU:HD11	2.00	0.42
3:G:1422:ASP:OD2	3:G:1568:LYS:NZ	2.37	0.42
3:G:3392:LEU:HD13	3:G:3395:ARG:HD2	2.01	0.42
9:G:5108:L9R:H32A	9:G:5108:L9R:H35A	1.75	0.42
3:I:233:ILE:HD12	3:I:242:ARG:HB3	2.01	0.42
3:I:1716:ILE:O	3:I:1721:GLU:N	2.51	0.42
3:I:1820:ARG:O	3:I:1824:GLN:HG2	2.18	0.42
3:I:3384:LYS:HD2	3:I:3386:GLU:HB3	2.01	0.42
3:I:3556:ASN:HB3	3:I:3559:LEU:HD13	1.99	0.42
3:A:169:LEU:HD22	3:A:202:MET:HG3	2.00	0.42
3:A:1753:LYS:HB3	3:A:1758:ARG:HA	2.01	0.42
3:A:2108:GLU:O	3:A:3694:LYS:NZ	2.51	0.42
3:A:2801:ASP:HA	3:A:2804:ILE:HG12	2.01	0.42
3:A:3414:ARG:HH21	3:A:3472:ALA:H	1.67	0.42
3:B:233:ILE:HD12	3:B:242:ARG:HB3	2.01	0.42
3:B:892:THR:HB	3:B:962:SER:H	1.84	0.42
3:G:719:LEU:HD11	2:H:7:ILE:HA	2.01	0.42
3:G:4152:GLU:OE1	3:G:4194:TYR:OH	2.28	0.42
3:I:2764:GLU:HG3	3:I:2857:PRO:HB3	2.01	0.42
2:H:25:HIS:CD2	2:H:104:LEU:HD11	2.54	0.42
1:K:30:LYS:HE3	1:K:30:LYS:HB3	1.94	0.42
1:E:1:ALA:HB3	3:G:3861:GLU:HG2	2.01	0.42
1:E:26:THR:HB	1:E:62:THR:HB	2.02	0.42
3:A:1690:ASP:OD2	3:A:1693:GLN:NE2	2.52	0.42
3:B:1000:ARG:HB3	3:B:1005:TRP:HB2	2.01	0.42
3:G:2661:TRP:HB3	3:G:2664:PHE:HB2	2.01	0.42
3:G:2751:LEU:HD23	3:G:2751:LEU:H	1.84	0.42
3:I:3123:LYS:HG3	3:I:3125:VAL:H	1.83	0.42
1:C:66:PRO:HG3	3:B:2186:MET:HB3	2.02	0.42
1:C:120:GLU:HA	1:C:123:GLU:HG3	2.02	0.42
3:A:2514:ASN:OD1	3:A:2514:ASN:N	2.53	0.42
3:A:4910:GLU:O	3:A:4914:VAL:HG13	2.19	0.42
3:B:938:HIS:HB3	3:B:1054:GLU:HB3	2.01	0.42
3:B:1947:CYS:SG	3:B:2127:GLN:NE2	2.92	0.42
3:B:2888:ARG:O	3:B:2892:GLN:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3003:LEU:HB2	3:B:3004:PRO:HD3	2.02	0.42
3:G:1154:ASP:OD1	3:G:1156:THR:OG1	2.37	0.42
3:G:2716:ASP:OD1	3:G:2716:ASP:N	2.53	0.42
3:G:2764:GLU:HG3	3:G:2857:PRO:HB3	2.01	0.42
3:I:788:LYS:HE3	3:I:788:LYS:HB2	1.84	0.42
3:I:3414:ARG:HH21	3:I:3472:ALA:H	1.67	0.42
1:D:111:ASN:O	3:I:1996:ARG:NH2	2.40	0.42
3:A:3235:SER:OG	3:A:3237:GLU:OE1	2.37	0.42
3:A:3269:VAL:HA	3:A:3273:THR:HB	2.01	0.42
3:B:1753:LYS:HB3	3:B:1758:ARG:HA	2.01	0.42
3:B:2751:LEU:HD23	3:B:2751:LEU:H	1.84	0.42
3:B:3284:TRP:HB3	3:B:3305:THR:HG21	2.02	0.42
3:G:169:LEU:HD22	3:G:202:MET:HG3	2.00	0.42
3:G:707:VAL:HG23	3:G:782:SER:HB3	2.02	0.42
3:G:1820:ARG:O	3:G:1824:GLN:HG2	2.18	0.42
3:G:2021:CYS:O	3:G:2028:ARG:NH2	2.52	0.42
3:G:3235:SER:OG	3:G:3237:GLU:OE1	2.37	0.42
3:G:3414:ARG:HH21	3:G:3472:ALA:H	1.67	0.42
3:I:2236:LEU:HD13	3:I:2250:MET:HE1	2.01	0.42
3:A:2677:LYS:HE2	3:A:2677:LYS:HB3	1.81	0.42
3:G:1000:ARG:HB3	3:G:1005:TRP:HB2	2.01	0.42
3:G:1206:GLN:HA	3:G:1227:ALA:O	2.18	0.42
3:G:1690:ASP:OD2	3:G:1693:GLN:NE2	2.52	0.42
3:G:1716:ILE:O	3:G:1721:GLU:N	2.51	0.42
3:I:1099:GLU:OE2	3:I:1125:ASN:ND2	2.50	0.42
3:I:2661:TRP:HB3	3:I:2664:PHE:HB2	2.02	0.42
3:I:3003:LEU:HB2	3:I:3004:PRO:HD3	2.02	0.42
3:I:4910:GLU:O	3:I:4914:VAL:HG13	2.19	0.42
3:I:4967:TYR:OH	3:I:5033:GLU:OE2	2.29	0.42
1:C:26:THR:HB	1:C:62:THR:HB	2.02	0.42
3:A:892:THR:HB	3:A:962:SER:H	1.84	0.42
3:A:2021:CYS:O	3:A:2028:ARG:NH2	2.52	0.42
3:A:3284:TRP:HB3	3:A:3305:THR:HG21	2.02	0.42
3:A:3384:LYS:HD2	3:A:3386:GLU:HB3	2.01	0.42
3:B:232:THR:HG21	3:B:252:VAL:HG21	2.01	0.42
3:B:863:LEU:HD11	3:B:930:LYS:NZ	2.35	0.42
3:B:901:LYS:HG3	3:B:903:LEU:HG	2.02	0.42
3:G:233:ILE:HD12	3:G:242:ARG:HB3	2.01	0.42
3:G:901:LYS:HD2	3:G:901:LYS:HA	1.84	0.42
3:G:1753:LYS:HB3	3:G:1758:ARG:HA	2.01	0.42
3:G:2236:LEU:HD13	3:G:2250:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3628:ARG:HG3	3:G:3631:ALA:HB3	2.01	0.42
3:G:3944:GLU:OE1	3:G:3946:GLN:N	2.47	0.42
3:G:4091:LYS:HE2	3:G:4091:LYS:HB2	1.89	0.42
3:I:707:VAL:HG23	3:I:782:SER:HB3	2.02	0.42
3:I:2021:CYS:O	3:I:2028:ARG:NH2	2.52	0.42
1:K:120:GLU:HA	1:K:123:GLU:HG3	2.02	0.42
3:A:863:LEU:HD11	3:A:930:LYS:NZ	2.35	0.42
3:B:1948:ASP:OD1	3:B:2126:ARG:NH2	2.48	0.42
3:B:3235:SER:OG	3:B:3237:GLU:OE1	2.37	0.42
3:B:3269:VAL:HA	3:B:3273:THR:HB	2.01	0.42
3:B:3628:ARG:HG3	3:B:3631:ALA:HB3	2.01	0.42
3:B:3946:GLN:OE1	3:B:3949:ARG:NH2	2.39	0.42
3:B:4888:TYR:HE1	3:I:4917:ASP:HB2	1.84	0.42
9:B:5308:L9R:H23	9:B:5308:L9R:H20	1.32	0.42
3:G:4910:GLU:O	3:G:4914:VAL:HG13	2.19	0.42
3:I:892:THR:HB	3:I:962:SER:H	1.84	0.42
3:I:1947:CYS:SG	3:I:2127:GLN:NE2	2.92	0.42
3:I:2514:ASN:OD1	3:I:2514:ASN:N	2.53	0.42
3:I:3390:GLY:HA2	3:I:3393:LEU:HD23	2.02	0.42
3:I:4712:PRO:O	3:I:4718:LYS:NZ	2.40	0.42
1:D:26:THR:HB	1:D:62:THR:HB	2.02	0.42
3:A:2212:VAL:HG11	3:A:2256:TYR:CE2	2.55	0.42
3:A:2263:ILE:HD12	3:A:2263:ILE:HA	1.95	0.42
3:A:2751:LEU:H	3:A:2751:LEU:HD23	1.84	0.42
3:B:1206:GLN:HA	3:B:1227:ALA:O	2.18	0.42
3:B:3390:GLY:HA2	3:B:3393:LEU:HD23	2.02	0.42
3:B:3535:LEU:O	3:B:3538:THR:OG1	2.31	0.42
3:G:870:ILE:HD12	3:G:870:ILE:HA	1.96	0.42
3:G:2907:PRO:O	3:G:2910:THR:OG1	2.35	0.42
3:I:2858:GLN:HB2	3:I:2859:PRO:HD3	2.02	0.42
3:I:3392:LEU:HD13	3:I:3395:ARG:HD2	2.01	0.42
1:D:120:GLU:HA	1:D:123:GLU:HG3	2.02	0.41
1:E:120:GLU:HA	1:E:123:GLU:HG3	2.02	0.41
3:A:1983:ALA:O	3:A:1987:SER:OG	2.30	0.41
3:B:336:PRO:HA	3:B:337:PRO:HD3	1.88	0.41
3:B:707:VAL:HG23	3:B:782:SER:HB3	2.02	0.41
3:B:872:GLU:HG2	3:B:922:LEU:HD21	2.02	0.41
3:B:1057:ASP:OD1	3:B:1057:ASP:N	2.31	0.41
3:B:2661:TRP:HB3	3:B:2664:PHE:HB2	2.01	0.41
3:G:232:THR:HG21	3:G:252:VAL:HG21	2.01	0.41
3:G:345:LEU:HB3	3:G:387:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:938:HIS:HB3	3:G:1054:GLU:HB3	2.01	0.41
3:G:1694:LEU:HB3	3:G:1715:LEU:HD12	2.00	0.41
3:G:2212:VAL:HG11	3:G:2256:TYR:CE2	2.55	0.41
3:G:4093:PHE:O	3:G:4097:MET:HG2	2.20	0.41
3:I:979:PRO:O	3:I:982:THR:OG1	2.33	0.41
3:I:1690:ASP:OD2	3:I:1693:GLN:NE2	2.52	0.41
3:I:3269:VAL:HA	3:I:3273:THR:HB	2.01	0.41
3:A:901:LYS:HG3	3:A:903:LEU:HG	2.02	0.41
3:B:881:LEU:HD13	3:B:881:LEU:HA	1.92	0.41
3:G:892:THR:HB	3:G:962:SER:H	1.84	0.41
3:I:3235:SER:OG	3:I:3237:GLU:OE1	2.37	0.41
3:I:4046:ASP:OD1	3:I:4159:ARG:NH2	2.48	0.41
1:K:66:PRO:HG3	3:A:2192:TYR:OH	2.21	0.41
3:A:232:THR:HG21	3:A:252:VAL:HG21	2.01	0.41
3:A:233:ILE:HD12	3:A:242:ARG:HB3	2.01	0.41
3:A:4861:LYS:H	3:A:4861:LYS:HG3	1.53	0.41
3:B:2514:ASN:OD1	3:B:2514:ASN:N	2.53	0.41
3:G:954:LYS:HB3	3:G:966:LYS:HE3	2.03	0.41
3:G:4238:CYS:HA	3:G:4989:MET:HE1	2.02	0.41
3:I:2751:LEU:H	3:I:2751:LEU:HD23	1.84	0.41
3:A:707:VAL:HG23	3:A:782:SER:HB3	2.02	0.41
3:A:1823:GLY:O	3:A:1825:HIS:ND1	2.52	0.41
3:G:233:ILE:O	3:G:257:ARG:NH1	2.49	0.41
3:G:3384:LYS:HD2	3:G:3386:GLU:HB3	2.01	0.41
3:G:3852:LYS:HE3	3:G:3852:LYS:HB3	1.89	0.41
3:I:901:LYS:HG3	3:I:903:LEU:HG	2.02	0.41
3:I:3107:VAL:HG21	3:I:3171:SER:HB2	2.03	0.41
3:I:3391:GLU:HG3	3:I:3395:ARG:HE	1.84	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.91	0.41
3:A:797:HIS:CG	3:A:821:LEU:HD23	2.56	0.41
3:A:901:LYS:HD2	3:A:901:LYS:HA	1.84	0.41
3:A:938:HIS:HB3	3:A:1054:GLU:HB3	2.01	0.41
3:A:2716:ASP:OD1	3:A:2716:ASP:N	2.53	0.41
3:A:3147:ILE:HG23	3:A:3152:PHE:HB2	2.02	0.41
3:A:4825:THR:O	3:A:4828:SER:OG	2.32	0.41
3:A:4917:ASP:HB2	3:G:4888:TYR:HE1	1.84	0.41
3:B:2749:GLU:HG3	3:B:2752:ASP:HB2	2.03	0.41
3:B:3391:GLU:HG3	3:B:3395:ARG:HE	1.84	0.41
3:B:4093:PHE:O	3:B:4097:MET:HG2	2.20	0.41
3:G:462:GLU:HG3	3:G:3710:LEU:HD13	2.02	0.41
3:G:2514:ASN:OD1	3:G:2514:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4060:LYS:HD2	3:G:4060:LYS:HA	1.91	0.41
3:I:938:HIS:HB3	3:I:1054:GLU:HB3	2.02	0.41
3:I:954:LYS:HB3	3:I:966:LYS:HE3	2.03	0.41
3:I:2775:TRP:CD2	3:I:2786:LYS:HE3	2.56	0.41
3:I:3628:ARG:HG3	3:I:3631:ALA:HB3	2.01	0.41
3:A:1154:ASP:OD1	3:A:1156:THR:OG1	2.37	0.41
3:A:2749:GLU:HG3	3:A:2752:ASP:HB2	2.03	0.41
3:A:2858:GLN:HB2	3:A:2859:PRO:HD3	2.02	0.41
3:A:3003:LEU:HB2	3:A:3004:PRO:HD3	2.02	0.41
3:B:330:ASP:OD1	3:B:330:ASP:N	2.53	0.41
3:B:2858:GLN:HB2	3:B:2859:PRO:HD3	2.02	0.41
3:B:4063:ASP:OD1	3:B:4064:MET:N	2.54	0.41
9:B:5308:L9R:H44	9:B:5308:L9R:H47A	1.52	0.41
3:G:144:GLU:OE1	3:I:2452:ARG:NH1	2.53	0.41
3:G:308:HIS:CE1	3:G:310:LYS:HB3	2.56	0.41
3:G:881:LEU:HD13	3:G:881:LEU:HA	1.92	0.41
3:G:2178:MET:HE3	3:G:2182:ILE:HD11	2.03	0.41
3:G:2801:ASP:HA	3:G:2804:ILE:HG12	2.01	0.41
3:G:2858:GLN:HB2	3:G:2859:PRO:HD3	2.02	0.41
3:G:3390:GLY:HA2	3:G:3393:LEU:HD23	2.02	0.41
3:G:5012:LYS:NZ	3:G:5016:GLU:OE2	2.41	0.41
3:I:4063:ASP:OD1	3:I:4064:MET:N	2.54	0.41
2:F:27:THR:HG23	2:F:38:SER:HB2	2.03	0.41
3:A:872:GLU:HG2	3:A:922:LEU:HD21	2.03	0.41
3:A:1000:ARG:HB3	3:A:1005:TRP:HB2	2.01	0.41
3:A:2495:VAL:HG22	3:A:2498:HIS:CE1	2.56	0.41
3:A:3249:LEU:HD23	3:A:3277:LEU:HD21	2.03	0.41
9:A:5308:L9R:H39	9:A:5308:L9R:H42A	1.76	0.41
3:B:2747:ILE:HD13	3:B:2814:LYS:HG2	2.02	0.41
3:B:3107:VAL:HG21	3:B:3171:SER:HB2	2.03	0.41
3:G:797:HIS:CG	3:G:821:LEU:HD23	2.56	0.41
3:G:1078:GLU:OE2	3:G:1654:SER:OG	2.26	0.41
3:G:3159:ASP:OD1	3:G:3159:ASP:N	2.52	0.41
3:G:3501:ASP:OD1	3:G:3501:ASP:N	2.54	0.41
3:I:1000:ARG:HB3	3:I:1005:TRP:HB2	2.01	0.41
3:I:2886:TRP:HA	3:I:2889:LYS:NZ	2.36	0.41
3:I:3284:TRP:HB3	3:I:3305:THR:HG21	2.02	0.41
3:A:2782:ASP:OD1	3:A:2782:ASP:N	2.54	0.41
3:A:3390:GLY:HA2	3:A:3393:LEU:HD23	2.02	0.41
3:A:3680:ALA:HB1	3:A:3683:GLN:NE2	2.36	0.41
3:B:462:GLU:HG3	3:B:3710:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2886:TRP:HA	3:B:2889:LYS:NZ	2.36	0.41
3:G:3147:ILE:HG23	3:G:3152:PHE:HB2	2.02	0.41
3:G:3680:ALA:HB1	3:G:3683:GLN:NE2	2.36	0.41
3:I:330:ASP:OD1	3:I:330:ASP:N	2.53	0.41
3:I:653:ALA:HB3	3:I:656:SER:HB2	2.03	0.41
3:I:863:LEU:HD11	3:I:930:LYS:NZ	2.35	0.41
3:I:872:GLU:HG2	3:I:922:LEU:HD21	2.03	0.41
3:I:1804:LEU:HD13	3:I:1853:ILE:HD12	2.03	0.41
3:I:2747:ILE:HD13	3:I:2814:LYS:HG2	2.02	0.41
3:I:4091:LYS:HB2	3:I:4091:LYS:HE2	1.89	0.41
3:A:1575:LEU:HD23	3:A:1575:LEU:HA	1.90	0.41
3:B:275:ARG:HH21	3:B:328:LYS:HG3	1.86	0.41
3:B:954:LYS:HB3	3:B:966:LYS:HE3	2.03	0.41
3:B:2212:VAL:HG11	3:B:2256:TYR:CE2	2.55	0.41
3:B:2495:VAL:HG22	3:B:2498:HIS:CE1	2.56	0.41
3:B:2801:ASP:HA	3:B:2804:ILE:HG12	2.01	0.41
3:B:3501:ASP:OD1	3:B:3501:ASP:N	2.54	0.41
3:B:4060:LYS:HD2	3:B:4060:LYS:HA	1.91	0.41
3:B:4687:TYR:OH	3:B:4699:GLY:O	2.26	0.41
3:G:901:LYS:HG3	3:G:903:LEU:HG	2.02	0.41
3:G:2749:GLU:HG3	3:G:2752:ASP:HB2	2.03	0.41
3:G:3107:VAL:HG21	3:G:3171:SER:HB2	2.03	0.41
3:G:3734:HIS:CG	3:G:3735:LEU:N	2.89	0.41
3:G:4661:TYR:OH	3:G:4786:ASP:OD2	2.33	0.41
3:G:4805:ASN:HD22	9:G:5101:L9R:C31	2.34	0.41
3:I:275:ARG:HH21	3:I:328:LYS:HG3	1.86	0.41
3:I:308:HIS:CE1	3:I:310:LYS:HB3	2.56	0.41
3:I:797:HIS:CG	3:I:821:LEU:HD23	2.56	0.41
3:I:870:ILE:HG12	3:I:1051:TYR:HE2	1.86	0.41
3:I:1997:GLU:O	3:I:2000:SER:OG	2.37	0.41
3:I:2212:VAL:HG11	3:I:2256:TYR:CE2	2.55	0.41
3:I:2587:TYR:O	3:I:2590:SER:OG	2.31	0.41
3:I:4093:PHE:O	3:I:4097:MET:HG2	2.20	0.41
9:I:5101:L9R:H23	9:I:5101:L9R:H20	1.32	0.41
1:K:26:THR:HB	1:K:62:THR:HB	2.02	0.41
3:A:345:LEU:HB3	3:A:387:ALA:HB1	2.02	0.41
3:A:2751:LEU:O	3:A:2755:ILE:HG12	2.21	0.41
3:A:3157:ILE:HG23	3:A:3161:VAL:HG12	2.03	0.41
3:A:4063:ASP:OD1	3:A:4064:MET:N	2.54	0.41
9:A:5308:L9R:H23	9:A:5308:L9R:H20	1.32	0.41
3:B:653:ALA:HB3	3:B:656:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:871:ARG:CZ	3:B:922:LEU:HD12	2.51	0.41
3:B:3147:ILE:HG23	3:B:3152:PHE:HB2	2.02	0.41
3:B:3414:ARG:HH21	3:B:3472:ALA:H	1.67	0.41
3:B:4152:GLU:OE1	3:B:4194:TYR:OH	2.28	0.41
3:G:2495:VAL:HG22	3:G:2498:HIS:CE1	2.56	0.41
3:G:3003:LEU:HB2	3:G:3004:PRO:HD3	2.02	0.41
3:G:3284:TRP:HB3	3:G:3305:THR:HG21	2.02	0.41
3:I:462:GLU:HG3	3:I:3710:LEU:HD13	2.02	0.41
3:I:3501:ASP:N	3:I:3501:ASP:OD1	2.54	0.41
2:H:27:THR:HG23	2:H:38:SER:HB2	2.03	0.41
1:D:85:ILE:H	1:D:85:ILE:HG13	1.57	0.40
3:A:308:HIS:CE1	3:A:310:LYS:HB3	2.56	0.40
3:A:2282:ASP:HA	3:A:2341:VAL:HG13	2.03	0.40
3:A:2413:GLU:OE2	3:A:2414:ASN:ND2	2.54	0.40
3:A:3501:ASP:OD1	3:A:3501:ASP:N	2.54	0.40
3:B:3734:HIS:CG	3:B:3735:LEU:N	2.89	0.40
3:G:871:ARG:CZ	3:G:922:LEU:HD12	2.51	0.40
3:G:2782:ASP:N	3:G:2782:ASP:OD1	2.54	0.40
3:G:4063:ASP:OD1	3:G:4064:MET:N	2.54	0.40
3:G:4754:ASN:OD1	3:G:4755:GLU:N	2.47	0.40
3:I:336:PRO:HA	3:I:337:PRO:HD3	1.88	0.40
3:I:2495:VAL:HG22	3:I:2498:HIS:CE1	2.56	0.40
3:I:2749:GLU:HG3	3:I:2752:ASP:HB2	2.03	0.40
3:I:2782:ASP:N	3:I:2782:ASP:OD1	2.54	0.40
3:I:3823:LYS:HA	3:I:3823:LYS:HD3	1.87	0.40
1:K:69:LEU:HD23	1:K:69:LEU:HA	1.91	0.40
3:A:462:GLU:HG3	3:A:3710:LEU:HD13	2.02	0.40
3:A:871:ARG:CZ	3:A:922:LEU:HD12	2.51	0.40
3:A:954:LYS:HB3	3:A:966:LYS:HE3	2.03	0.40
3:A:2886:TRP:HA	3:A:2889:LYS:NZ	2.36	0.40
3:A:3341:PHE:O	3:A:3344:PRO:HD2	2.21	0.40
3:A:3535:LEU:O	3:A:3538:THR:OG1	2.31	0.40
3:A:4093:PHE:O	3:A:4097:MET:HG2	2.20	0.40
3:A:4154:VAL:HG12	3:A:4157:ASP:HB2	2.03	0.40
3:B:1634:LEU:HD23	3:B:1634:LEU:HA	1.92	0.40
3:B:1690:ASP:OD2	3:B:1693:GLN:NE2	2.52	0.40
3:B:2751:LEU:O	3:B:2755:ILE:HG12	2.21	0.40
3:B:4940:PHE:HZ	3:I:4931:ILE:HG23	1.87	0.40
3:G:863:LEU:HD11	3:G:930:LYS:NZ	2.35	0.40
3:G:2775:TRP:CD2	3:G:2786:LYS:HE3	2.56	0.40
3:G:2881:ASN:HA	3:G:2884:ASN:HD21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3249:LEU:HD23	3:G:3277:LEU:HD21	2.03	0.40
3:G:3341:PHE:O	3:G:3344:PRO:HD2	2.21	0.40
3:I:871:ARG:HB2	3:I:929:LEU:HD12	2.04	0.40
3:I:2758:PHE:HA	3:I:2761:TYR:HB2	2.04	0.40
3:I:3341:PHE:O	3:I:3344:PRO:HD2	2.21	0.40
3:I:3562:LYS:HE2	3:I:3562:LYS:HB2	1.91	0.40
3:I:4651:THR:HG23	3:I:4796:MET:HE1	2.03	0.40
2:O:27:THR:HG23	2:O:38:SER:HB2	2.03	0.40
3:A:870:ILE:HG12	3:A:1051:TYR:HE2	1.86	0.40
3:A:1079:LYS:HA	3:A:1189:LEU:HD11	2.04	0.40
3:A:2740:VAL:HG21	3:A:2819:TRP:HE1	1.87	0.40
3:A:2747:ILE:HD13	3:A:2814:LYS:HG2	2.02	0.40
3:A:3971:GLY:N	3:A:3972:PRO:HA	2.37	0.40
3:B:308:HIS:CE1	3:B:310:LYS:HB3	2.56	0.40
3:B:797:HIS:CG	3:B:821:LEU:HD23	2.56	0.40
3:B:961:MET:HE2	3:B:961:MET:HB2	1.93	0.40
3:B:2413:GLU:OE2	3:B:2414:ASN:ND2	2.54	0.40
3:B:4825:THR:O	3:B:4828:SER:OG	2.32	0.40
3:B:4967:TYR:OH	3:B:5033:GLU:OE2	2.29	0.40
3:G:2001:PRO:O	3:G:2005:GLN:HG3	2.21	0.40
3:G:2282:ASP:HA	3:G:2341:VAL:HG13	2.03	0.40
3:G:2413:GLU:OE2	3:G:2414:ASN:ND2	2.54	0.40
3:G:2759:ALA:HB1	3:G:2806:ARG:HB2	2.04	0.40
9:G:5101:L9R:H42A	9:G:5101:L9R:H39	1.76	0.40
3:I:345:LEU:HB3	3:I:387:ALA:HB1	2.02	0.40
3:I:871:ARG:CZ	3:I:922:LEU:HD12	2.51	0.40
3:I:2001:PRO:O	3:I:2005:GLN:HG3	2.21	0.40
3:I:2527:LEU:HD12	3:I:2527:LEU:HA	1.92	0.40
3:I:2759:ALA:HB1	3:I:2806:ARG:HB2	2.04	0.40
3:I:3734:HIS:CG	3:I:3735:LEU:N	2.89	0.40
3:A:275:ARG:HE	3:A:328:LYS:HE2	1.87	0.40
3:A:3107:VAL:HG21	3:A:3171:SER:HB2	2.03	0.40
3:B:683:ARG:HG2	3:B:717:ASP:HB3	2.04	0.40
3:B:1488:LYS:HE3	3:B:1488:LYS:HB2	1.86	0.40
3:B:2001:PRO:O	3:B:2005:GLN:HG3	2.22	0.40
3:B:2740:VAL:HG21	3:B:2819:TRP:HE1	1.86	0.40
3:B:2758:PHE:HA	3:B:2761:TYR:HB2	2.04	0.40
3:B:2775:TRP:CD2	3:B:2786:LYS:HE3	2.56	0.40
3:B:3157:ILE:HG23	3:B:3161:VAL:HG12	2.03	0.40
3:G:653:ALA:HB3	3:G:656:SER:HB2	2.03	0.40
3:G:1948:ASP:OD1	3:G:2126:ARG:NH2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4090:LYS:HG2	3:G:4123:ILE:HD11	2.03	0.40
3:G:4967:TYR:OH	3:G:5033:GLU:OE2	2.29	0.40
3:I:1079:LYS:HA	3:I:1189:LEU:HD11	2.04	0.40
3:I:4090:LYS:HG2	3:I:4123:ILE:HD11	2.04	0.40
3:I:4813:LEU:HD23	3:I:4813:LEU:HA	1.87	0.40
2:J:17:LYS:HE3	2:J:17:LYS:HB3	1.84	0.40
1:E:130:ILE:H	1:E:130:ILE:HG13	1.72	0.40
3:A:1947:CYS:SG	3:A:2127:GLN:NE2	2.92	0.40
3:A:3717:ASP:OD1	3:A:3717:ASP:N	2.55	0.40
3:A:4090:LYS:HG2	3:A:4123:ILE:HD11	2.03	0.40
3:B:979:PRO:O	3:B:982:THR:OG1	2.33	0.40
3:B:1451:GLY:HA3	3:B:1494:MET:HA	2.04	0.40
3:B:3159:ASP:OD1	3:B:3159:ASP:N	2.52	0.40
3:G:1079:LYS:HA	3:G:1189:LEU:HD11	2.04	0.40
3:G:3226:GLU:C	3:G:3228:ALA:H	2.25	0.40
3:G:4900:GLU:H	3:G:4900:GLU:HG2	1.70	0.40
3:G:4917:ASP:HB2	3:I:4888:TYR:HE1	1.87	0.40
3:I:1488:LYS:HB2	3:I:1488:LYS:HE3	1.86	0.40
3:I:1823:GLY:O	3:I:1825:HIS:ND1	2.52	0.40
3:I:3147:ILE:HG23	3:I:3152:PHE:HB2	2.02	0.40
3:I:3226:GLU:C	3:I:3228:ALA:H	2.25	0.40
3:I:3249:LEU:HD23	3:I:3277:LEU:HD21	2.03	0.40
3:I:3717:ASP:N	3:I:3717:ASP:OD1	2.55	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	C	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	D	147/150 (98%)	146 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	K	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
2	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	H	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	J	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	O	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
3	A	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	B	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	G	4385/5037 (87%)	4274 (98%)	111 (2%)	0	100	100
3	I	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
All	All	18548/21176 (88%)	18089 (98%)	459 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	127/128 (99%)	122 (96%)	5 (4%)	32	42
1	D	127/128 (99%)	122 (96%)	5 (4%)	32	42
1	E	127/128 (99%)	122 (96%)	5 (4%)	32	42
1	K	127/128 (99%)	122 (96%)	5 (4%)	32	42
2	F	89/89 (100%)	86 (97%)	3 (3%)	37	48
2	H	89/89 (100%)	86 (97%)	3 (3%)	37	48
2	J	89/89 (100%)	86 (97%)	3 (3%)	37	48
2	O	89/89 (100%)	86 (97%)	3 (3%)	37	48
3	A	3836/4276 (90%)	3760 (98%)	76 (2%)	55	67
3	B	3836/4276 (90%)	3760 (98%)	76 (2%)	55	67
3	G	3836/4276 (90%)	3760 (98%)	76 (2%)	55	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	3836/4276 (90%)	3760 (98%)	76 (2%)	55 67
All	All	16208/17972 (90%)	15872 (98%)	336 (2%)	56 66

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	21	LYS
1	K	30	LYS
1	K	105	LEU
1	K	124	MET
1	K	145	MET
2	F	17	LYS
2	F	29	MET
2	F	79	ASP
1	D	21	LYS
1	D	30	LYS
1	D	105	LEU
1	D	124	MET
1	D	145	MET
1	E	21	LYS
1	E	30	LYS
1	E	105	LEU
1	E	124	MET
1	E	145	MET
1	C	21	LYS
1	C	30	LYS
1	C	105	LEU
1	C	124	MET
1	C	145	MET
3	A	81	MET
3	A	125	ARG
3	A	155	LYS
3	A	860	GLN
3	A	862	VAL
3	A	869	ARG
3	A	873	LYS
3	A	882	TRP
3	A	887	ILE
3	A	897	ARG
3	A	898	ASP
3	A	907	LEU
3	A	908	VAL

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Mol	Chain	Res	Type
3	A	911	HIS
3	A	922	LEU
3	A	945	LYS
3	A	957	LYS
3	A	958	THR
3	A	959	TYR
3	A	961	MET
3	A	962	SER
3	A	963	ASN
3	A	972	LEU
3	A	984	LEU
3	A	998	ARG
3	A	999	ASP
3	A	1021	LEU
3	A	1022	VAL
3	A	1044	ARG
3	A	1057	ASP
3	A	1143	TRP
3	A	1186	ASP
3	A	1506	GLN
3	A	1511	HIS
3	A	1752	ARG
3	A	1758	ARG
3	A	1872	THR
3	A	1923	GLU
3	A	1990	GLU
3	A	2037	ASP
3	A	2100[A]	HIS
3	A	2100[B]	HIS
3	A	2221	LYS
3	A	2224	ARG
3	A	2336	ARG
3	A	2482	ASP
3	A	2738	ARG
3	A	2761	TYR
3	A	2786	LYS
3	A	2797	PHE
3	A	2806	ARG
3	A	2827	ARG
3	A	2862	LEU
3	A	2876	GLU
3	A	2914	LYS

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Mol	Chain	Res	Type
3	A	2932	MET
3	A	3053	ARG
3	A	3296	LEU
3	A	3382	GLU
3	A	3451	PHE
3	A	3614	LYS
3	A	3619	VAL
3	A	3622	LYS
3	A	3639	THR
3	A	3752	SER
3	A	3756	LYS
3	A	3899	PHE
3	A	3933	PHE
3	A	4580	TYR
3	A	4662	ASN
3	A	4796	MET
3	A	4821	LYS
3	A	4861	LYS
3	A	4871	GLU
3	A	4903	ASP
3	A	4911	LEU
3	B	81	MET
3	B	125	ARG
3	B	155	LYS
3	B	860	GLN
3	B	862	VAL
3	B	869	ARG
3	B	873	LYS
3	B	882	TRP
3	B	887	ILE
3	B	897	ARG
3	B	898	ASP
3	B	907	LEU
3	B	908	VAL
3	B	911	HIS
3	B	922	LEU
3	B	945	LYS
3	B	957	LYS
3	B	958	THR
3	B	959	TYR
3	B	961	MET
3	B	962	SER

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Mol	Chain	Res	Type
3	B	963	ASN
3	B	972	LEU
3	B	984	LEU
3	B	998	ARG
3	B	999	ASP
3	B	1021	LEU
3	B	1022	VAL
3	B	1044	ARG
3	B	1057	ASP
3	B	1143	TRP
3	B	1186	ASP
3	B	1506	GLN
3	B	1511	HIS
3	B	1752	ARG
3	B	1758	ARG
3	B	1872	THR
3	B	1923	GLU
3	B	1990	GLU
3	B	2037	ASP
3	B	2100[A]	HIS
3	B	2100[B]	HIS
3	B	2221	LYS
3	B	2224	ARG
3	B	2336	ARG
3	B	2482	ASP
3	B	2738	ARG
3	B	2761	TYR
3	B	2786	LYS
3	B	2797	PHE
3	B	2806	ARG
3	B	2827	ARG
3	B	2862	LEU
3	B	2876	GLU
3	B	2914	LYS
3	B	2932	MET
3	B	3053	ARG
3	B	3296	LEU
3	B	3382	GLU
3	B	3451	PHE
3	B	3614	LYS
3	B	3619	VAL
3	B	3622	LYS

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Mol	Chain	Res	Type
3	B	3639	THR
3	B	3752	SER
3	B	3756	LYS
3	B	3899	PHE
3	B	3933	PHE
3	B	4580	TYR
3	B	4662	ASN
3	B	4796	MET
3	B	4821	LYS
3	B	4861	LYS
3	B	4871	GLU
3	B	4903	ASP
3	B	4911	LEU
3	G	81	MET
3	G	125	ARG
3	G	155	LYS
3	G	860	GLN
3	G	862	VAL
3	G	869	ARG
3	G	873	LYS
3	G	882	TRP
3	G	887	ILE
3	G	897	ARG
3	G	898	ASP
3	G	907	LEU
3	G	908	VAL
3	G	911	HIS
3	G	922	LEU
3	G	945	LYS
3	G	957	LYS
3	G	958	THR
3	G	959	TYR
3	G	961	MET
3	G	962	SER
3	G	963	ASN
3	G	972	LEU
3	G	984	LEU
3	G	998	ARG
3	G	999	ASP
3	G	1021	LEU
3	G	1022	VAL
3	G	1044	ARG

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Mol	Chain	Res	Type
3	G	1057	ASP
3	G	1143	TRP
3	G	1186	ASP
3	G	1506	GLN
3	G	1511	HIS
3	G	1752	ARG
3	G	1758	ARG
3	G	1872	THR
3	G	1923	GLU
3	G	1990	GLU
3	G	2037	ASP
3	G	2100[A]	HIS
3	G	2100[B]	HIS
3	G	2221	LYS
3	G	2224	ARG
3	G	2336	ARG
3	G	2482	ASP
3	G	2738	ARG
3	G	2761	TYR
3	G	2786	LYS
3	G	2797	PHE
3	G	2806	ARG
3	G	2827	ARG
3	G	2862	LEU
3	G	2876	GLU
3	G	2914	LYS
3	G	2932	MET
3	G	3053	ARG
3	G	3296	LEU
3	G	3382	GLU
3	G	3451	PHE
3	G	3614	LYS
3	G	3619	VAL
3	G	3622	LYS
3	G	3639	THR
3	G	3752	SER
3	G	3756	LYS
3	G	3899	PHE
3	G	3933	PHE
3	G	4580	TYR
3	G	4662	ASN
3	G	4796	MET

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Mol	Chain	Res	Type
3	G	4821	LYS
3	G	4861	LYS
3	G	4871	GLU
3	G	4903	ASP
3	G	4911	LEU
3	I	81	MET
3	I	125	ARG
3	I	155	LYS
3	I	860	GLN
3	I	862	VAL
3	I	869	ARG
3	I	873	LYS
3	I	882	TRP
3	I	887	ILE
3	I	897	ARG
3	I	898	ASP
3	I	907	LEU
3	I	908	VAL
3	I	911	HIS
3	I	922	LEU
3	I	945	LYS
3	I	957	LYS
3	I	958	THR
3	I	959	TYR
3	I	961	MET
3	I	962	SER
3	I	963	ASN
3	I	972	LEU
3	I	984	LEU
3	I	998	ARG
3	I	999	ASP
3	I	1021	LEU
3	I	1022	VAL
3	I	1044	ARG
3	I	1057	ASP
3	I	1143	TRP
3	I	1186	ASP
3	I	1506	GLN
3	I	1511	HIS
3	I	1752	ARG
3	I	1758	ARG
3	I	1872	THR

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Mol	Chain	Res	Type
3	I	1923	GLU
3	I	1990	GLU
3	I	2037	ASP
3	I	2100[A]	HIS
3	I	2100[B]	HIS
3	I	2221	LYS
3	I	2224	ARG
3	I	2336	ARG
3	I	2482	ASP
3	I	2738	ARG
3	I	2761	TYR
3	I	2786	LYS
3	I	2797	PHE
3	I	2806	ARG
3	I	2827	ARG
3	I	2862	LEU
3	I	2876	GLU
3	I	2914	LYS
3	I	2932	MET
3	I	3053	ARG
3	I	3296	LEU
3	I	3382	GLU
3	I	3451	PHE
3	I	3614	LYS
3	I	3619	VAL
3	I	3622	LYS
3	I	3639	THR
3	I	3752	SER
3	I	3756	LYS
3	I	3899	PHE
3	I	3933	PHE
3	I	4580	TYR
3	I	4662	ASN
3	I	4796	MET
3	I	4821	LYS
3	I	4861	LYS
3	I	4871	GLU
3	I	4903	ASP
3	I	4911	LEU
2	H	17	LYS
2	H	29	MET
2	H	79	ASP

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Mol	Chain	Res	Type
2	J	17	LYS
2	J	29	MET
2	J	79	ASP
2	O	17	LYS
2	O	29	MET
2	O	79	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	991	ASN
3	A	2180	GLN
3	A	2881	ASN
3	B	991	ASN
3	B	2180	GLN
3	B	2881	ASN
3	B	3734	HIS
3	B	3761	GLN
3	G	991	ASN
3	G	2881	ASN
3	I	991	ASN
3	I	2180	GLN
3	I	2881	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 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
8	KVR	G	5107	-	24,25,25	1.38	3 (12%)	32,34,34	1.54	4 (12%)
8	KVR	B	5306	-	24,25,25	1.39	3 (12%)	32,34,34	1.54	4 (12%)
9	L9R	B	5308	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
9	L9R	A	5307	-	53,53,53	1.22	5 (9%)	59,61,61	1.11	3 (5%)
5	ATP	B	5301	-	26,33,33	0.60	0	31,52,52	0.82	2 (6%)
5	ATP	G	5102	-	26,33,33	0.58	0	31,52,52	0.82	2 (6%)
5	ATP	I	5106	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
8	KVR	A	5306	-	24,25,25	1.38	3 (12%)	32,34,34	1.54	4 (12%)
9	L9R	B	5307	-	53,53,53	1.22	5 (9%)	59,61,61	1.11	3 (5%)
7	CFF	B	5304	-	8,15,15	2.35	3 (37%)	8,23,23	1.42	1 (12%)
7	CFF	A	5304	-	8,15,15	2.35	3 (37%)	8,23,23	1.42	1 (12%)
9	L9R	I	5101	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
5	ATP	G	5106	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)
9	L9R	I	5108	-	53,53,53	1.21	4 (7%)	59,61,61	1.11	3 (5%)
9	L9R	G	5108	-	53,53,53	1.22	4 (7%)	59,61,61	1.11	3 (5%)
7	CFF	I	5105	-	8,15,15	2.35	3 (37%)	8,23,23	1.43	1 (12%)
7	CFF	G	5105	-	8,15,15	2.35	3 (37%)	8,23,23	1.43	1 (12%)
9	L9R	G	5101	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
5	ATP	B	5305	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
5	ATP	I	5102	-	26,33,33	0.61	0	31,52,52	0.82	2 (6%)
9	L9R	A	5308	-	53,53,53	1.18	4 (7%)	59,61,61	1.11	2 (3%)
5	ATP	A	5301	-	26,33,33	0.59	0	31,52,52	0.82	2 (6%)
8	KVR	I	5107	-	24,25,25	1.38	3 (12%)	32,34,34	1.54	4 (12%)
5	ATP	A	5305	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)

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
8	KVR	G	5107	-	-	2/10/20/20	0/2/3/3
8	KVR	B	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5308	-	-	34/57/57/57	-
9	L9R	A	5307	-	-	31/57/57/57	-
5	ATP	B	5301	-	-	8/18/38/38	0/3/3/3
5	ATP	G	5102	-	-	8/18/38/38	0/3/3/3
5	ATP	I	5106	-	-	6/18/38/38	0/3/3/3
8	KVR	A	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5307	-	-	31/57/57/57	-
7	CFF	B	5304	-	-	-	0/2/2/2
7	CFF	A	5304	-	-	-	0/2/2/2
9	L9R	I	5101	-	-	34/57/57/57	-
5	ATP	G	5106	-	-	6/18/38/38	0/3/3/3
9	L9R	I	5108	-	-	31/57/57/57	-
9	L9R	G	5108	-	-	31/57/57/57	-
7	CFF	I	5105	-	-	-	0/2/2/2
9	L9R	G	5101	-	-	34/57/57/57	-
7	CFF	G	5105	-	-	-	0/2/2/2
5	ATP	B	5305	-	-	6/18/38/38	0/3/3/3
5	ATP	I	5102	-	-	8/18/38/38	0/3/3/3
9	L9R	A	5308	-	-	34/57/57/57	-
5	ATP	A	5301	-	-	8/18/38/38	0/3/3/3
8	KVR	I	5107	-	-	2/10/20/20	0/2/3/3
5	ATP	A	5305	-	-	6/18/38/38	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	5306	KVR	C06-S09	4.85	1.82	1.77
8	I	5107	KVR	C06-S09	4.84	1.82	1.77
8	A	5306	KVR	C06-S09	4.82	1.82	1.77
8	G	5107	KVR	C06-S09	4.80	1.82	1.77
7	G	5105	CFF	C5-C4	-4.24	1.33	1.39
7	I	5105	CFF	C5-C4	-4.24	1.33	1.39
7	A	5304	CFF	C5-C4	-4.22	1.33	1.39
7	B	5304	CFF	C5-C4	-4.22	1.33	1.39
7	B	5304	CFF	C6-N1	-3.95	1.32	1.38
7	A	5304	CFF	C6-N1	-3.93	1.32	1.38
7	G	5105	CFF	C6-N1	-3.93	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	5105	CFF	C6-N1	-3.93	1.32	1.38
9	A	5307	L9R	O2-C31	3.59	1.44	1.34
9	B	5307	L9R	O2-C31	3.59	1.44	1.34
9	G	5108	L9R	O2-C31	3.59	1.44	1.34
9	I	5108	L9R	O2-C31	3.59	1.44	1.34
9	A	5308	L9R	O2-C31	3.54	1.44	1.34
9	I	5101	L9R	O2-C31	3.53	1.44	1.34
9	B	5308	L9R	O2-C31	3.52	1.44	1.34
9	G	5101	L9R	O2-C31	3.52	1.44	1.34
9	G	5108	L9R	O3-C11	3.16	1.42	1.33
9	A	5307	L9R	O3-C11	3.13	1.42	1.33
9	I	5108	L9R	O3-C11	3.13	1.42	1.33
9	B	5307	L9R	O3-C11	3.13	1.42	1.33
9	A	5308	L9R	O3-C11	3.03	1.42	1.33
9	B	5308	L9R	O3-C11	3.03	1.42	1.33
9	G	5101	L9R	O3-C11	3.03	1.42	1.33
9	I	5101	L9R	O3-C11	3.03	1.42	1.33
8	G	5107	KVR	C13-C05	2.56	1.55	1.51
8	A	5306	KVR	C13-C05	2.55	1.55	1.51
8	B	5306	KVR	C13-C05	2.52	1.55	1.51
9	A	5307	L9R	C32-C31	2.52	1.58	1.50
9	I	5108	L9R	C32-C31	2.52	1.58	1.50
9	B	5307	L9R	C32-C31	2.51	1.58	1.50
8	I	5107	KVR	C13-C05	2.51	1.55	1.51
9	G	5108	L9R	C32-C31	2.51	1.58	1.50
9	I	5101	L9R	C32-C31	2.32	1.57	1.50
9	A	5308	L9R	C32-C31	2.32	1.57	1.50
9	B	5308	L9R	C32-C31	2.31	1.57	1.50
9	G	5101	L9R	C32-C31	2.31	1.57	1.50
7	G	5105	CFF	O13-C6	-2.30	1.18	1.24
7	A	5304	CFF	O13-C6	-2.29	1.18	1.24
7	B	5304	CFF	O13-C6	-2.29	1.18	1.24
8	A	5306	KVR	C13-N12	-2.28	1.45	1.47
8	I	5107	KVR	C13-N12	-2.28	1.45	1.47
8	B	5306	KVR	C13-N12	-2.28	1.45	1.47
8	G	5107	KVR	C13-N12	-2.27	1.45	1.47
7	I	5105	CFF	O13-C6	-2.27	1.18	1.24
9	I	5101	L9R	O2-C2	-2.14	1.41	1.46
9	B	5308	L9R	O2-C2	-2.11	1.41	1.46
9	G	5101	L9R	O2-C2	-2.11	1.41	1.46
9	A	5308	L9R	O2-C2	-2.11	1.41	1.46
9	I	5108	L9R	P-O3P	2.04	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	5307	L9R	P-O3P	2.04	1.67	1.59
9	G	5108	L9R	P-O3P	2.04	1.67	1.59
9	B	5307	L9R	P-O3P	2.03	1.67	1.59
9	A	5307	L9R	O2-C2	-2.01	1.41	1.46
9	B	5307	L9R	O2-C2	-2.00	1.41	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	5107	KVR	C10-S09-C06	5.26	110.17	102.71
8	A	5306	KVR	C10-S09-C06	5.26	110.16	102.71
8	B	5306	KVR	C10-S09-C06	5.24	110.14	102.71
8	I	5107	KVR	C10-S09-C06	5.24	110.13	102.71
9	B	5308	L9R	O2-C31-C32	4.04	120.20	111.50
9	G	5101	L9R	O2-C31-C32	4.04	120.20	111.50
9	A	5308	L9R	O2-C31-C32	4.03	120.20	111.50
9	I	5101	L9R	O2-C31-C32	4.02	120.17	111.50
9	B	5307	L9R	O2-C31-C32	3.93	119.96	111.50
9	A	5307	L9R	O2-C31-C32	3.92	119.95	111.50
9	I	5108	L9R	O2-C31-C32	3.92	119.95	111.50
9	G	5108	L9R	O2-C31-C32	3.90	119.90	111.50
8	G	5107	KVR	C11-C10-S09	-3.25	110.15	114.22
8	A	5306	KVR	C11-C10-S09	-3.23	110.16	114.22
8	B	5306	KVR	C11-C10-S09	-3.22	110.18	114.22
8	I	5107	KVR	C11-C10-S09	-3.21	110.19	114.22
7	I	5105	CFF	C14-N7-C8	-3.11	110.47	125.43
7	A	5304	CFF	C14-N7-C8	-3.10	110.51	125.43
7	B	5304	CFF	C14-N7-C8	-3.10	110.52	125.43
7	G	5105	CFF	C14-N7-C8	-3.09	110.54	125.43
8	I	5107	KVR	C14-N12-C11	-2.77	106.56	111.06
8	G	5107	KVR	C14-N12-C11	-2.77	106.57	111.06
9	I	5108	L9R	O3-C11-C12	2.76	120.56	111.91
9	B	5307	L9R	O3-C11-C12	2.76	120.56	111.91
8	A	5306	KVR	C14-N12-C11	-2.75	106.60	111.06
9	A	5307	L9R	O3-C11-C12	2.75	120.53	111.91
9	G	5108	L9R	O3-C11-C12	2.73	120.48	111.91
8	B	5306	KVR	C14-N12-C11	-2.71	106.66	111.06
9	A	5308	L9R	O3-C11-C12	2.66	120.24	111.91
9	B	5308	L9R	O3-C11-C12	2.65	120.22	111.91
9	G	5101	L9R	O3-C11-C12	2.65	120.22	111.91
9	I	5101	L9R	O3-C11-C12	2.64	120.18	111.91
5	I	5102	ATP	C5-C6-N6	2.32	123.88	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	5301	ATP	C5-C6-N6	2.32	123.87	120.35
5	G	5102	ATP	C5-C6-N6	2.31	123.87	120.35
5	G	5106	ATP	C5-C6-N6	2.30	123.84	120.35
5	B	5301	ATP	C5-C6-N6	2.29	123.84	120.35
5	A	5305	ATP	C5-C6-N6	2.29	123.83	120.35
5	I	5106	ATP	C5-C6-N6	2.27	123.81	120.35
5	B	5305	ATP	C5-C6-N6	2.26	123.79	120.35
8	A	5306	KVR	O23-C21-C18	2.23	120.64	114.85
8	I	5107	KVR	O23-C21-C18	2.23	120.64	114.85
8	B	5306	KVR	O23-C21-C18	2.23	120.63	114.85
9	I	5108	L9R	C4-C5-N	-2.22	108.36	115.78
9	B	5307	L9R	C4-C5-N	-2.22	108.36	115.78
9	G	5108	L9R	C4-C5-N	-2.21	108.39	115.78
9	A	5307	L9R	C4-C5-N	-2.21	108.40	115.78
8	G	5107	KVR	O23-C21-C18	2.21	120.57	114.85
5	G	5106	ATP	PB-O3B-PG	2.08	139.95	132.83
5	A	5305	ATP	PB-O3B-PG	2.07	139.95	132.83
5	I	5106	ATP	PB-O3B-PG	2.07	139.94	132.83
5	I	5102	ATP	PB-O3B-PG	2.07	139.93	132.83
5	B	5305	ATP	PB-O3B-PG	2.07	139.92	132.83
5	A	5301	ATP	PB-O3B-PG	2.06	139.90	132.83
5	G	5102	ATP	PB-O3B-PG	2.06	139.90	132.83
5	B	5301	ATP	PB-O3B-PG	2.05	139.86	132.83

There are no chirality outliers.

All (324) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5301	ATP	C5'-O5'-PA-O1A
5	A	5301	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O3A
5	B	5301	ATP	C5'-O5'-PA-O1A
5	B	5301	ATP	C5'-O5'-PA-O2A
5	B	5305	ATP	C5'-O5'-PA-O2A
5	B	5305	ATP	C5'-O5'-PA-O3A
5	G	5102	ATP	C5'-O5'-PA-O1A
5	G	5102	ATP	C5'-O5'-PA-O2A
5	G	5106	ATP	C5'-O5'-PA-O2A
5	G	5106	ATP	C5'-O5'-PA-O3A
5	I	5102	ATP	C5'-O5'-PA-O1A
5	I	5102	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	I	5106	ATP	C5'-O5'-PA-O2A
5	I	5106	ATP	C5'-O5'-PA-O3A
8	A	5306	KVR	C15-C14-N12-C11
8	A	5306	KVR	C15-C14-N12-C13
8	B	5306	KVR	C15-C14-N12-C11
8	B	5306	KVR	C15-C14-N12-C13
8	G	5107	KVR	C15-C14-N12-C11
8	G	5107	KVR	C15-C14-N12-C13
8	I	5107	KVR	C15-C14-N12-C11
8	I	5107	KVR	C15-C14-N12-C13
9	A	5308	L9R	C1-O3P-P-O1P
9	A	5308	L9R	C1-O3P-P-O4P
9	A	5308	L9R	C4-O4P-P-O1P
9	A	5308	L9R	C4-O4P-P-O2P
9	A	5308	L9R	O4P-C4-C5-N
9	B	5308	L9R	C1-O3P-P-O1P
9	B	5308	L9R	C1-O3P-P-O4P
9	B	5308	L9R	C4-O4P-P-O1P
9	B	5308	L9R	C4-O4P-P-O2P
9	B	5308	L9R	O4P-C4-C5-N
9	G	5101	L9R	C1-O3P-P-O1P
9	G	5101	L9R	C1-O3P-P-O4P
9	G	5101	L9R	C4-O4P-P-O1P
9	G	5101	L9R	C4-O4P-P-O2P
9	G	5101	L9R	O4P-C4-C5-N
9	I	5101	L9R	C1-O3P-P-O1P
9	I	5101	L9R	C1-O3P-P-O4P
9	I	5101	L9R	C4-O4P-P-O1P
9	I	5101	L9R	C4-O4P-P-O2P
9	I	5101	L9R	O4P-C4-C5-N
9	B	5308	L9R	C20-C21-C22-C23
9	I	5101	L9R	C20-C21-C22-C23
9	A	5308	L9R	C20-C21-C22-C23
9	G	5101	L9R	C20-C21-C22-C23
9	A	5307	L9R	C32-C31-O2-C2
9	B	5307	L9R	C32-C31-O2-C2
9	G	5108	L9R	C32-C31-O2-C2
9	I	5108	L9R	C32-C31-O2-C2
9	A	5308	L9R	C13-C14-C15-C16
9	B	5308	L9R	C13-C14-C15-C16
9	G	5101	L9R	C13-C14-C15-C16
9	I	5101	L9R	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
9	A	5307	L9R	C12-C11-O3-C3
9	B	5307	L9R	C12-C11-O3-C3
9	G	5108	L9R	C12-C11-O3-C3
9	I	5108	L9R	C12-C11-O3-C3
9	A	5307	L9R	O11-C11-O3-C3
9	B	5307	L9R	O11-C11-O3-C3
9	G	5108	L9R	O11-C11-O3-C3
9	I	5108	L9R	O11-C11-O3-C3
9	A	5307	L9R	O31-C31-O2-C2
9	B	5307	L9R	O31-C31-O2-C2
9	G	5108	L9R	O31-C31-O2-C2
9	I	5108	L9R	O31-C31-O2-C2
9	A	5308	L9R	C11-C12-C13-C14
9	B	5308	L9R	C11-C12-C13-C14
9	G	5101	L9R	C11-C12-C13-C14
9	I	5101	L9R	C11-C12-C13-C14
9	A	5307	L9R	C32-C33-C34-C35
9	B	5307	L9R	C32-C33-C34-C35
9	G	5108	L9R	C32-C33-C34-C35
9	I	5108	L9R	C32-C33-C34-C35
9	A	5307	L9R	C33-C34-C35-C36
9	B	5307	L9R	C33-C34-C35-C36
9	A	5308	L9R	C35-C36-C37-C38
9	B	5308	L9R	C35-C36-C37-C38
9	G	5101	L9R	C35-C36-C37-C38
9	G	5108	L9R	C33-C34-C35-C36
9	I	5101	L9R	C35-C36-C37-C38
9	I	5108	L9R	C33-C34-C35-C36
9	A	5308	L9R	C22-C23-C24-C25
9	B	5308	L9R	C22-C23-C24-C25
9	G	5101	L9R	C22-C23-C24-C25
9	I	5101	L9R	C22-C23-C24-C25
9	A	5307	L9R	C16-C17-C18-C19
9	B	5307	L9R	C16-C17-C18-C19
9	G	5108	L9R	C16-C17-C18-C19
9	I	5108	L9R	C16-C17-C18-C19
9	A	5308	L9R	C16-C17-C18-C19
9	B	5307	L9R	C20-C21-C22-C23
9	B	5308	L9R	C16-C17-C18-C19
9	G	5101	L9R	C16-C17-C18-C19
9	G	5108	L9R	C20-C21-C22-C23
9	I	5101	L9R	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	A	5307	L9R	C20-C21-C22-C23
9	I	5108	L9R	C20-C21-C22-C23
9	A	5307	L9R	C21-C22-C23-C24
9	B	5307	L9R	C21-C22-C23-C24
9	B	5308	L9R	C15-C16-C17-C18
9	G	5108	L9R	C21-C22-C23-C24
9	G	5108	L9R	C44-C45-C46-C47
9	I	5108	L9R	C44-C45-C46-C47
9	A	5307	L9R	C44-C45-C46-C47
9	A	5308	L9R	C15-C16-C17-C18
9	B	5307	L9R	C44-C45-C46-C47
9	G	5101	L9R	C15-C16-C17-C18
9	I	5101	L9R	C15-C16-C17-C18
9	I	5108	L9R	C21-C22-C23-C24
9	A	5308	L9R	C12-C13-C14-C15
9	B	5308	L9R	C12-C13-C14-C15
9	G	5101	L9R	C12-C13-C14-C15
9	I	5101	L9R	C12-C13-C14-C15
9	A	5308	L9R	C42-C43-C44-C45
9	B	5308	L9R	C42-C43-C44-C45
9	G	5101	L9R	C42-C43-C44-C45
9	I	5101	L9R	C42-C43-C44-C45
9	A	5308	L9R	C24-C25-C26-C27
9	B	5308	L9R	C24-C25-C26-C27
9	G	5101	L9R	C24-C25-C26-C27
9	I	5101	L9R	C24-C25-C26-C27
9	A	5307	L9R	C4-C5-N-C6
9	B	5307	L9R	C4-C5-N-C6
9	G	5108	L9R	C4-C5-N-C6
9	I	5108	L9R	C4-C5-N-C6
9	A	5307	L9R	O3P-C1-C2-O2
9	B	5307	L9R	O3P-C1-C2-O2
9	G	5108	L9R	O3P-C1-C2-O2
9	I	5108	L9R	O3P-C1-C2-O2
9	A	5308	L9R	C32-C33-C34-C35
9	B	5308	L9R	C32-C33-C34-C35
9	G	5101	L9R	C32-C33-C34-C35
9	I	5101	L9R	C32-C33-C34-C35
9	A	5308	L9R	C41-C42-C43-C44
9	B	5308	L9R	C41-C42-C43-C44
9	G	5101	L9R	C41-C42-C43-C44
5	A	5301	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	B	5301	ATP	O4'-C4'-C5'-O5'
5	G	5102	ATP	O4'-C4'-C5'-O5'
5	I	5102	ATP	O4'-C4'-C5'-O5'
9	A	5307	L9R	C41-C42-C43-C44
9	B	5307	L9R	C41-C42-C43-C44
9	G	5108	L9R	C41-C42-C43-C44
9	I	5101	L9R	C41-C42-C43-C44
9	I	5108	L9R	C41-C42-C43-C44
9	A	5308	L9R	C4-O4P-P-O3P
9	B	5308	L9R	C4-O4P-P-O3P
9	G	5101	L9R	C4-O4P-P-O3P
9	I	5101	L9R	C4-O4P-P-O3P
9	A	5308	L9R	C17-C18-C19-C20
9	B	5308	L9R	C17-C18-C19-C20
9	G	5101	L9R	C17-C18-C19-C20
9	I	5101	L9R	C17-C18-C19-C20
9	A	5307	L9R	C4-C5-N-C8
9	B	5307	L9R	C4-C5-N-C8
9	G	5108	L9R	C4-C5-N-C8
9	I	5108	L9R	C4-C5-N-C8
9	A	5308	L9R	C33-C34-C35-C36
9	B	5308	L9R	C33-C34-C35-C36
9	G	5101	L9R	C33-C34-C35-C36
9	I	5101	L9R	C33-C34-C35-C36
9	A	5308	L9R	C40-C41-C42-C43
9	B	5308	L9R	C40-C41-C42-C43
9	G	5101	L9R	C40-C41-C42-C43
9	I	5101	L9R	C40-C41-C42-C43
9	A	5307	L9R	C35-C36-C37-C38
9	B	5307	L9R	C35-C36-C37-C38
9	B	5307	L9R	C4-C5-N-C7
9	G	5108	L9R	C35-C36-C37-C38
9	I	5108	L9R	C35-C36-C37-C38
9	A	5308	L9R	C19-C20-C21-C22
9	B	5308	L9R	C19-C20-C21-C22
9	G	5101	L9R	C19-C20-C21-C22
9	I	5101	L9R	C19-C20-C21-C22
9	B	5308	L9R	C14-C15-C16-C17
9	I	5101	L9R	C14-C15-C16-C17
9	A	5308	L9R	C14-C15-C16-C17
9	G	5101	L9R	C14-C15-C16-C17
9	A	5308	L9R	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
9	B	5308	L9R	C44-C45-C46-C47
9	G	5101	L9R	C44-C45-C46-C47
9	I	5101	L9R	C44-C45-C46-C47
9	A	5307	L9R	C37-C38-C39-C40
9	B	5307	L9R	C37-C38-C39-C40
9	G	5108	L9R	C37-C38-C39-C40
9	I	5108	L9R	C37-C38-C39-C40
9	A	5307	L9R	C4-C5-N-C7
9	G	5108	L9R	C4-C5-N-C7
9	I	5108	L9R	C4-C5-N-C7
5	A	5301	ATP	C3'-C4'-C5'-O5'
5	B	5301	ATP	C3'-C4'-C5'-O5'
5	G	5102	ATP	C3'-C4'-C5'-O5'
5	I	5102	ATP	C3'-C4'-C5'-O5'
9	A	5308	L9R	C12-C11-O3-C3
9	B	5308	L9R	C12-C11-O3-C3
9	G	5101	L9R	C12-C11-O3-C3
9	I	5101	L9R	C12-C11-O3-C3
9	A	5307	L9R	C1-C2-C3-O3
9	B	5307	L9R	C1-C2-C3-O3
9	G	5108	L9R	C1-C2-C3-O3
9	I	5108	L9R	C1-C2-C3-O3
9	A	5308	L9R	C18-C19-C20-C21
9	B	5308	L9R	C18-C19-C20-C21
9	G	5101	L9R	C18-C19-C20-C21
9	I	5101	L9R	C18-C19-C20-C21
9	A	5307	L9R	C24-C25-C26-C27
9	B	5307	L9R	C24-C25-C26-C27
9	G	5108	L9R	C24-C25-C26-C27
9	I	5108	L9R	C24-C25-C26-C27
9	G	5108	L9R	C45-C46-C47-C48
9	A	5307	L9R	C45-C46-C47-C48
9	B	5307	L9R	C45-C46-C47-C48
9	I	5108	L9R	C45-C46-C47-C48
9	A	5307	L9R	O3P-C1-C2-C3
9	B	5307	L9R	O3P-C1-C2-C3
9	G	5108	L9R	O3P-C1-C2-C3
9	I	5108	L9R	O3P-C1-C2-C3
9	A	5307	L9R	C13-C14-C15-C16
9	A	5307	L9R	C15-C16-C17-C18
9	B	5307	L9R	C13-C14-C15-C16
9	G	5108	L9R	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
9	I	5108	L9R	C13-C14-C15-C16
9	B	5307	L9R	C15-C16-C17-C18
9	G	5108	L9R	C15-C16-C17-C18
9	I	5108	L9R	C15-C16-C17-C18
9	A	5308	L9R	O11-C11-O3-C3
9	G	5101	L9R	O11-C11-O3-C3
9	I	5101	L9R	O11-C11-O3-C3
9	A	5307	L9R	O2-C2-C3-O3
9	B	5307	L9R	O2-C2-C3-O3
9	G	5108	L9R	O2-C2-C3-O3
9	I	5108	L9R	O2-C2-C3-O3
9	B	5308	L9R	O11-C11-O3-C3
9	A	5308	L9R	C39-C40-C41-C42
9	B	5308	L9R	C39-C40-C41-C42
9	G	5101	L9R	C39-C40-C41-C42
9	I	5101	L9R	C39-C40-C41-C42
9	A	5308	L9R	C4-C5-N-C7
9	B	5308	L9R	C4-C5-N-C7
9	G	5101	L9R	C4-C5-N-C7
9	I	5101	L9R	C4-C5-N-C7
9	A	5307	L9R	C1-O3P-P-O4P
9	B	5307	L9R	C1-O3P-P-O4P
9	G	5108	L9R	C1-O3P-P-O4P
9	I	5108	L9R	C1-O3P-P-O4P
5	A	5305	ATP	C3'-C4'-C5'-O5'
5	B	5305	ATP	C3'-C4'-C5'-O5'
5	G	5106	ATP	C3'-C4'-C5'-O5'
5	I	5106	ATP	C3'-C4'-C5'-O5'
9	A	5308	L9R	C4-C5-N-C6
9	B	5308	L9R	C4-C5-N-C6
9	A	5308	L9R	C23-C24-C25-C26
9	B	5308	L9R	C23-C24-C25-C26
9	I	5101	L9R	C23-C24-C25-C26
9	G	5101	L9R	C23-C24-C25-C26
9	G	5101	L9R	C4-C5-N-C6
9	I	5101	L9R	C4-C5-N-C6
5	A	5301	ATP	PG-O3B-PB-O3A
5	G	5102	ATP	PG-O3B-PB-O3A
9	A	5308	L9R	C4-C5-N-C8
9	B	5308	L9R	C4-C5-N-C8
9	G	5101	L9R	C4-C5-N-C8
9	I	5101	L9R	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
9	A	5307	L9R	C40-C41-C42-C43
9	B	5307	L9R	C40-C41-C42-C43
9	G	5108	L9R	C40-C41-C42-C43
9	I	5108	L9R	C40-C41-C42-C43
5	A	5305	ATP	O4'-C4'-C5'-O5'
5	B	5305	ATP	O4'-C4'-C5'-O5'
5	G	5106	ATP	O4'-C4'-C5'-O5'
5	I	5106	ATP	O4'-C4'-C5'-O5'
5	B	5301	ATP	PG-O3B-PB-O3A
5	I	5102	ATP	PG-O3B-PB-O3A
9	B	5308	L9R	C25-C26-C27-C28
9	G	5101	L9R	C25-C26-C27-C28
9	I	5101	L9R	C25-C26-C27-C28
9	A	5308	L9R	C25-C26-C27-C28
5	A	5301	ATP	C5'-O5'-PA-O3A
5	B	5301	ATP	C5'-O5'-PA-O3A
5	G	5102	ATP	C5'-O5'-PA-O3A
5	I	5102	ATP	C5'-O5'-PA-O3A
9	A	5307	L9R	O2-C31-C32-C33
9	B	5307	L9R	O2-C31-C32-C33
9	G	5108	L9R	O2-C31-C32-C33
9	I	5108	L9R	O2-C31-C32-C33
9	I	5108	L9R	C12-C13-C14-C15
9	A	5307	L9R	C12-C13-C14-C15
9	G	5108	L9R	C12-C13-C14-C15
9	B	5307	L9R	C12-C13-C14-C15
5	A	5301	ATP	PG-O3B-PB-O1B
5	A	5305	ATP	PG-O3B-PB-O1B
5	A	5305	ATP	PG-O3B-PB-O2B
5	B	5301	ATP	PG-O3B-PB-O1B
5	B	5305	ATP	PG-O3B-PB-O1B
5	B	5305	ATP	PG-O3B-PB-O2B
5	G	5102	ATP	PG-O3B-PB-O1B
5	G	5106	ATP	PG-O3B-PB-O1B
5	G	5106	ATP	PG-O3B-PB-O2B
5	I	5102	ATP	PG-O3B-PB-O1B
5	I	5106	ATP	PG-O3B-PB-O1B
5	I	5106	ATP	PG-O3B-PB-O2B
9	A	5307	L9R	C43-C44-C45-C46
9	B	5307	L9R	C43-C44-C45-C46
9	G	5108	L9R	C43-C44-C45-C46
9	I	5108	L9R	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
5	A	5301	ATP	C4'-C5'-O5'-PA
5	B	5301	ATP	C4'-C5'-O5'-PA
5	G	5102	ATP	C4'-C5'-O5'-PA
5	I	5102	ATP	C4'-C5'-O5'-PA
9	A	5307	L9R	C4-O4P-P-O1P
9	B	5307	L9R	C4-O4P-P-O1P
9	G	5108	L9R	C4-O4P-P-O1P
9	I	5108	L9R	C4-O4P-P-O1P
9	B	5307	L9R	O31-C31-C32-C33
9	I	5108	L9R	O31-C31-C32-C33
9	A	5307	L9R	O31-C31-C32-C33
9	G	5108	L9R	O31-C31-C32-C33
9	I	5101	L9R	C45-C46-C47-C48
9	A	5308	L9R	C45-C46-C47-C48
9	G	5101	L9R	C45-C46-C47-C48
9	B	5308	L9R	C45-C46-C47-C48

There are no ring outliers.

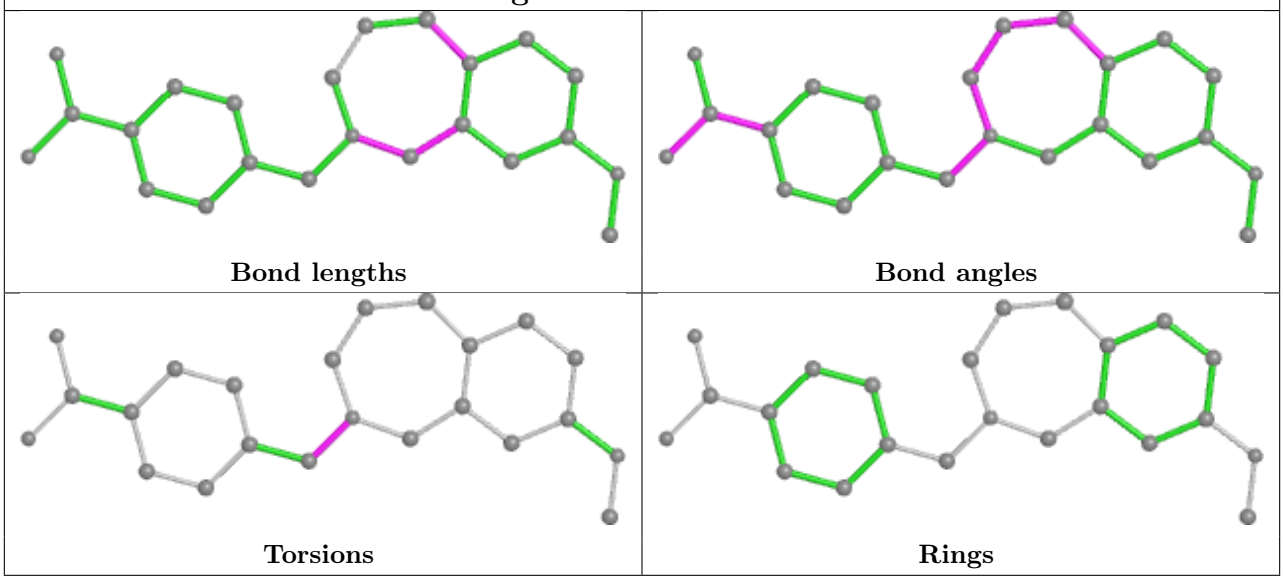
16 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	5308	L9R	4	0
9	A	5307	L9R	3	0
5	B	5301	ATP	1	0
5	G	5102	ATP	1	0
5	I	5106	ATP	1	0
9	B	5307	L9R	2	0
9	I	5101	L9R	5	0
5	G	5106	ATP	1	0
9	I	5108	L9R	3	0
9	G	5108	L9R	3	0
9	G	5101	L9R	6	0
5	B	5305	ATP	1	0
5	I	5102	ATP	1	0
9	A	5308	L9R	6	0
5	A	5301	ATP	1	0
5	A	5305	ATP	1	0

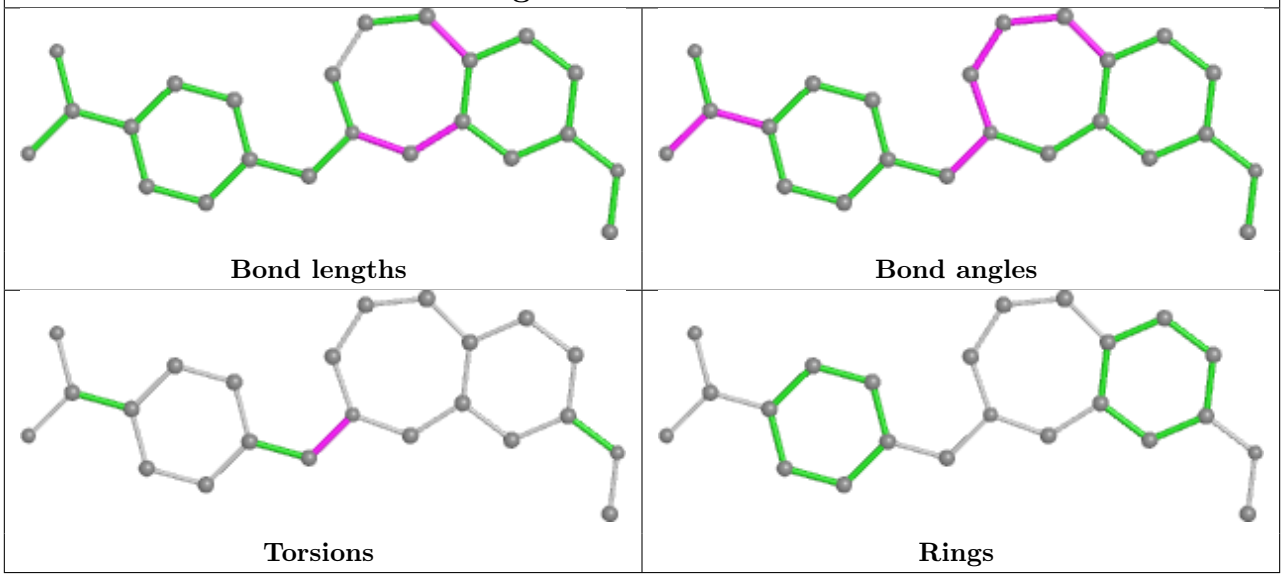
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

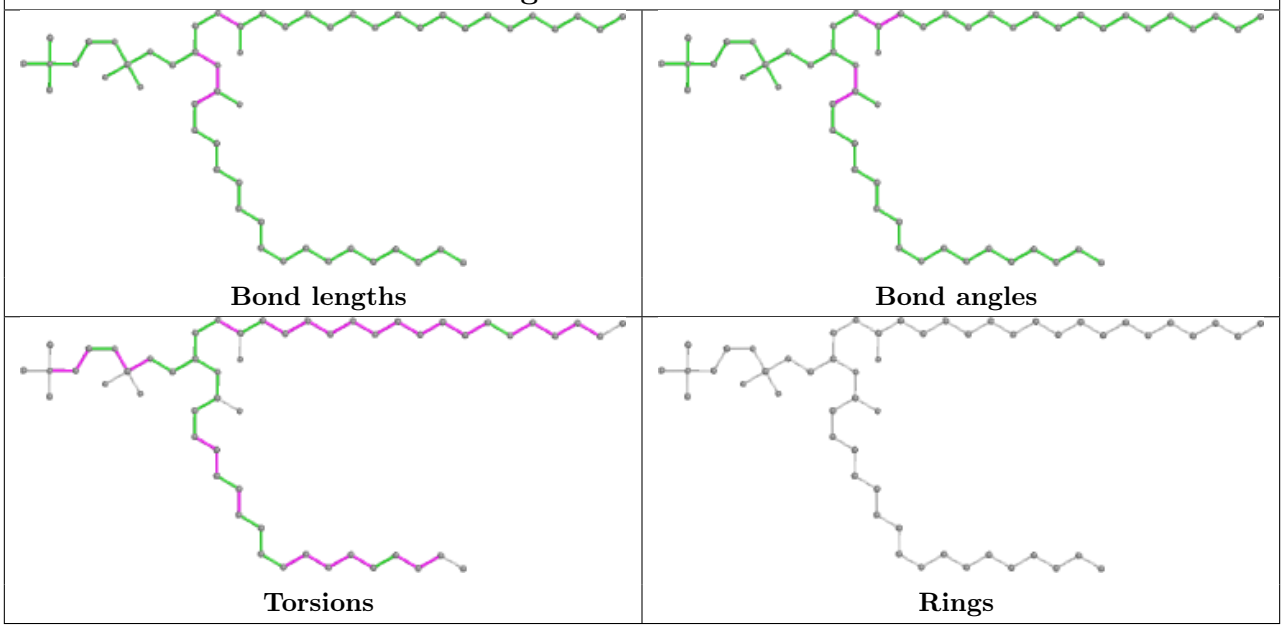
Ligand KVR G 5107



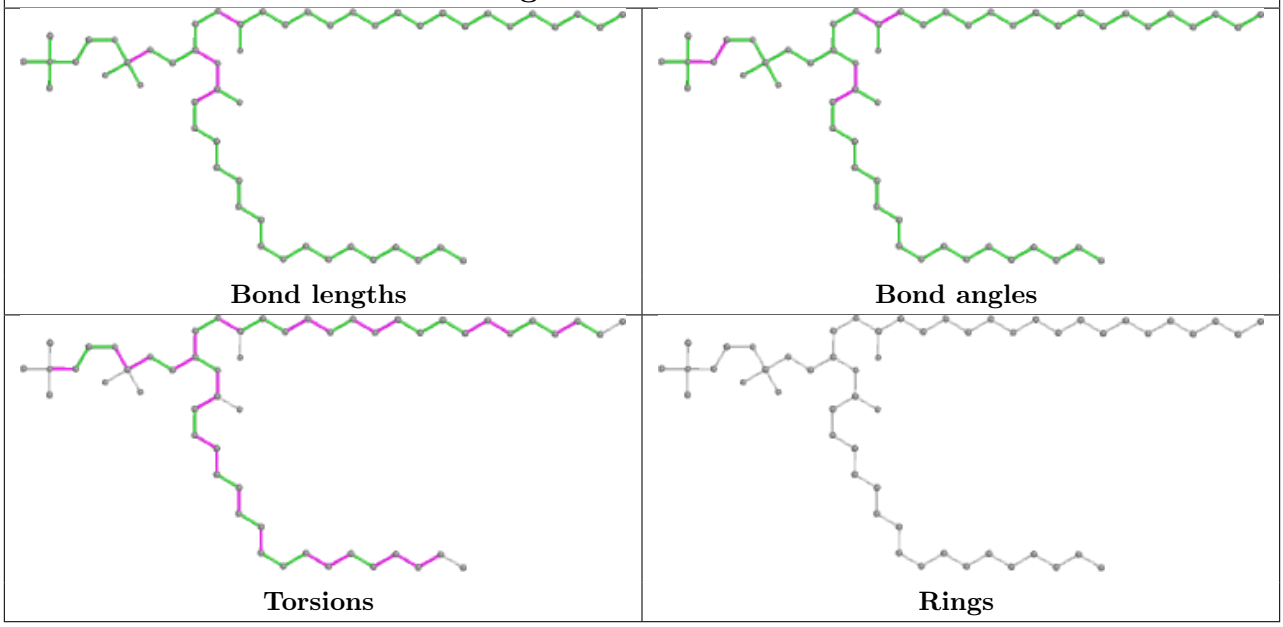
Ligand KVR B 5306



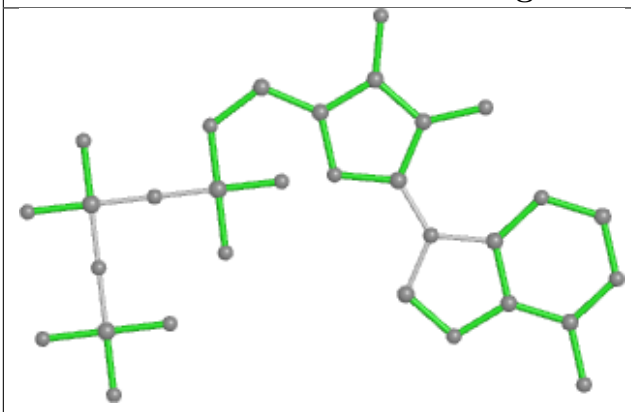
Ligand L9R B 5308



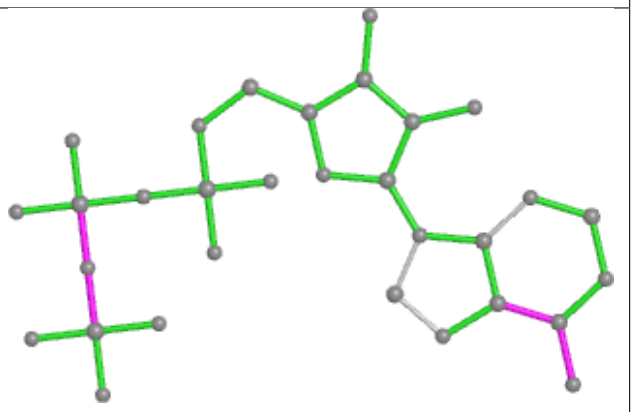
Ligand L9R A 5307



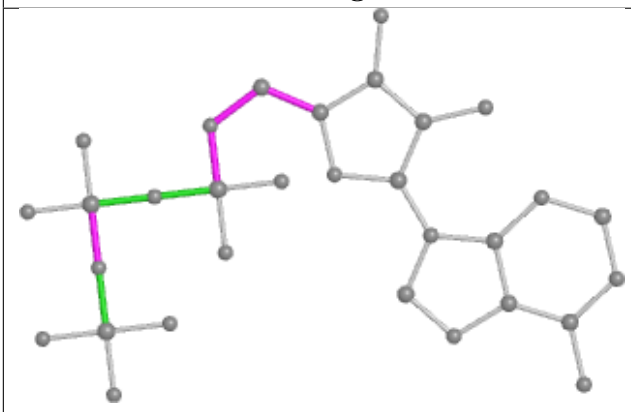
Ligand ATP B 5301



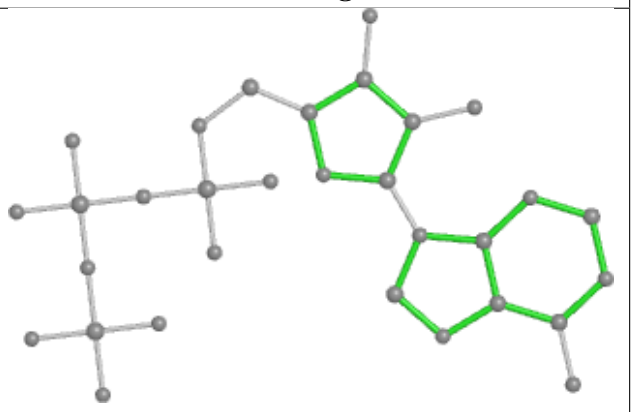
Bond lengths



Bond angles

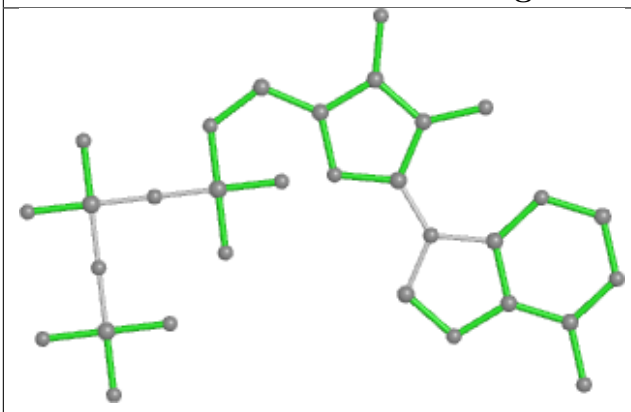


Torsions

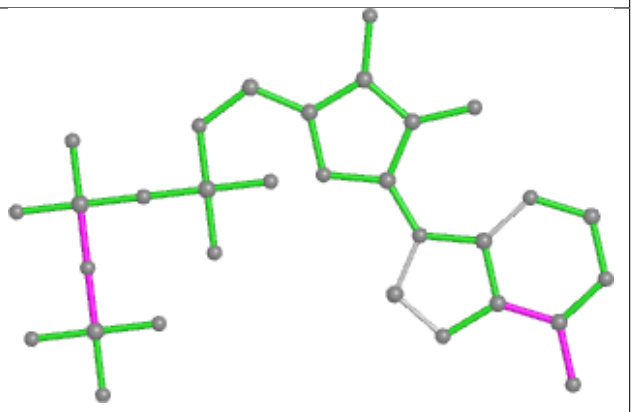


Rings

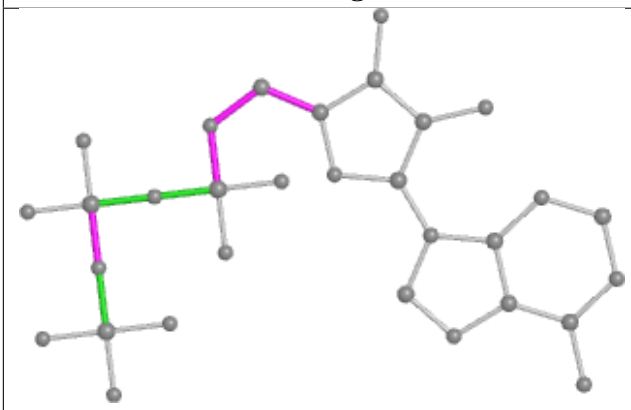
Ligand ATP G 5102



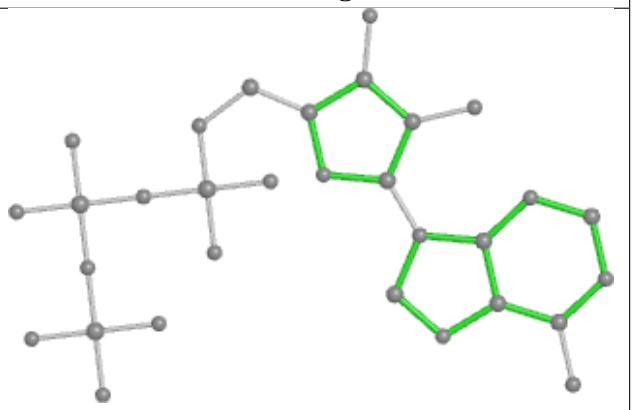
Bond lengths



Bond angles

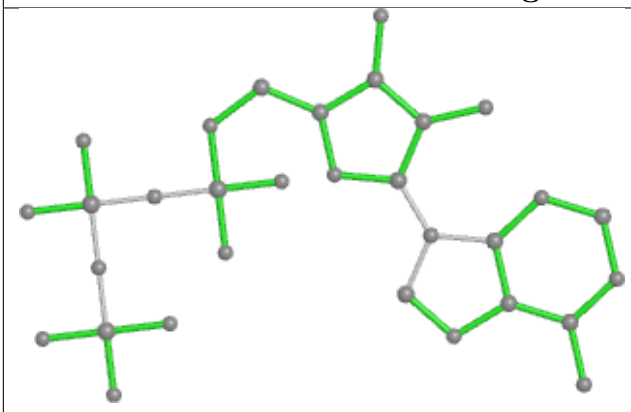


Torsions

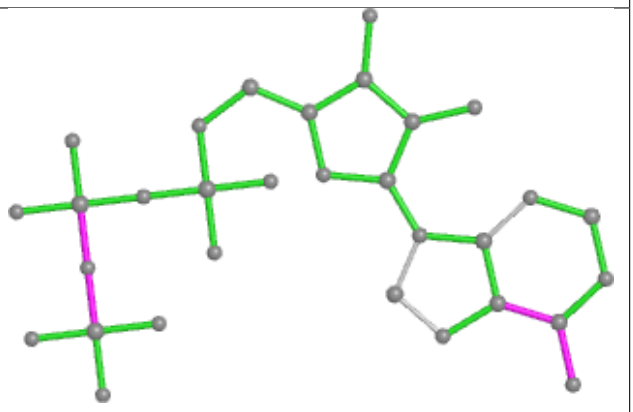


Rings

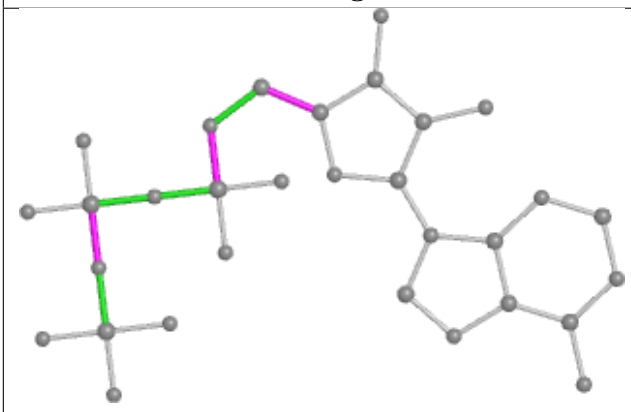
Ligand ATP I 5106



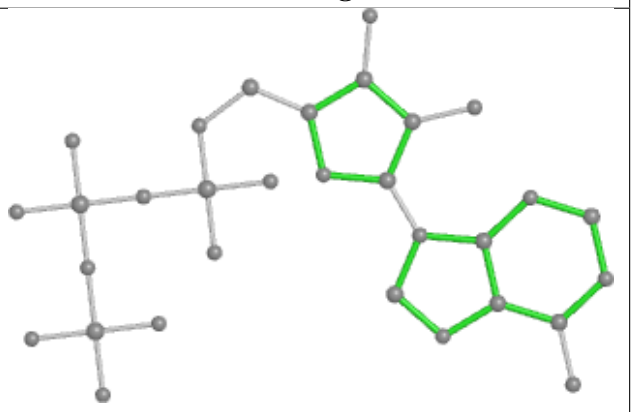
Bond lengths



Bond angles

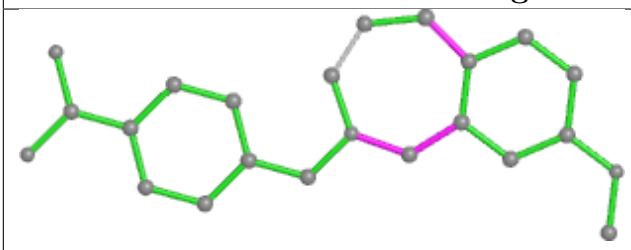


Torsions

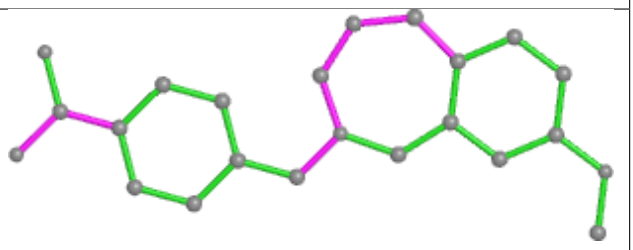


Rings

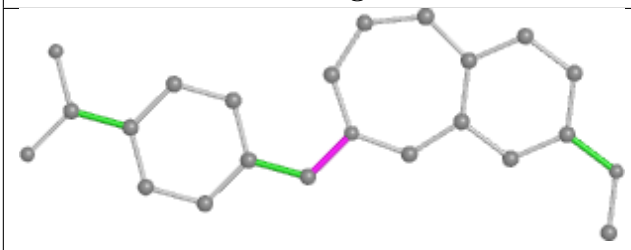
Ligand KVR A 5306



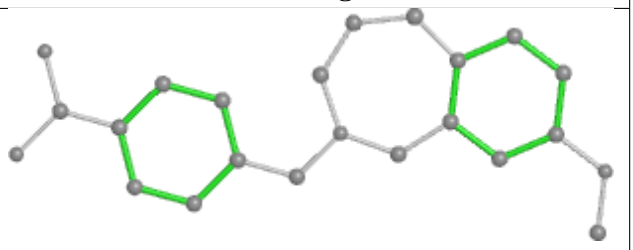
Bond lengths



Bond angles

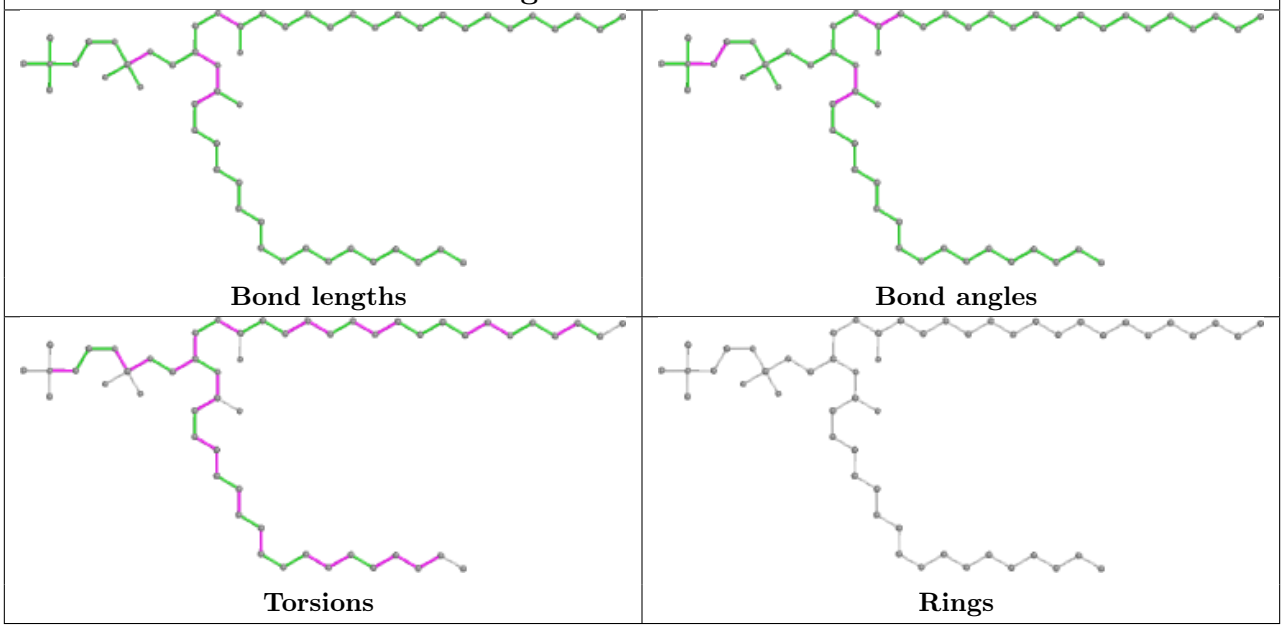


Torsions

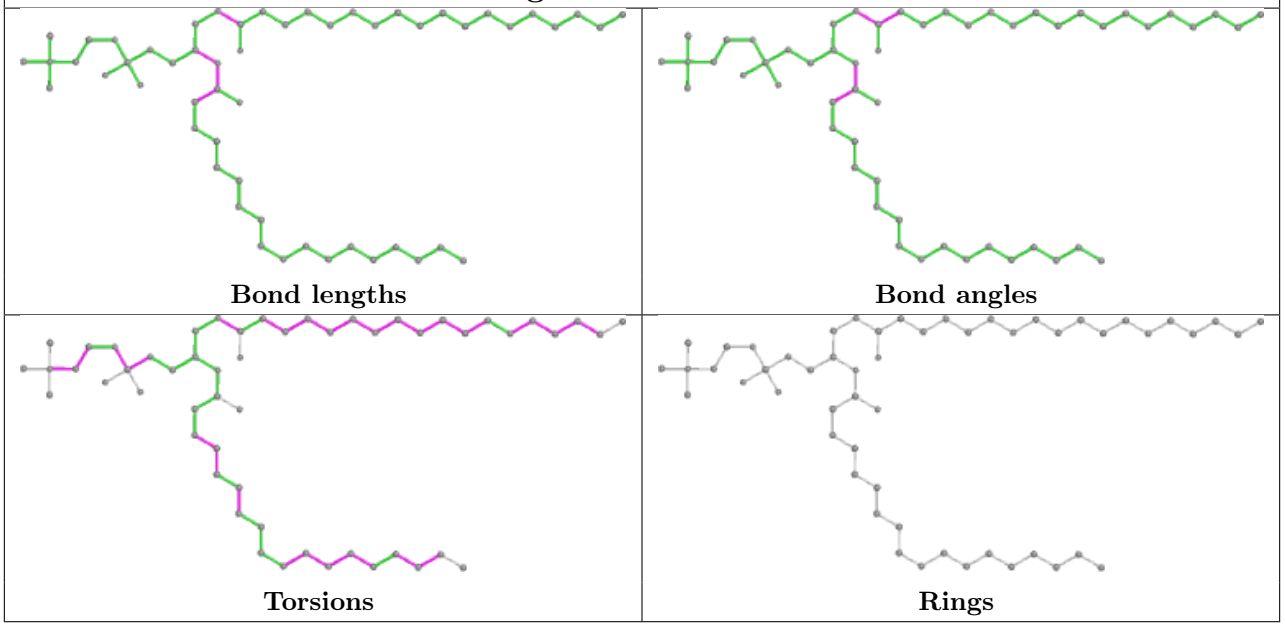


Rings

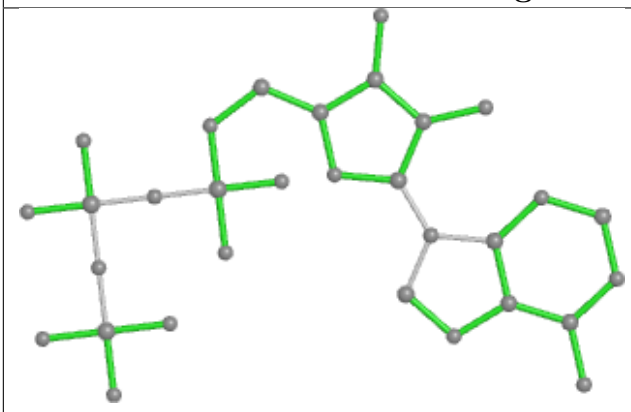
Ligand L9R B 5307



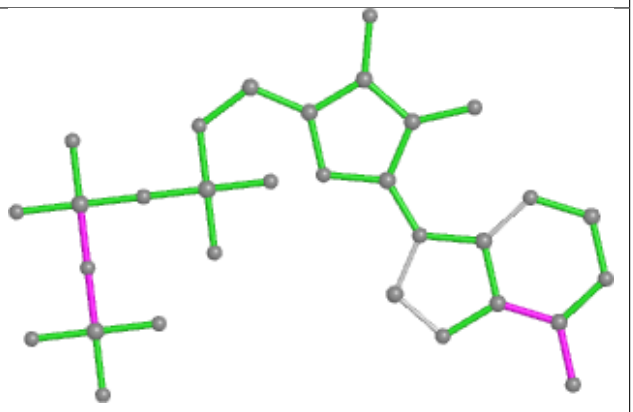
Ligand L9R I 5101



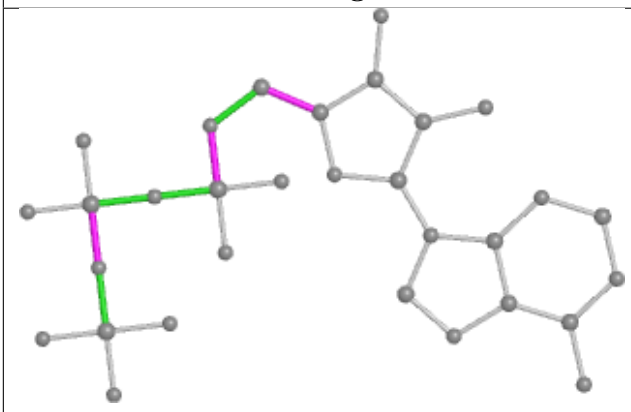
Ligand ATP G 5106



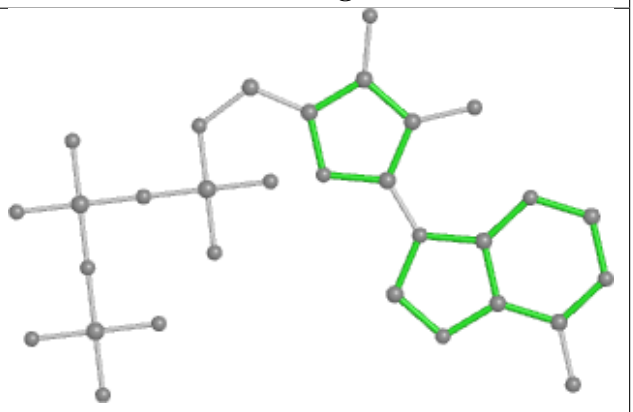
Bond lengths



Bond angles

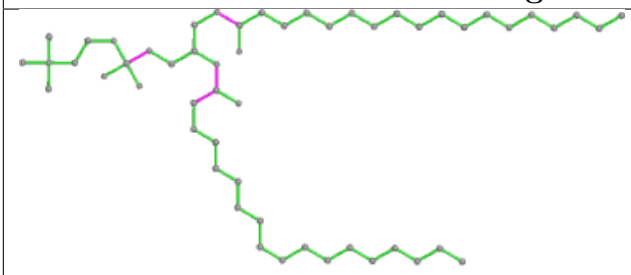


Torsions

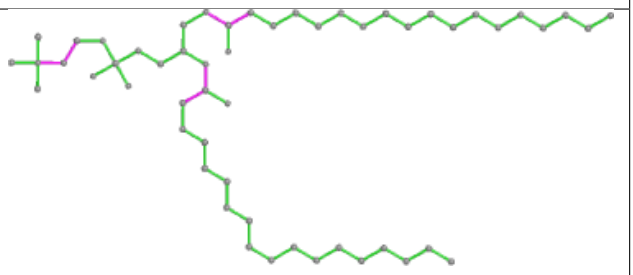


Rings

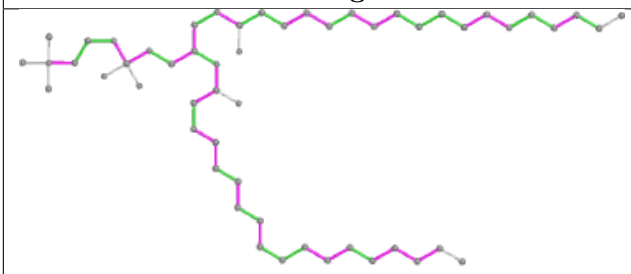
Ligand L9R I 5108



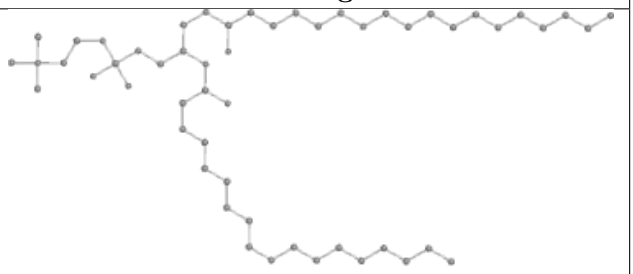
Bond lengths



Bond angles

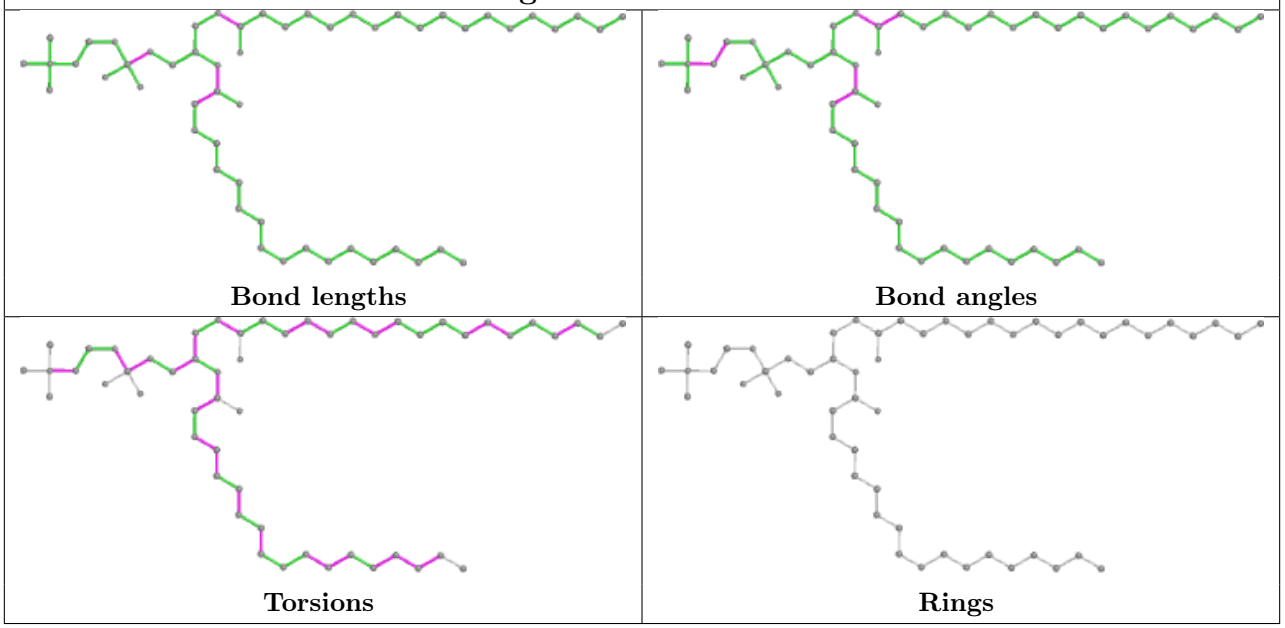


Torsions

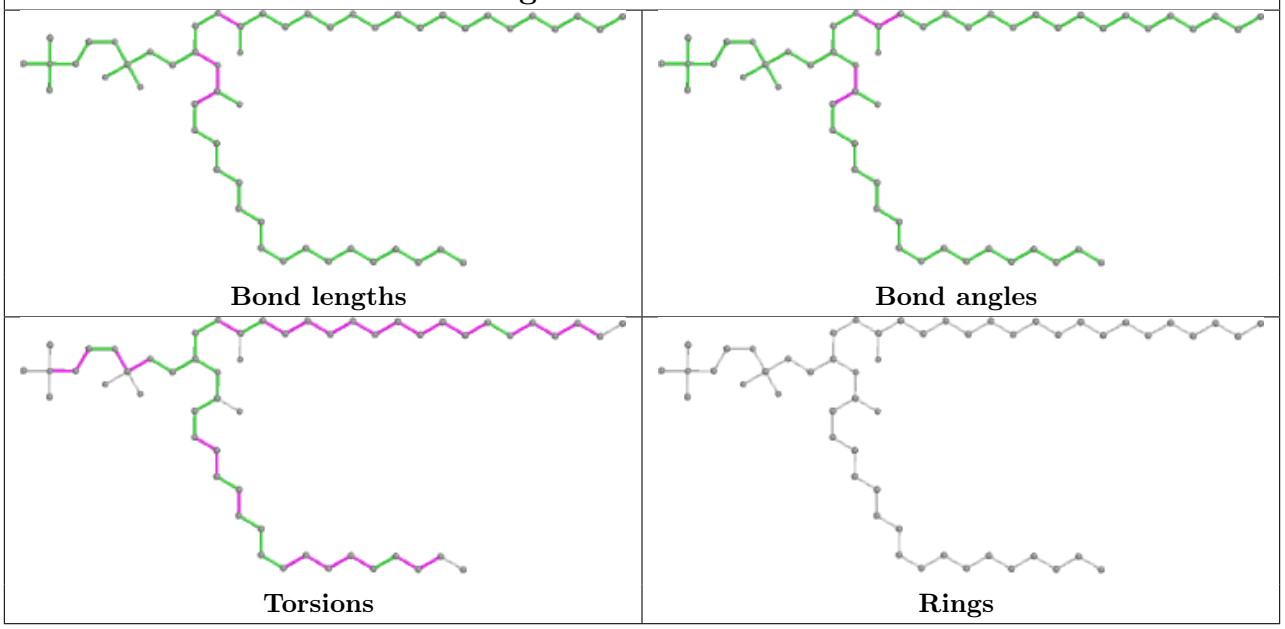


Rings

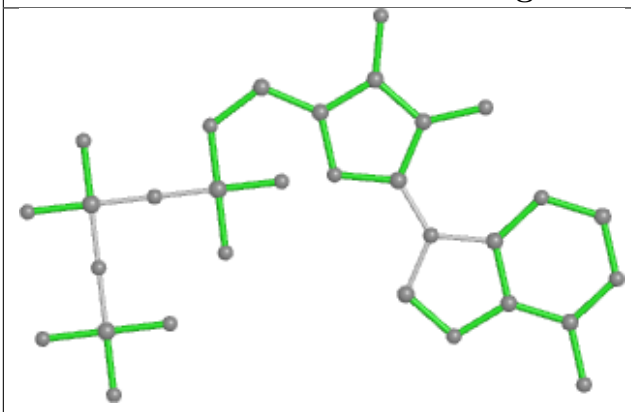
Ligand L9R G 5108



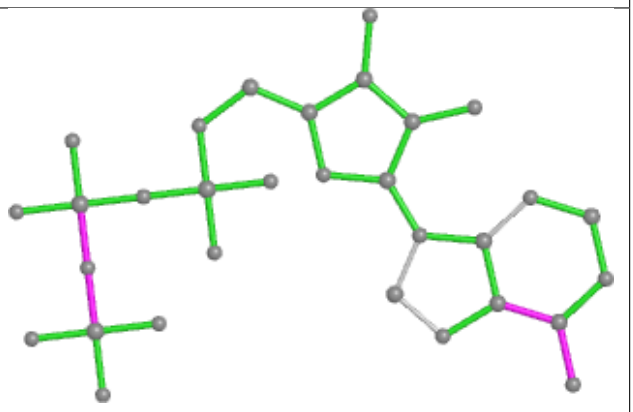
Ligand L9R G 5101



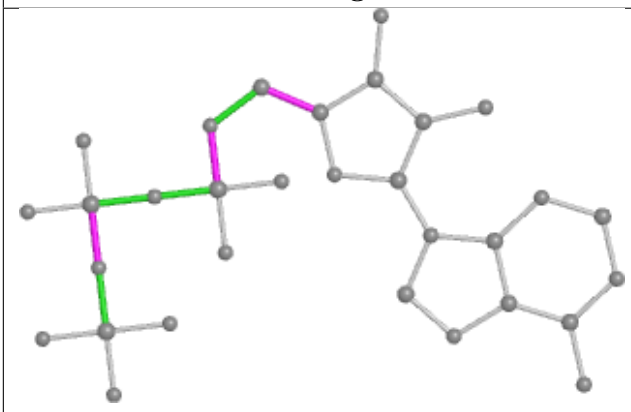
Ligand ATP B 5305



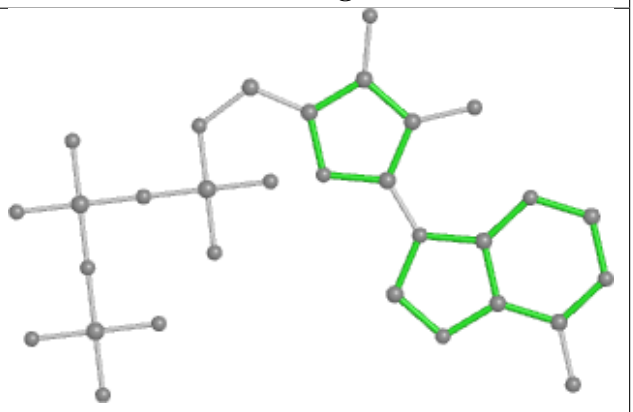
Bond lengths



Bond angles

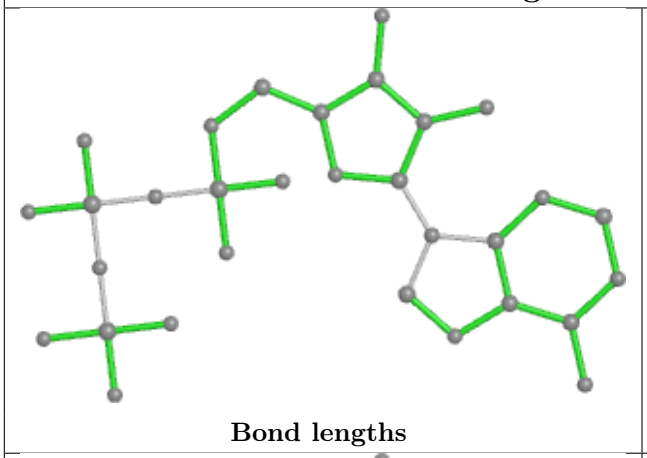


Torsions

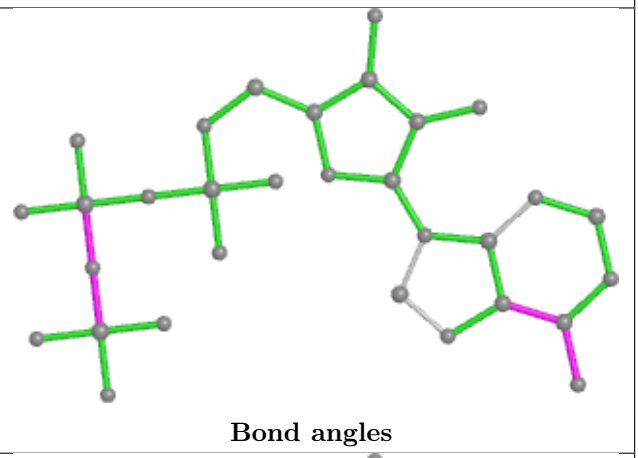


Rings

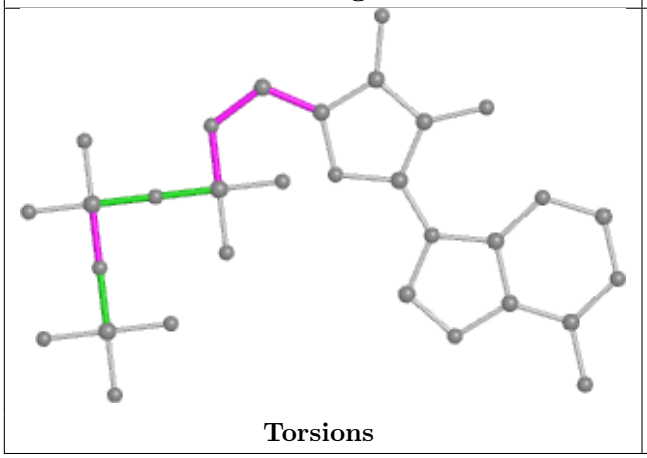
Ligand ATP I 5102



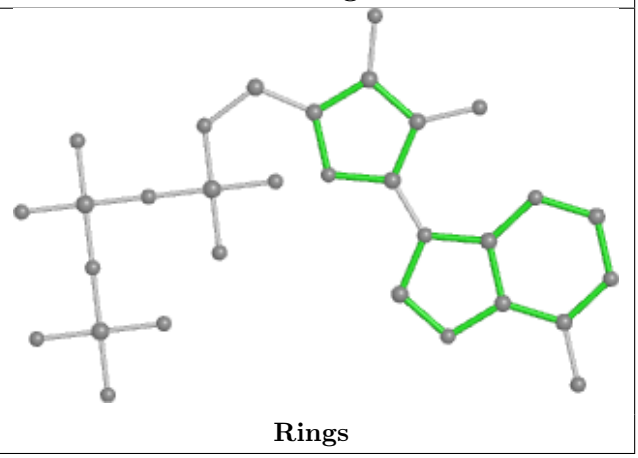
Bond lengths



Bond angles

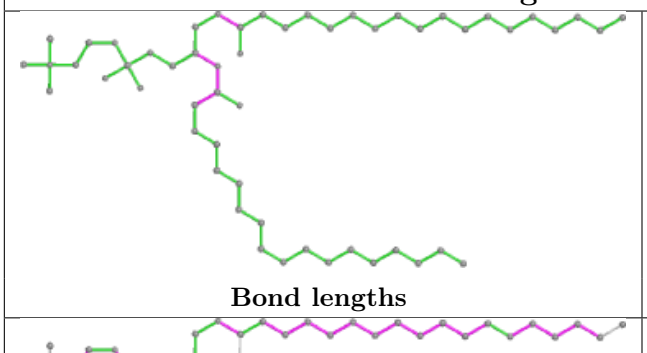


Torsions

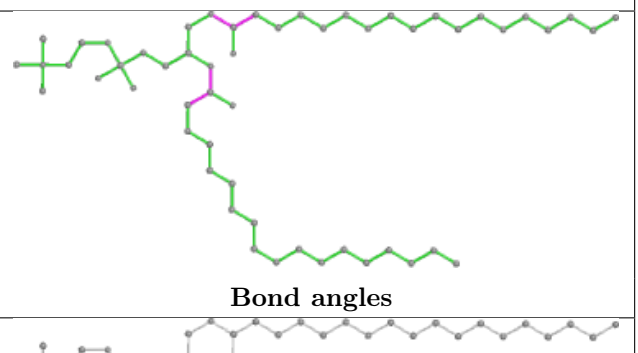


Rings

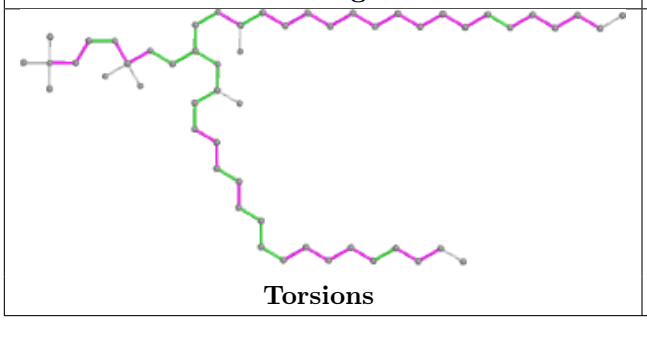
Ligand L9R A 5308



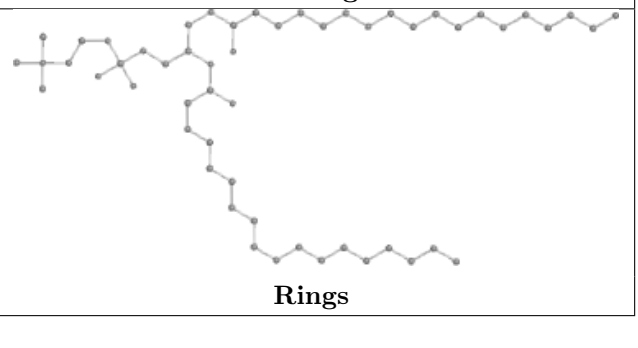
Bond lengths



Bond angles

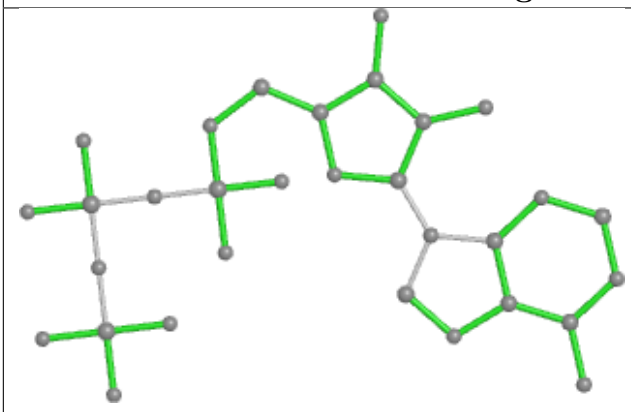


Torsions

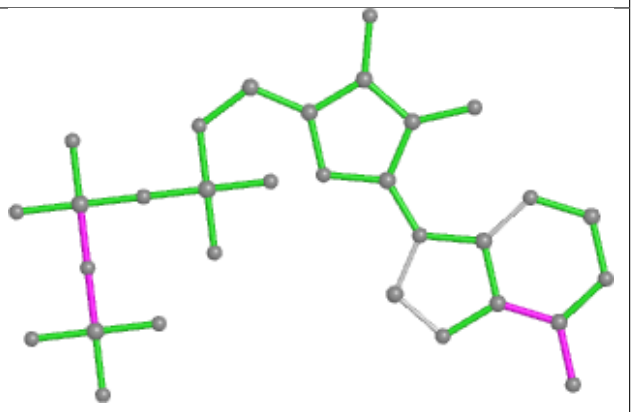


Rings

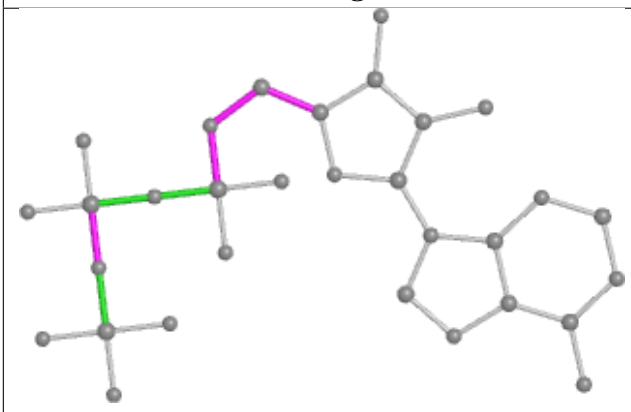
Ligand ATP A 5301



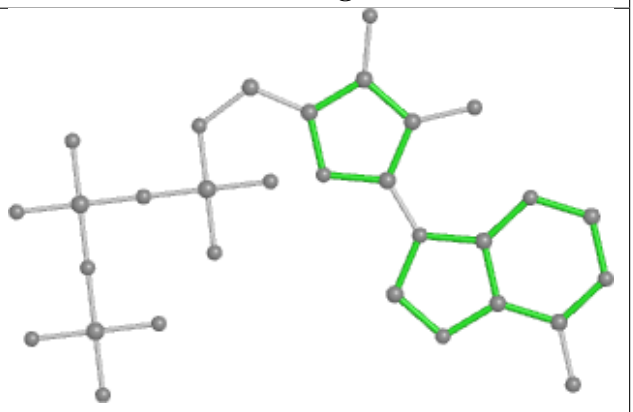
Bond lengths



Bond angles

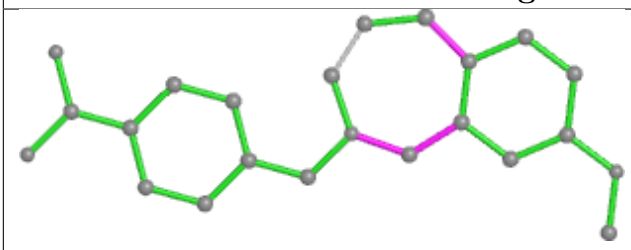


Torsions

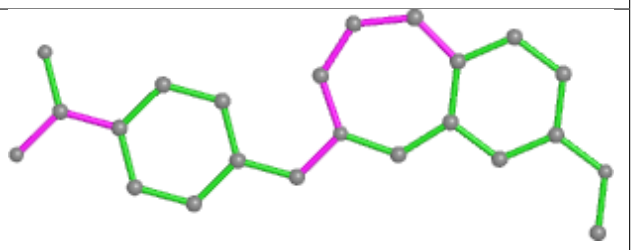


Rings

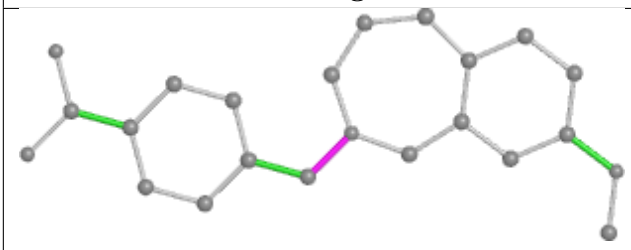
Ligand KVR I 5107



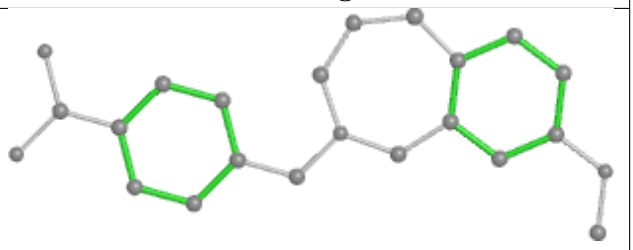
Bond lengths



Bond angles

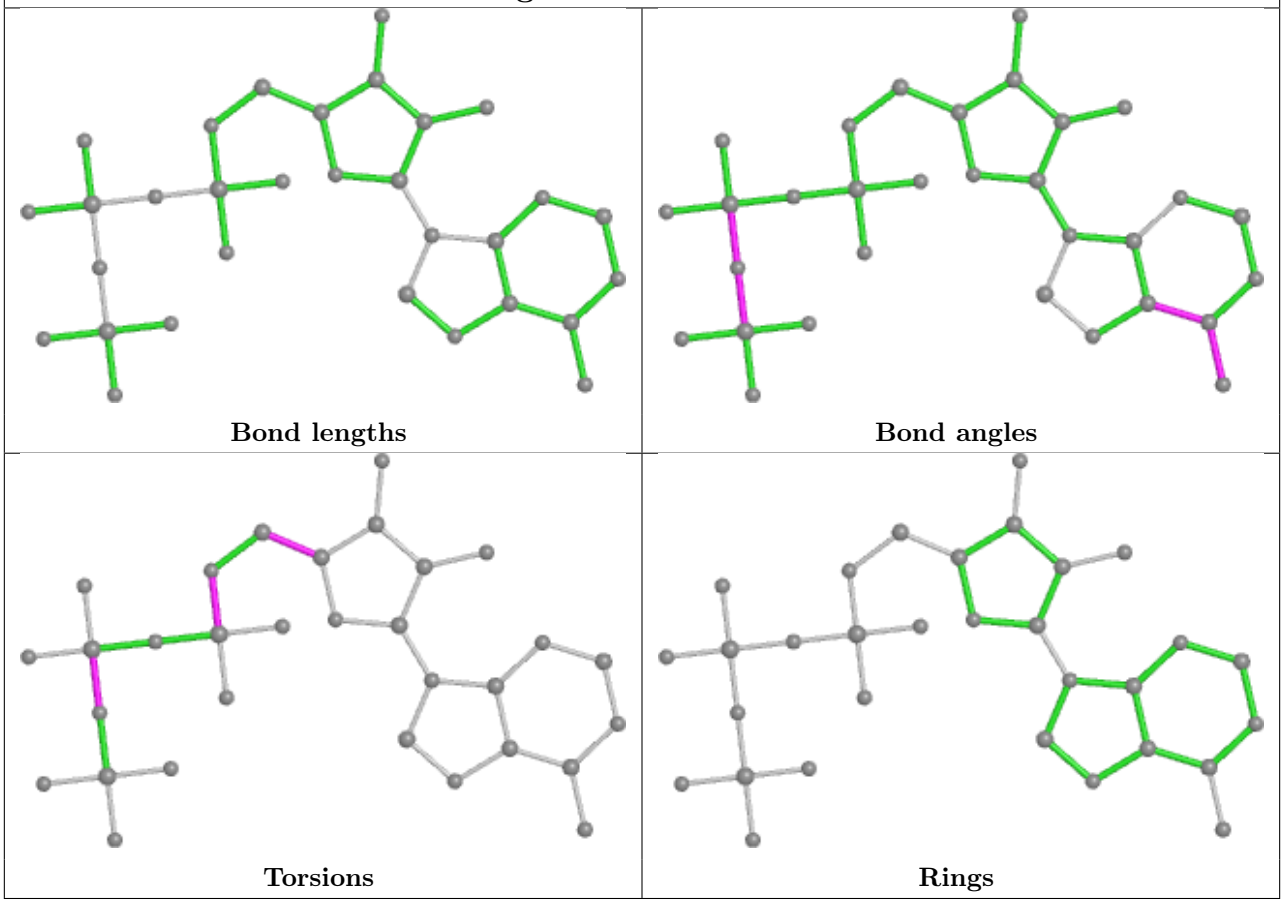


Torsions



Rings

Ligand ATP A 5305



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26205. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.