



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:21 PM BST

PDB ID : 4V94  
Title : Molecular architecture of the eukaryotic chaperonin TRiC/CCT derived by a combination of chemical crosslinking and mass-spectrometry, XL-MS  
Authors : Leitner, A.; Joachimiak, L.A.; Bracher, A.; Walzthoeni, T.; Chen, B.; Monke-meyer, L.; Pechmann, S.; Holmes, S.; Cong, Y.; Ma, B.; Ludtke, S.; Chiu, W.; Hartl, F.U.; Aebersold, R.; Frydman, J.  
Deposited on : 2012-01-11  
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

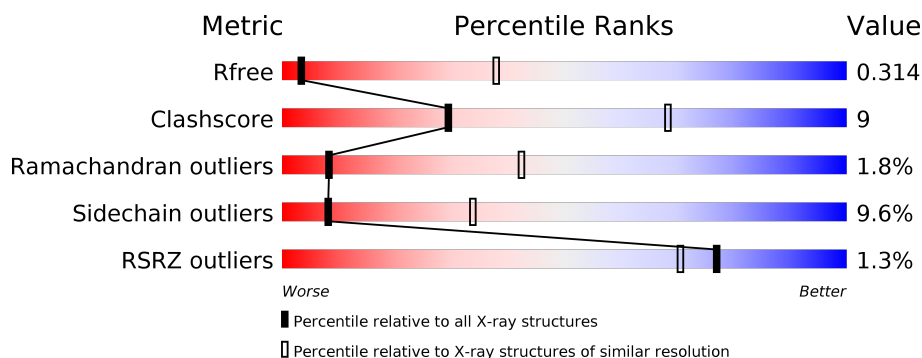
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





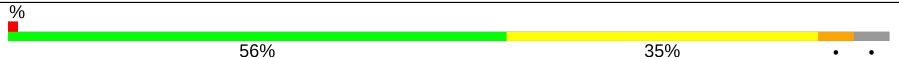
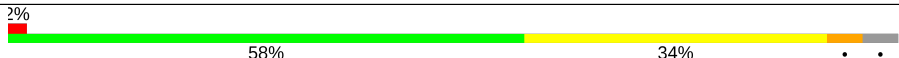
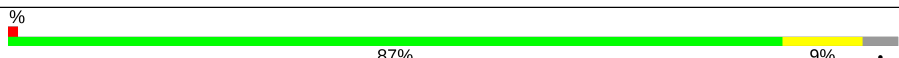
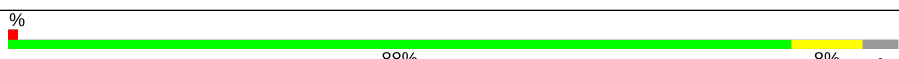
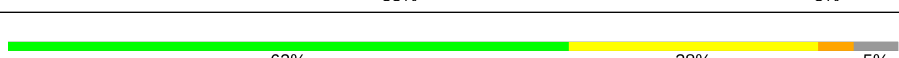
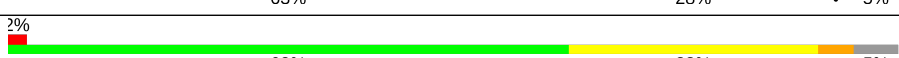
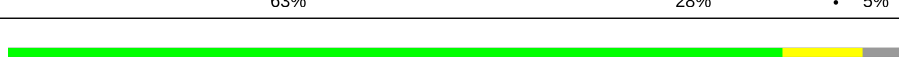

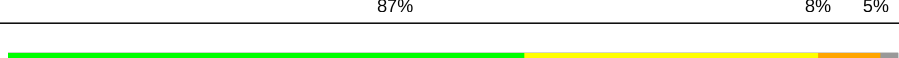



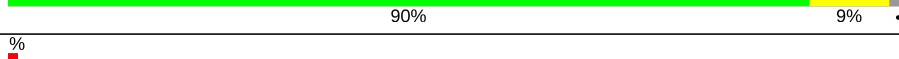


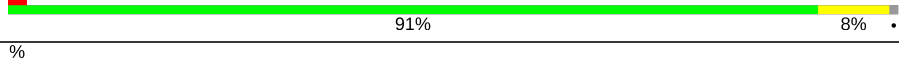
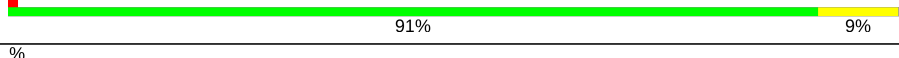
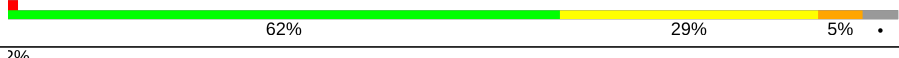

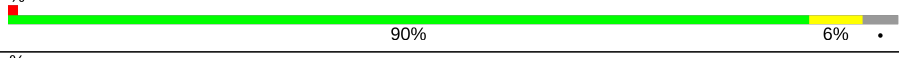
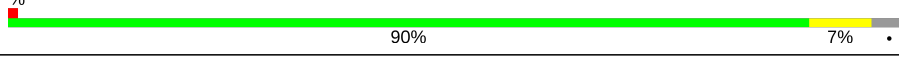


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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

Mol	Chain	Length	Quality of chain
1	F	546	<div> <div>2%</div> <div>63% 31% 5%</div> </div>
1	N	546	<div> <div>3%</div> <div>67% 28%</div> </div>
1	f	546	<div> <div>3%</div> <div>93% 5%</div> </div>
1	n	546	<div> <div>2%</div> <div>93% 5%</div> </div>
2	H	568	<div> <div>60% 27% 8%</div> </div>
2	P	568	<div> <div>2%</div> <div>62% 27% 8%</div> </div>


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Mol	Chain	Length	Quality of chain
2	h	568	
2	p	568	
3	G	550	
3	O	550	
3	g	550	
3	o	550	
4	E	562	
4	M	562	
4	e	562	
4	m	562	
5	B	527	
5	J	527	
5	b	527	
5	j	527	
6	D	528	
6	L	528	
6	d	528	
6	l	528	
7	A	559	
7	I	559	
7	a	559	
7	i	559	
8	C	590	
8	K	590	
8	c	590	

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Mol	Chain	Length	Quality of chain
8	k	590	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	BEF	B	603	-	-	X	-
11	BEF	C	1103	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 120080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	N	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	f	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	n	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			

- Molecule 2 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	P	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	h	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	p	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			

- Molecule 3 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	O	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	g	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	o	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	M	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	e	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	m	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			

- Molecule 5 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	J	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	b	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	j	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			

- Molecule 6 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	L	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	d	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	l	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
L	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
d	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
l	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078

- Molecule 7 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	I	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	a	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	i	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			

- Molecule 8 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	K	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	c	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	k	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1001	GLY	-	SEE REMARK 999	UNP P39077
C	1002	SER	-	SEE REMARK 999	UNP P39077
C	1003	GLY	-	SEE REMARK 999	UNP P39077
C	1004	SER	-	SEE REMARK 999	UNP P39077
C	1005	GLY	-	SEE REMARK 999	UNP P39077
C	1006	TRP	-	SEE REMARK 999	UNP P39077
C	1007	SER	-	SEE REMARK 999	UNP P39077
C	1008	HIS	-	SEE REMARK 999	UNP P39077
C	1009	PRO	-	SEE REMARK 999	UNP P39077
C	1010	GLN	-	SEE REMARK 999	UNP P39077
C	1011	PHE	-	SEE REMARK 999	UNP P39077
C	1012	GLU	-	SEE REMARK 999	UNP P39077
C	1013	LYS	-	SEE REMARK 999	UNP P39077
C	1014	GLY	-	SEE REMARK 999	UNP P39077
C	1015	SER	-	SEE REMARK 999	UNP P39077
C	1016	GLY	-	SEE REMARK 999	UNP P39077
C	1017	LYS	-	SEE REMARK 999	UNP P39077
C	1018	ARG	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1019	ARG	-	SEE REMARK 999	UNP P39077
C	1020	TRP	-	SEE REMARK 999	UNP P39077
C	1021	LYS	-	SEE REMARK 999	UNP P39077
C	1022	LYS	-	SEE REMARK 999	UNP P39077
C	1023	ASN	-	SEE REMARK 999	UNP P39077
C	1024	PHE	-	SEE REMARK 999	UNP P39077
C	1025	ILE	-	SEE REMARK 999	UNP P39077
C	1026	ALA	-	SEE REMARK 999	UNP P39077
C	1027	VAL	-	SEE REMARK 999	UNP P39077
C	1028	SER	-	SEE REMARK 999	UNP P39077
C	1029	ALA	-	SEE REMARK 999	UNP P39077
C	1030	ALA	-	SEE REMARK 999	UNP P39077
C	1031	ASN	-	SEE REMARK 999	UNP P39077
C	1032	ARG	-	SEE REMARK 999	UNP P39077
C	1033	PHE	-	SEE REMARK 999	UNP P39077
C	1034	LYS	-	SEE REMARK 999	UNP P39077
C	1035	LYS	-	SEE REMARK 999	UNP P39077
C	1036	ILE	-	SEE REMARK 999	UNP P39077
C	1037	SER	-	SEE REMARK 999	UNP P39077
C	1038	SER	-	SEE REMARK 999	UNP P39077
C	1039	SER	-	SEE REMARK 999	UNP P39077
C	1040	GLY	-	SEE REMARK 999	UNP P39077
C	1041	ALA	-	SEE REMARK 999	UNP P39077
C	1042	LEU	-	SEE REMARK 999	UNP P39077
C	1043	GLY	-	SEE REMARK 999	UNP P39077
C	1044	SER	-	SEE REMARK 999	UNP P39077
C	1045	GLY	-	SEE REMARK 999	UNP P39077
C	1046	HIS	-	SEE REMARK 999	UNP P39077
C	1047	HIS	-	SEE REMARK 999	UNP P39077
C	1048	HIS	-	SEE REMARK 999	UNP P39077
C	1049	HIS	-	SEE REMARK 999	UNP P39077
C	1050	HIS	-	SEE REMARK 999	UNP P39077
C	1051	HIS	-	SEE REMARK 999	UNP P39077
C	1052	HIS	-	SEE REMARK 999	UNP P39077
C	1053	HIS	-	SEE REMARK 999	UNP P39077
C	1054	GLY	-	SEE REMARK 999	UNP P39077
C	1055	SER	-	SEE REMARK 999	UNP P39077
C	1056	GLY	-	SEE REMARK 999	UNP P39077
K	1001	GLY	-	SEE REMARK 999	UNP P39077
K	1002	SER	-	SEE REMARK 999	UNP P39077
K	1003	GLY	-	SEE REMARK 999	UNP P39077
K	1004	SER	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1005	GLY	-	SEE REMARK 999	UNP P39077
K	1006	TRP	-	SEE REMARK 999	UNP P39077
K	1007	SER	-	SEE REMARK 999	UNP P39077
K	1008	HIS	-	SEE REMARK 999	UNP P39077
K	1009	PRO	-	SEE REMARK 999	UNP P39077
K	1010	GLN	-	SEE REMARK 999	UNP P39077
K	1011	PHE	-	SEE REMARK 999	UNP P39077
K	1012	GLU	-	SEE REMARK 999	UNP P39077
K	1013	LYS	-	SEE REMARK 999	UNP P39077
K	1014	GLY	-	SEE REMARK 999	UNP P39077
K	1015	SER	-	SEE REMARK 999	UNP P39077
K	1016	GLY	-	SEE REMARK 999	UNP P39077
K	1017	LYS	-	SEE REMARK 999	UNP P39077
K	1018	ARG	-	SEE REMARK 999	UNP P39077
K	1019	ARG	-	SEE REMARK 999	UNP P39077
K	1020	TRP	-	SEE REMARK 999	UNP P39077
K	1021	LYS	-	SEE REMARK 999	UNP P39077
K	1022	LYS	-	SEE REMARK 999	UNP P39077
K	1023	ASN	-	SEE REMARK 999	UNP P39077
K	1024	PHE	-	SEE REMARK 999	UNP P39077
K	1025	ILE	-	SEE REMARK 999	UNP P39077
K	1026	ALA	-	SEE REMARK 999	UNP P39077
K	1027	VAL	-	SEE REMARK 999	UNP P39077
K	1028	SER	-	SEE REMARK 999	UNP P39077
K	1029	ALA	-	SEE REMARK 999	UNP P39077
K	1030	ALA	-	SEE REMARK 999	UNP P39077
K	1031	ASN	-	SEE REMARK 999	UNP P39077
K	1032	ARG	-	SEE REMARK 999	UNP P39077
K	1033	PHE	-	SEE REMARK 999	UNP P39077
K	1034	LYS	-	SEE REMARK 999	UNP P39077
K	1035	LYS	-	SEE REMARK 999	UNP P39077
K	1036	ILE	-	SEE REMARK 999	UNP P39077
K	1037	SER	-	SEE REMARK 999	UNP P39077
K	1038	SER	-	SEE REMARK 999	UNP P39077
K	1039	SER	-	SEE REMARK 999	UNP P39077
K	1040	GLY	-	SEE REMARK 999	UNP P39077
K	1041	ALA	-	SEE REMARK 999	UNP P39077
K	1042	LEU	-	SEE REMARK 999	UNP P39077
K	1043	GLY	-	SEE REMARK 999	UNP P39077
K	1044	SER	-	SEE REMARK 999	UNP P39077
K	1045	GLY	-	SEE REMARK 999	UNP P39077
K	1046	HIS	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1047	HIS	-	SEE REMARK 999	UNP P39077
K	1048	HIS	-	SEE REMARK 999	UNP P39077
K	1049	HIS	-	SEE REMARK 999	UNP P39077
K	1050	HIS	-	SEE REMARK 999	UNP P39077
K	1051	HIS	-	SEE REMARK 999	UNP P39077
K	1052	HIS	-	SEE REMARK 999	UNP P39077
K	1053	HIS	-	SEE REMARK 999	UNP P39077
K	1054	GLY	-	SEE REMARK 999	UNP P39077
K	1055	SER	-	SEE REMARK 999	UNP P39077
K	1056	GLY	-	SEE REMARK 999	UNP P39077
c	1001	GLY	-	SEE REMARK 999	UNP P39077
c	1002	SER	-	SEE REMARK 999	UNP P39077
c	1003	GLY	-	SEE REMARK 999	UNP P39077
c	1004	SER	-	SEE REMARK 999	UNP P39077
c	1005	GLY	-	SEE REMARK 999	UNP P39077
c	1006	TRP	-	SEE REMARK 999	UNP P39077
c	1007	SER	-	SEE REMARK 999	UNP P39077
c	1008	HIS	-	SEE REMARK 999	UNP P39077
c	1009	PRO	-	SEE REMARK 999	UNP P39077
c	1010	GLN	-	SEE REMARK 999	UNP P39077
c	1011	PHE	-	SEE REMARK 999	UNP P39077
c	1012	GLU	-	SEE REMARK 999	UNP P39077
c	1013	LYS	-	SEE REMARK 999	UNP P39077
c	1014	GLY	-	SEE REMARK 999	UNP P39077
c	1015	SER	-	SEE REMARK 999	UNP P39077
c	1016	GLY	-	SEE REMARK 999	UNP P39077
c	1017	LYS	-	SEE REMARK 999	UNP P39077
c	1018	ARG	-	SEE REMARK 999	UNP P39077
c	1019	ARG	-	SEE REMARK 999	UNP P39077
c	1020	TRP	-	SEE REMARK 999	UNP P39077
c	1021	LYS	-	SEE REMARK 999	UNP P39077
c	1022	LYS	-	SEE REMARK 999	UNP P39077
c	1023	ASN	-	SEE REMARK 999	UNP P39077
c	1024	PHE	-	SEE REMARK 999	UNP P39077
c	1025	ILE	-	SEE REMARK 999	UNP P39077
c	1026	ALA	-	SEE REMARK 999	UNP P39077
c	1027	VAL	-	SEE REMARK 999	UNP P39077
c	1028	SER	-	SEE REMARK 999	UNP P39077
c	1029	ALA	-	SEE REMARK 999	UNP P39077
c	1030	ALA	-	SEE REMARK 999	UNP P39077
c	1031	ASN	-	SEE REMARK 999	UNP P39077
c	1032	ARG	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
c	1033	PHE	-	SEE REMARK 999	UNP P39077
c	1034	LYS	-	SEE REMARK 999	UNP P39077
c	1035	LYS	-	SEE REMARK 999	UNP P39077
c	1036	ILE	-	SEE REMARK 999	UNP P39077
c	1037	SER	-	SEE REMARK 999	UNP P39077
c	1038	SER	-	SEE REMARK 999	UNP P39077
c	1039	SER	-	SEE REMARK 999	UNP P39077
c	1040	GLY	-	SEE REMARK 999	UNP P39077
c	1041	ALA	-	SEE REMARK 999	UNP P39077
c	1042	LEU	-	SEE REMARK 999	UNP P39077
c	1043	GLY	-	SEE REMARK 999	UNP P39077
c	1044	SER	-	SEE REMARK 999	UNP P39077
c	1045	GLY	-	SEE REMARK 999	UNP P39077
c	1046	HIS	-	SEE REMARK 999	UNP P39077
c	1047	HIS	-	SEE REMARK 999	UNP P39077
c	1048	HIS	-	SEE REMARK 999	UNP P39077
c	1049	HIS	-	SEE REMARK 999	UNP P39077
c	1050	HIS	-	SEE REMARK 999	UNP P39077
c	1051	HIS	-	SEE REMARK 999	UNP P39077
c	1052	HIS	-	SEE REMARK 999	UNP P39077
c	1053	HIS	-	SEE REMARK 999	UNP P39077
c	1054	GLY	-	SEE REMARK 999	UNP P39077
c	1055	SER	-	SEE REMARK 999	UNP P39077
c	1056	GLY	-	SEE REMARK 999	UNP P39077
k	1001	GLY	-	SEE REMARK 999	UNP P39077
k	1002	SER	-	SEE REMARK 999	UNP P39077
k	1003	GLY	-	SEE REMARK 999	UNP P39077
k	1004	SER	-	SEE REMARK 999	UNP P39077
k	1005	GLY	-	SEE REMARK 999	UNP P39077
k	1006	TRP	-	SEE REMARK 999	UNP P39077
k	1007	SER	-	SEE REMARK 999	UNP P39077
k	1008	HIS	-	SEE REMARK 999	UNP P39077
k	1009	PRO	-	SEE REMARK 999	UNP P39077
k	1010	GLN	-	SEE REMARK 999	UNP P39077
k	1011	PHE	-	SEE REMARK 999	UNP P39077
k	1012	GLU	-	SEE REMARK 999	UNP P39077
k	1013	LYS	-	SEE REMARK 999	UNP P39077
k	1014	GLY	-	SEE REMARK 999	UNP P39077
k	1015	SER	-	SEE REMARK 999	UNP P39077
k	1016	GLY	-	SEE REMARK 999	UNP P39077
k	1017	LYS	-	SEE REMARK 999	UNP P39077
k	1018	ARG	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	1019	ARG	-	SEE REMARK 999	UNP P39077
k	1020	TRP	-	SEE REMARK 999	UNP P39077
k	1021	LYS	-	SEE REMARK 999	UNP P39077
k	1022	LYS	-	SEE REMARK 999	UNP P39077
k	1023	ASN	-	SEE REMARK 999	UNP P39077
k	1024	PHE	-	SEE REMARK 999	UNP P39077
k	1025	ILE	-	SEE REMARK 999	UNP P39077
k	1026	ALA	-	SEE REMARK 999	UNP P39077
k	1027	VAL	-	SEE REMARK 999	UNP P39077
k	1028	SER	-	SEE REMARK 999	UNP P39077
k	1029	ALA	-	SEE REMARK 999	UNP P39077
k	1030	ALA	-	SEE REMARK 999	UNP P39077
k	1031	ASN	-	SEE REMARK 999	UNP P39077
k	1032	ARG	-	SEE REMARK 999	UNP P39077
k	1033	PHE	-	SEE REMARK 999	UNP P39077
k	1034	LYS	-	SEE REMARK 999	UNP P39077
k	1035	LYS	-	SEE REMARK 999	UNP P39077
k	1036	ILE	-	SEE REMARK 999	UNP P39077
k	1037	SER	-	SEE REMARK 999	UNP P39077
k	1038	SER	-	SEE REMARK 999	UNP P39077
k	1039	SER	-	SEE REMARK 999	UNP P39077
k	1040	GLY	-	SEE REMARK 999	UNP P39077
k	1041	ALA	-	SEE REMARK 999	UNP P39077
k	1042	LEU	-	SEE REMARK 999	UNP P39077
k	1043	GLY	-	SEE REMARK 999	UNP P39077
k	1044	SER	-	SEE REMARK 999	UNP P39077
k	1045	GLY	-	SEE REMARK 999	UNP P39077
k	1046	HIS	-	SEE REMARK 999	UNP P39077
k	1047	HIS	-	SEE REMARK 999	UNP P39077
k	1048	HIS	-	SEE REMARK 999	UNP P39077
k	1049	HIS	-	SEE REMARK 999	UNP P39077
k	1050	HIS	-	SEE REMARK 999	UNP P39077
k	1051	HIS	-	SEE REMARK 999	UNP P39077
k	1052	HIS	-	SEE REMARK 999	UNP P39077
k	1053	HIS	-	SEE REMARK 999	UNP P39077
k	1054	GLY	-	SEE REMARK 999	UNP P39077
k	1055	SER	-	SEE REMARK 999	UNP P39077
k	1056	GLY	-	SEE REMARK 999	UNP P39077

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

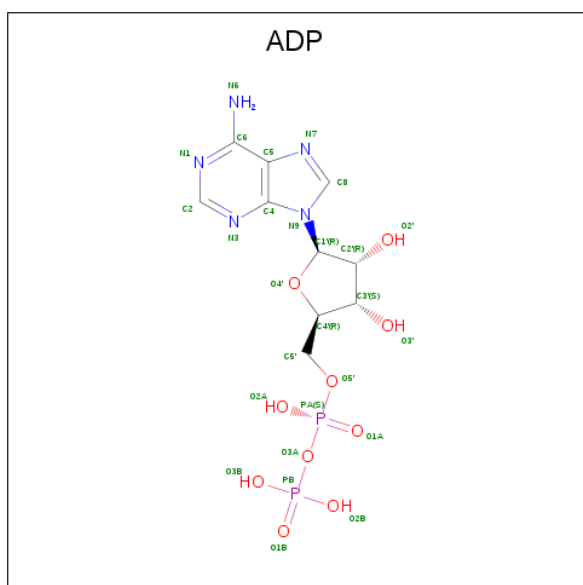
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	P	1	Total Mg 1 1	0	0
9	g	1	Total Mg 1 1	0	0
9	K	1	Total Mg 1 1	0	0
9	h	1	Total Mg 1 1	0	0
9	B	1	Total Mg 1 1	0	0
9	c	1	Total Mg 1 1	0	0
9	N	1	Total Mg 1 1	0	0
9	o	1	Total Mg 1 1	0	0
9	f	1	Total Mg 1 1	0	0
9	p	1	Total Mg 1 1	0	0
9	J	1	Total Mg 1 1	0	0
9	k	1	Total Mg 1 1	0	0
9	E	1	Total Mg 1 1	0	0
9	b	1	Total Mg 1 1	0	0
9	A	1	Total Mg 1 1	0	0
9	n	1	Total Mg 1 1	0	0
9	M	1	Total Mg 1 1	0	0
9	j	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	e	1	Total Mg 1 1	0	0
9	I	1	Total Mg 1 1	0	0
9	a	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	1	Total	Mg	0	0
			1	1		
9	m	1	Total	Mg	0	0
			1	1		
9	G	1	Total	Mg	0	0
			1	1		
9	d	1	Total	Mg	0	0
			1	1		
9	H	1	Total	Mg	0	0
			1	1		
9	i	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		
9	O	1	Total	Mg	0	0
			1	1		
9	l	1	Total	Mg	0	0
			1	1		
9	F	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	F	1	Total	C	N	O P	0	0
			27	10	5	10 2		

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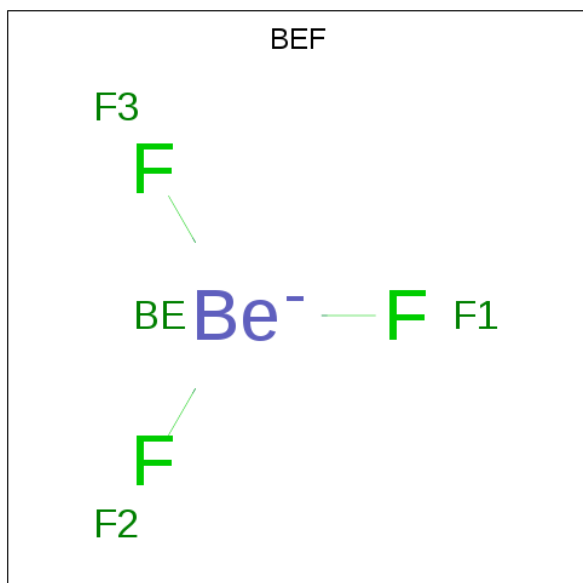
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	N	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	P	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	O	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	f	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	h	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	g	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	e	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	b	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	d	1	Total 27	C 10	N 5	O 10	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	a	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	n	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	p	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	o	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	m	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	j	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	l	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	i	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	k	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total	Be	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total 4	Be 1	F 3	0	0
11	G	1	Total 4	Be 1	F 3	0	0
11	E	1	Total 4	Be 1	F 3	0	0
11	B	1	Total 4	Be 1	F 3	0	0
11	D	1	Total 4	Be 1	F 3	0	0
11	A	1	Total 4	Be 1	F 3	0	0
11	C	1	Total 4	Be 1	F 3	0	0
11	N	1	Total 4	Be 1	F 3	0	0
11	P	1	Total 4	Be 1	F 3	0	0
11	O	1	Total 4	Be 1	F 3	0	0
11	M	1	Total 4	Be 1	F 3	0	0
11	J	1	Total 4	Be 1	F 3	0	0
11	L	1	Total 4	Be 1	F 3	0	0
11	I	1	Total 4	Be 1	F 3	0	0
11	K	1	Total 4	Be 1	F 3	0	0
11	f	1	Total 4	Be 1	F 3	0	0
11	h	1	Total 4	Be 1	F 3	0	0
11	g	1	Total 4	Be 1	F 3	0	0
11	e	1	Total 4	Be 1	F 3	0	0
11	b	1	Total 4	Be 1	F 3	0	0
11	d	1	Total 4	Be 1	F 3	0	0

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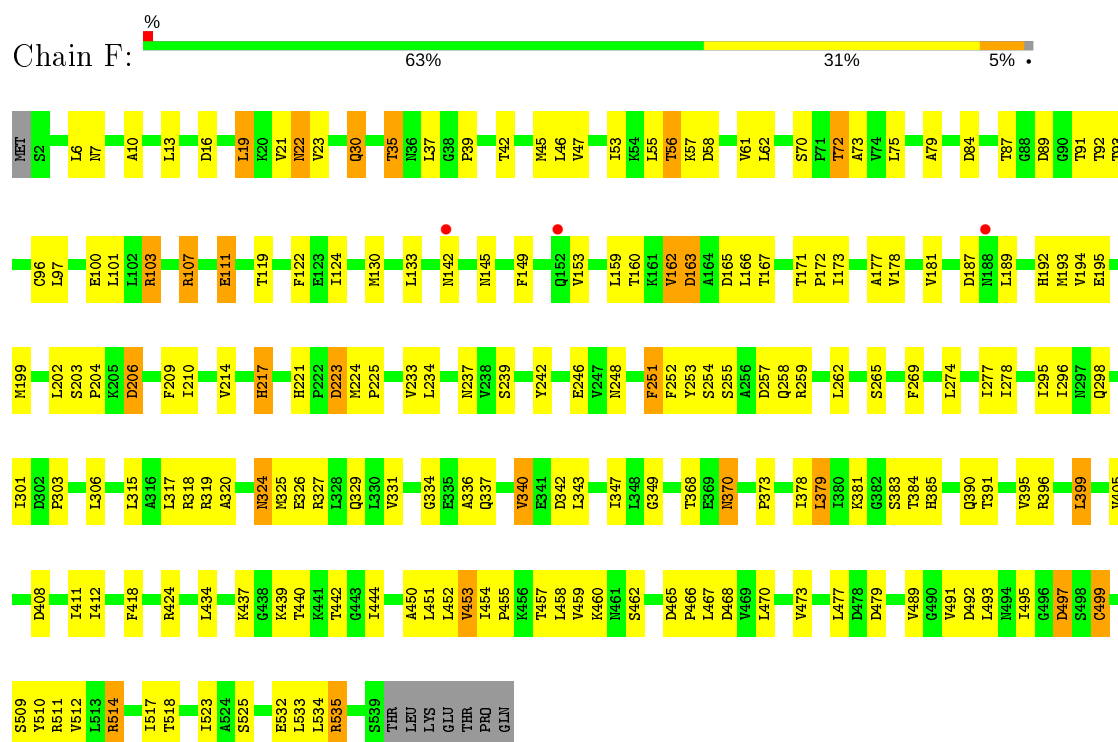
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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11	c	1	Total 4	Be 1	F 3	0	0
11	n	1	Total 4	Be 1	F 3	0	0
11	p	1	Total 4	Be 1	F 3	0	0
11	o	1	Total 4	Be 1	F 3	0	0
11	m	1	Total 4	Be 1	F 3	0	0
11	j	1	Total 4	Be 1	F 3	0	0
11	l	1	Total 4	Be 1	F 3	0	0
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11	k	1	Total 4	Be 1	F 3	0	0

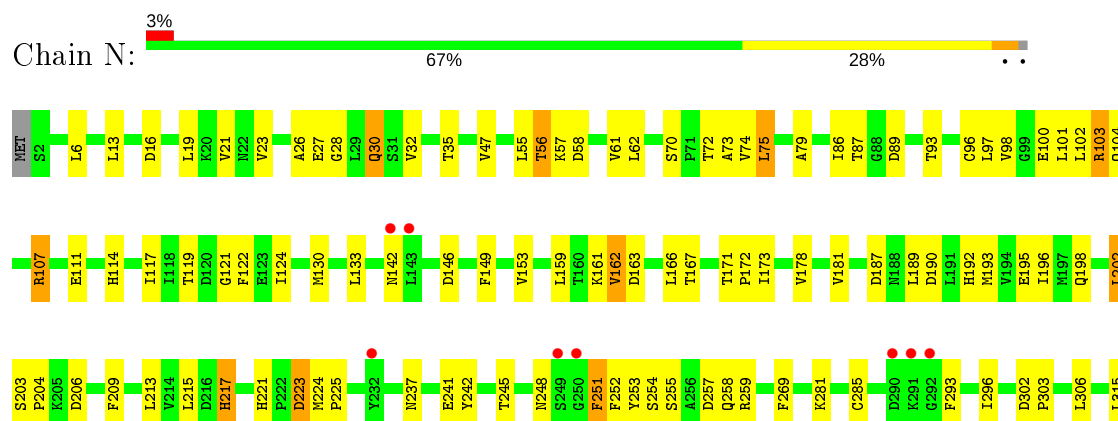
### 3 Residue-property plots [i](#)

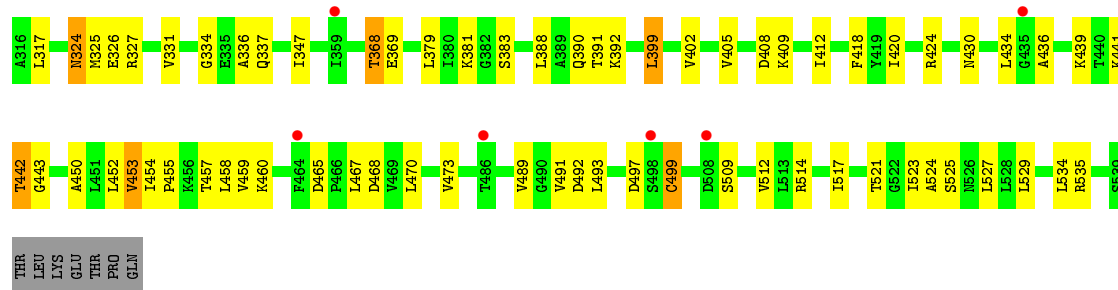
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: T-complex protein 1 subunit zeta

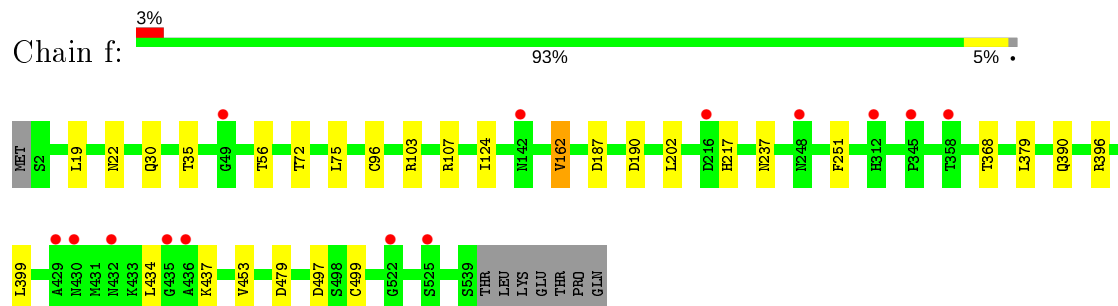


- Molecule 1: T-complex protein 1 subunit zeta

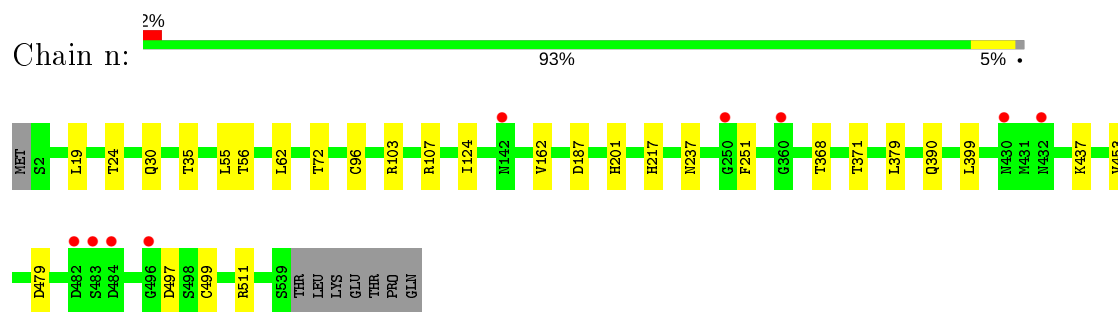




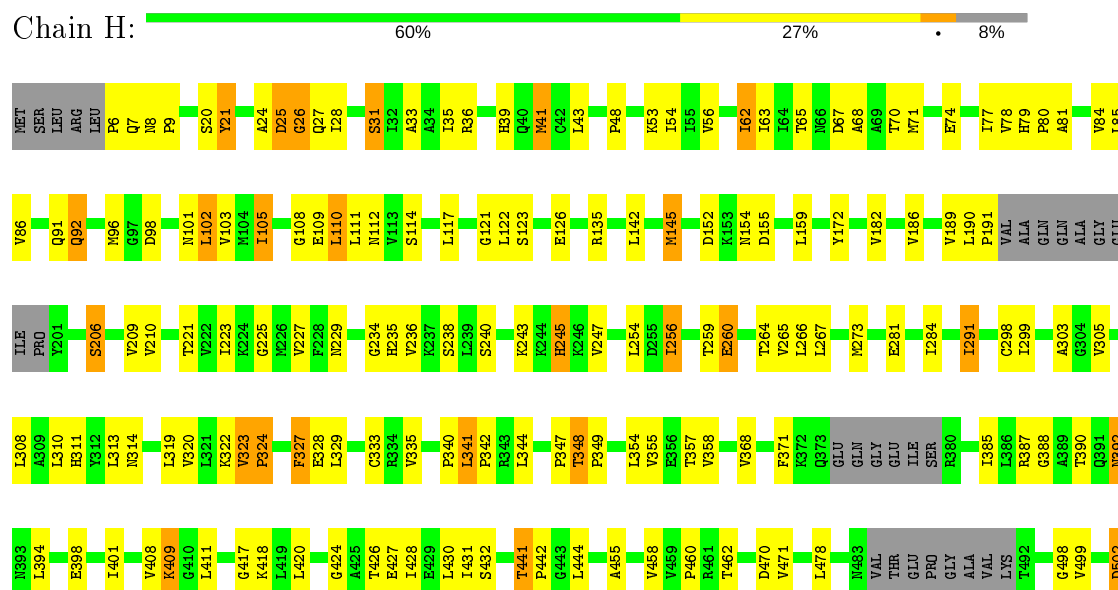
- Molecule 1: T-complex protein 1 subunit zeta



- Molecule 1: T-complex protein 1 subunit zeta

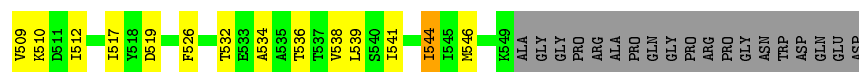
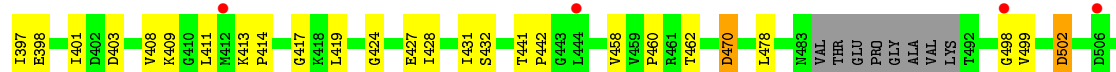
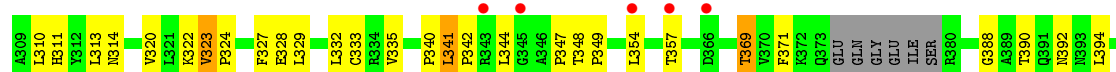
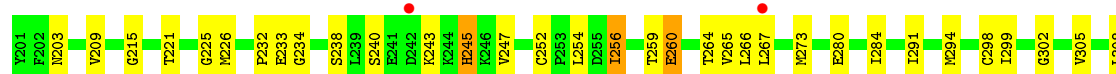
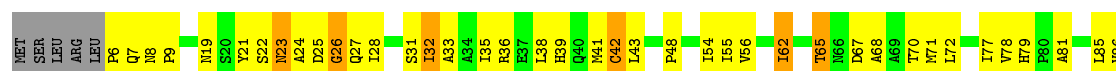


- Molecule 2: T-complex protein 1 subunit theta

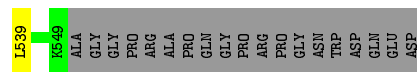
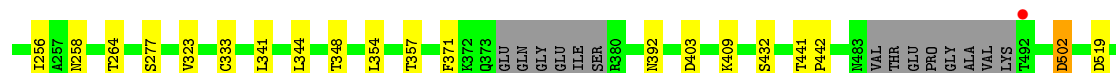
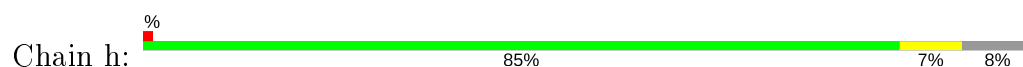




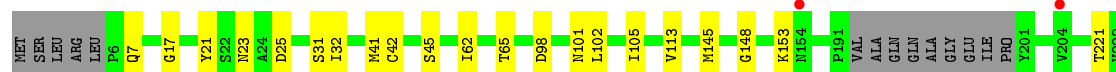
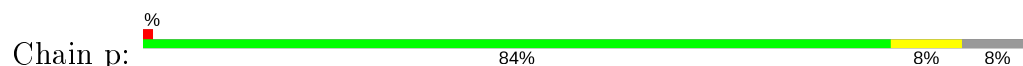
• Molecule 2: T-complex protein 1 subunit theta

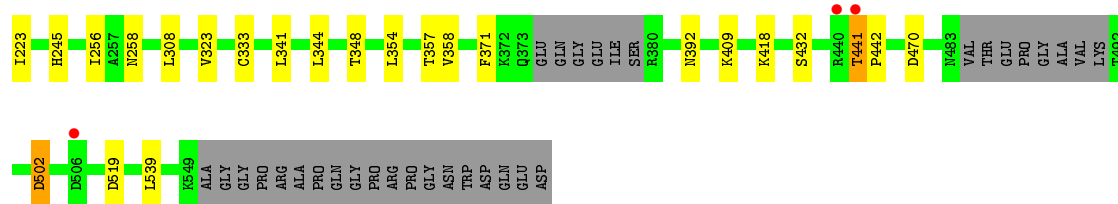


• Molecule 2: T-complex protein 1 subunit theta

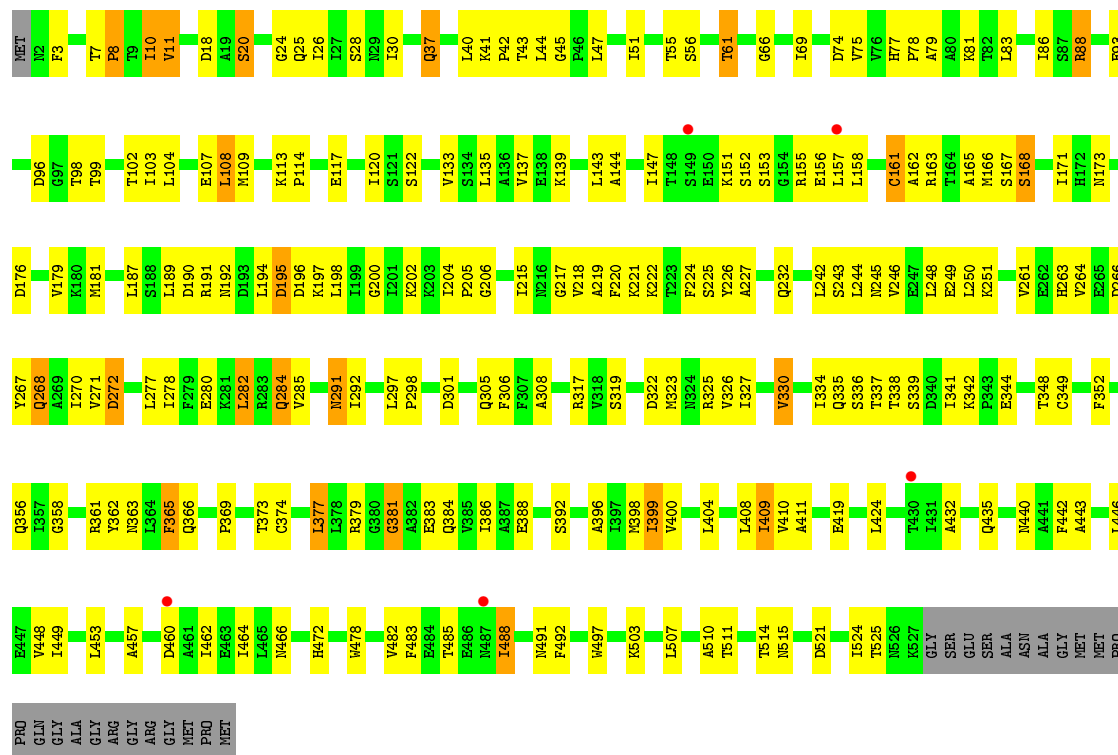


• Molecule 2: T-complex protein 1 subunit theta

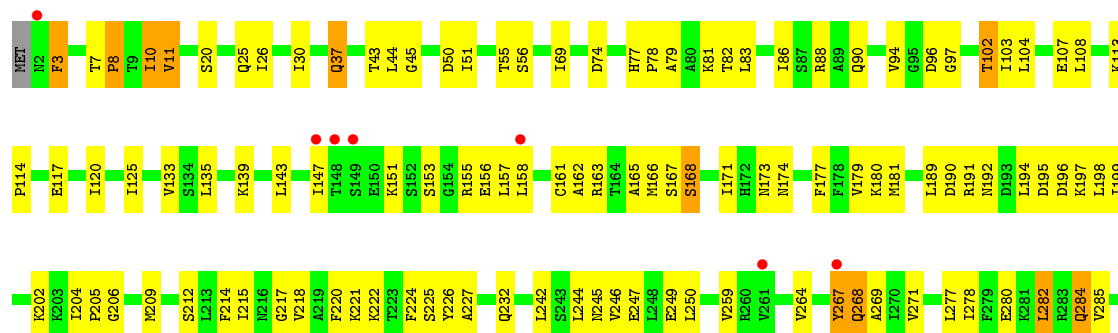


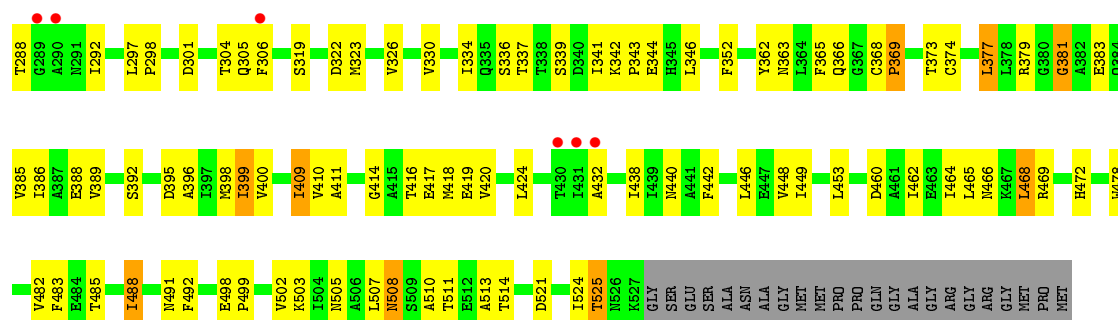


• Molecule 3: T-complex protein 1 subunit eta

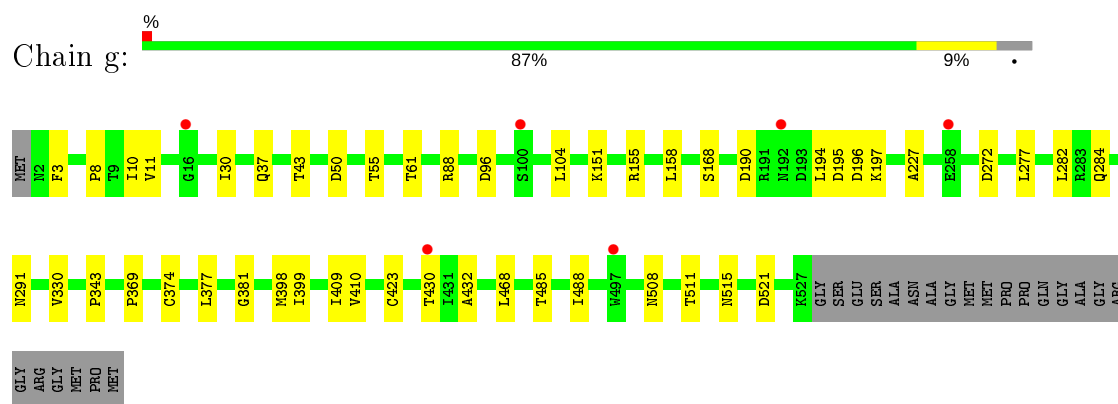


• Molecule 3: T-complex protein 1 subunit eta

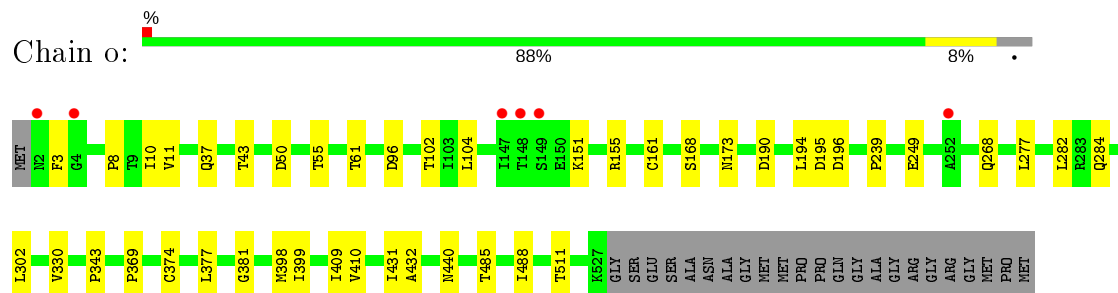




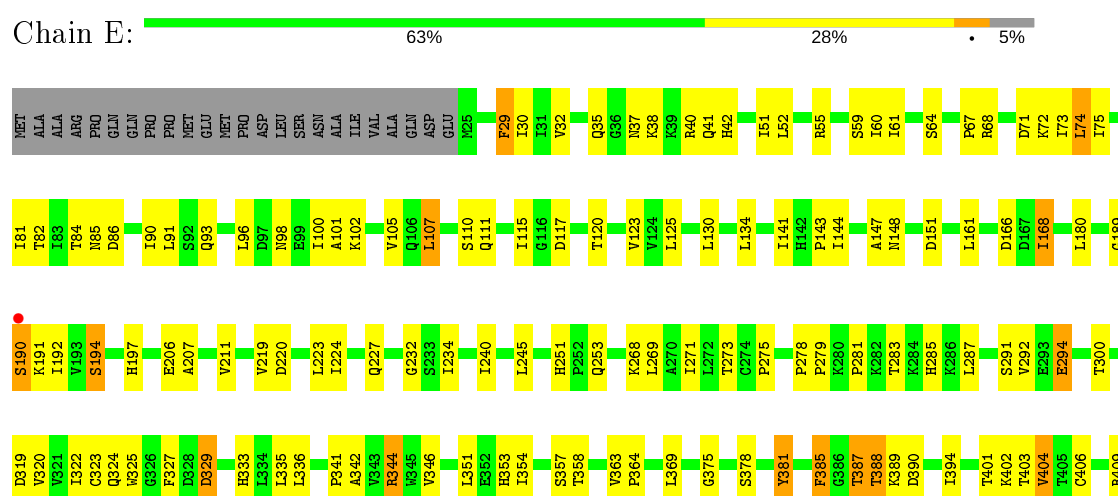
• Molecule 3: T-complex protein 1 subunit eta

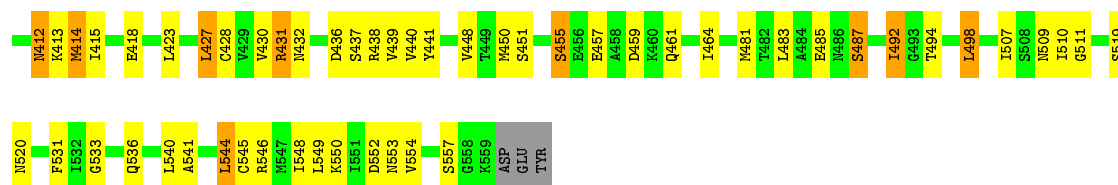


• Molecule 3: T-complex protein 1 subunit eta

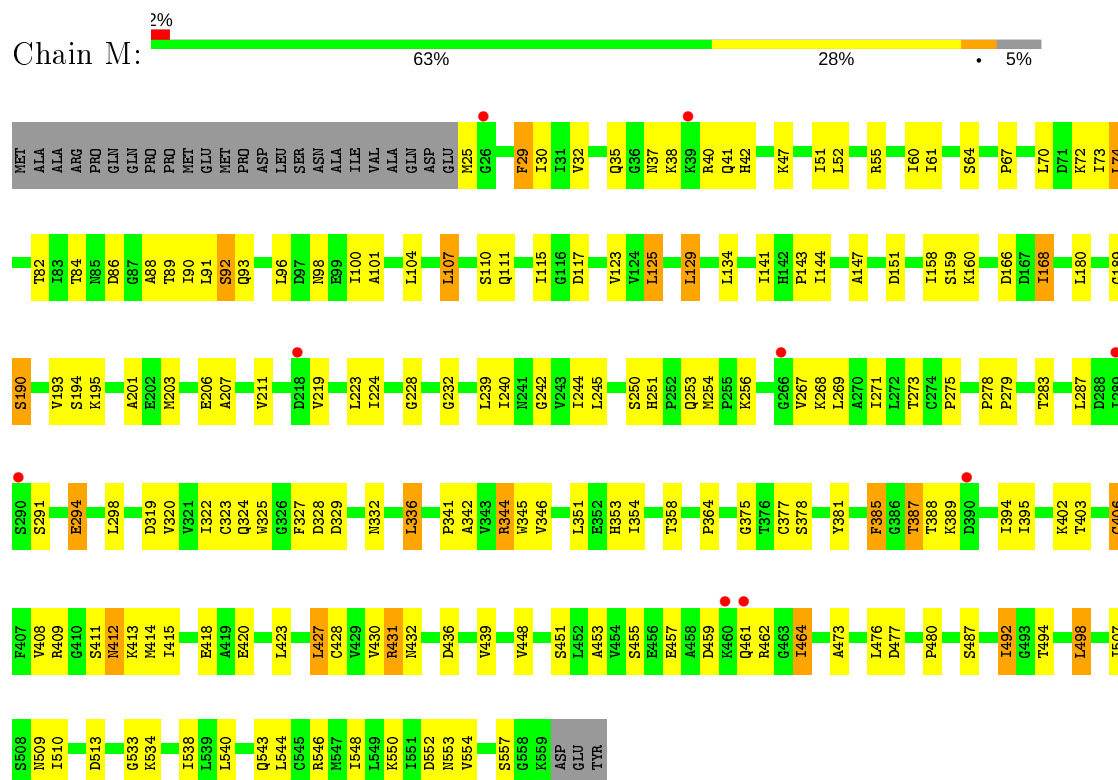


• Molecule 4: T-complex protein 1 subunit epsilon

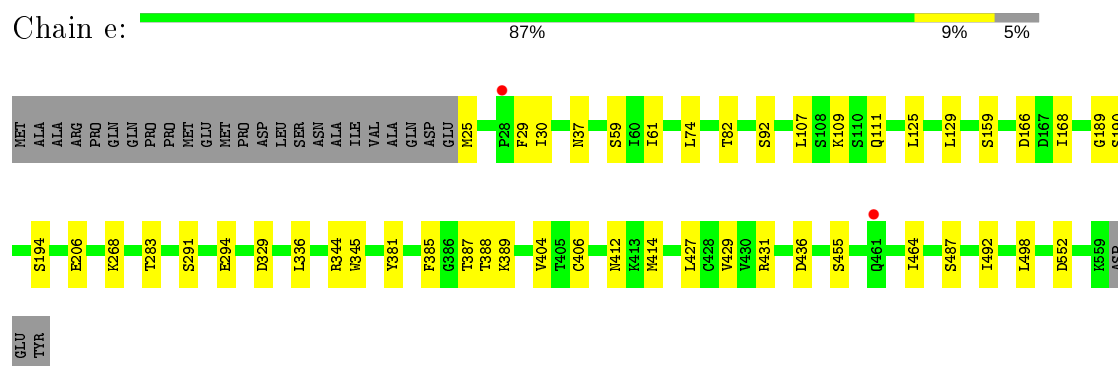




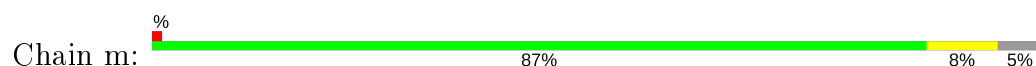
- Molecule 4: T-complex protein 1 subunit epsilon



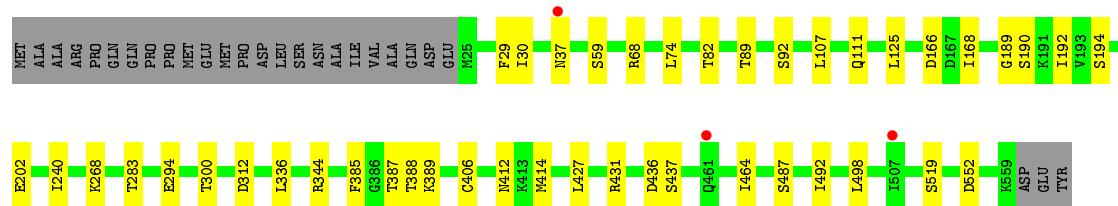
- Molecule 4: T-complex protein 1 subunit epsilon



- Molecule 4: T-complex protein 1 subunit epsilon

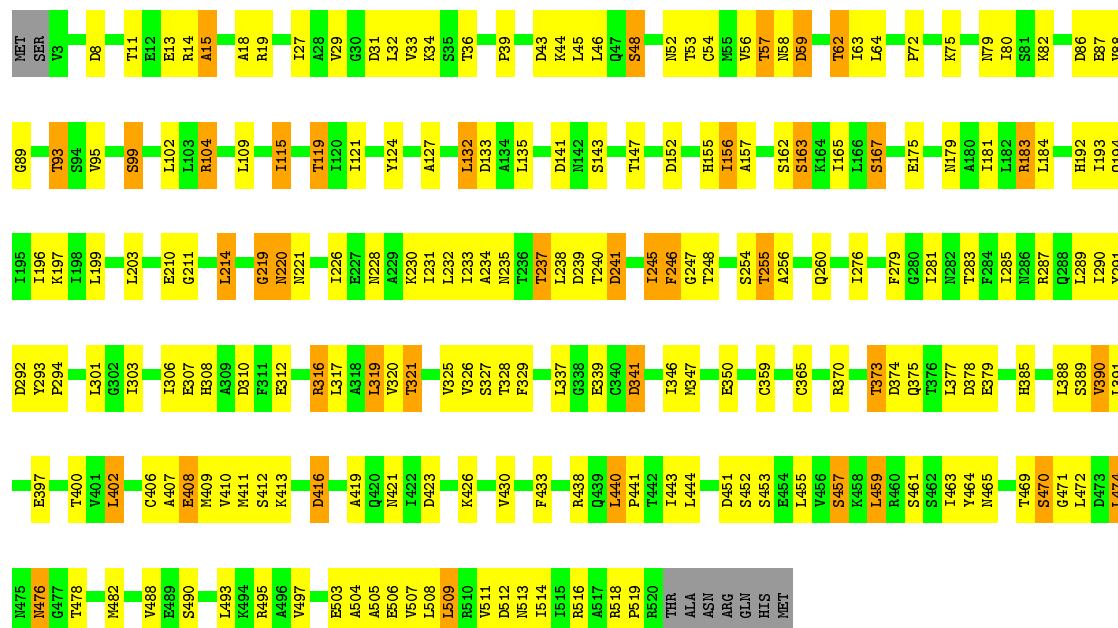






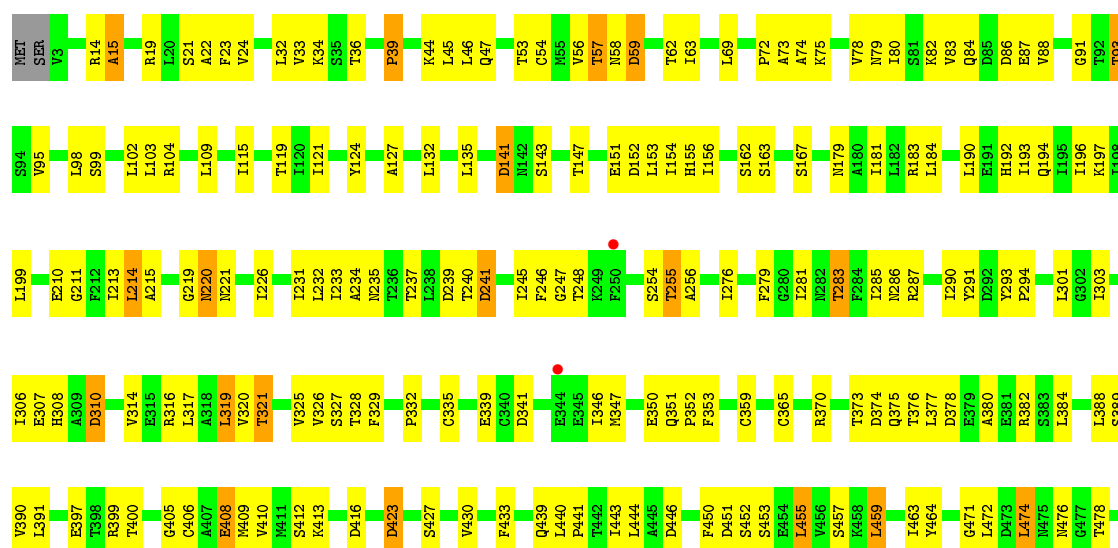
• Molecule 5: T-complex protein 1 subunit beta

Chain B: 58% 33% 7% .



• Molecule 5: T-complex protein 1 subunit beta

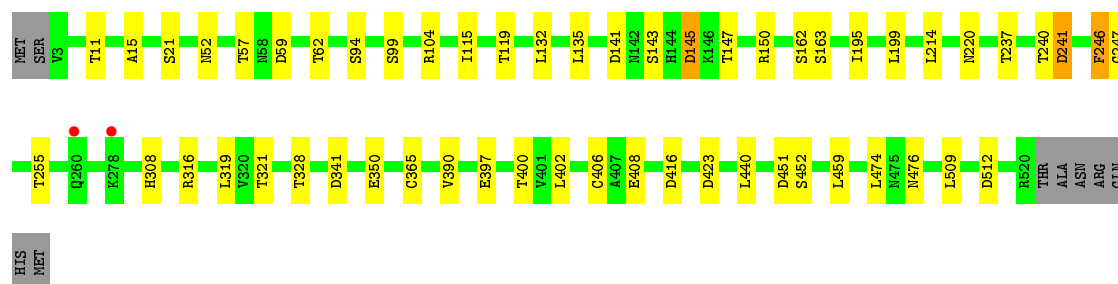
Chain J: 59% 35% . .





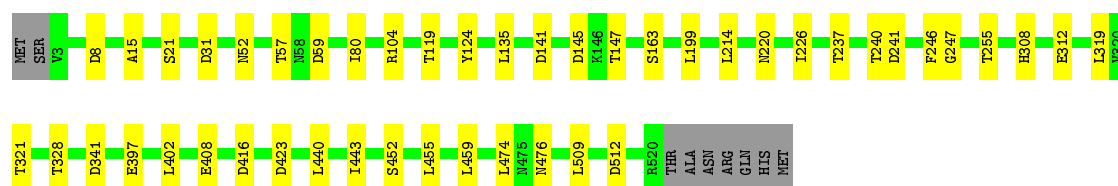
• Molecule 5: T-complex protein 1 subunit beta

Chain b: 88% 10% ..



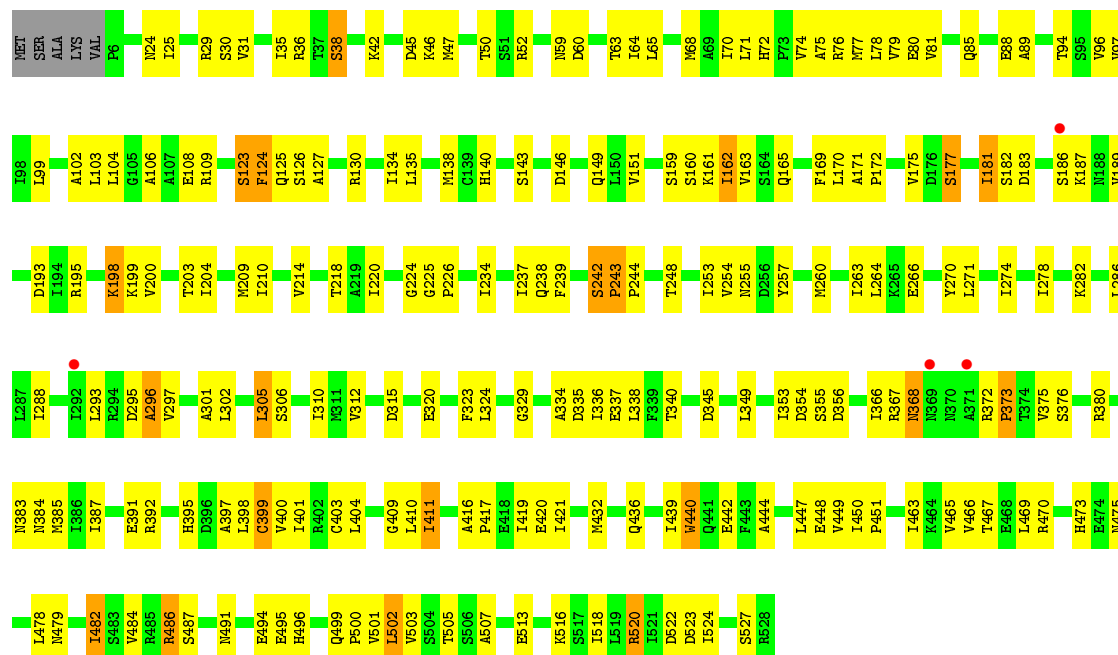
• Molecule 5: T-complex protein 1 subunit beta

Chain j: 90% 9% .



• Molecule 6: T-complex protein 1 subunit delta

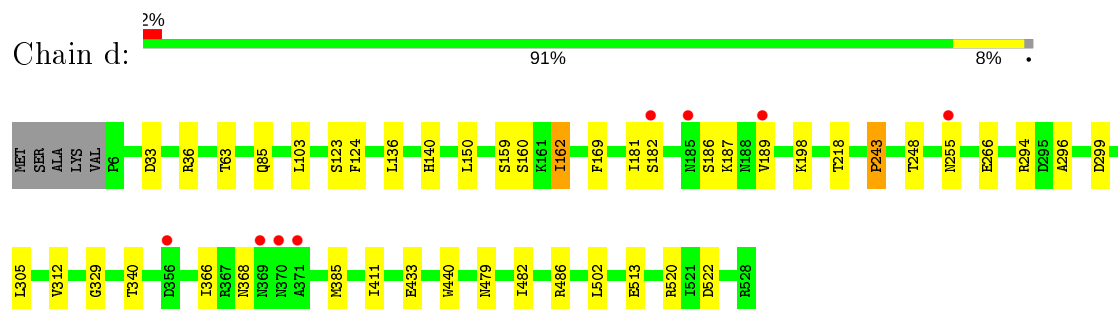
Chain D: 58% 37% ..



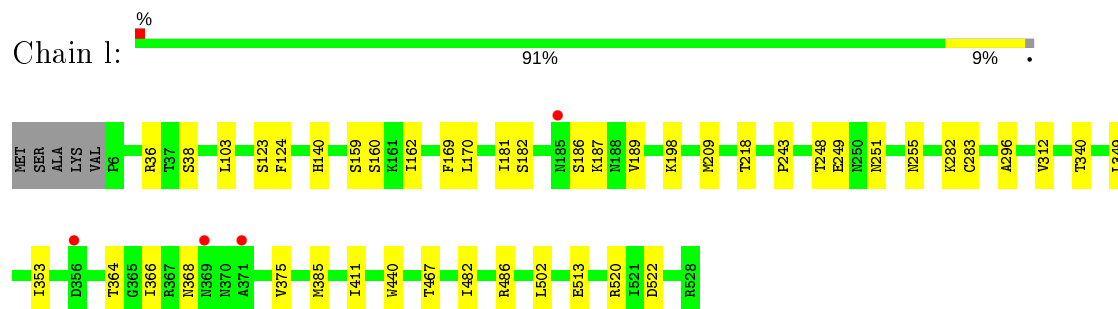
- Molecule 6: T-complex protein 1 subunit delta



- Molecule 6: T-complex protein 1 subunit delta



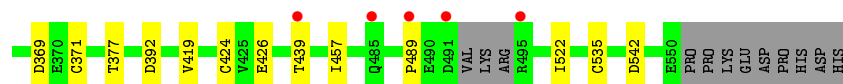
- Molecule 6: T-complex protein 1 subunit delta



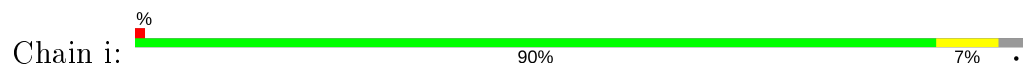
- Molecule 7: T-complex protein 1 subunit alpha



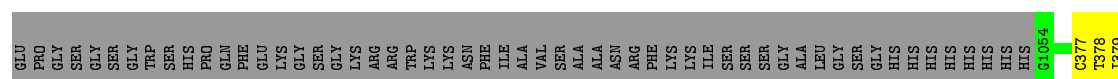
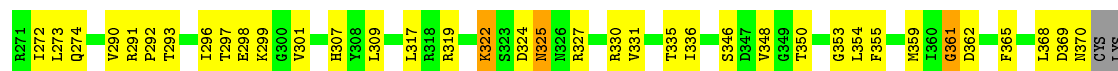
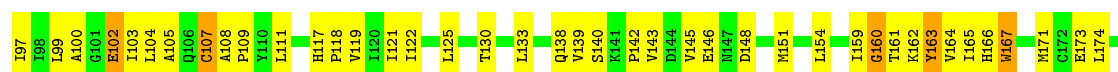
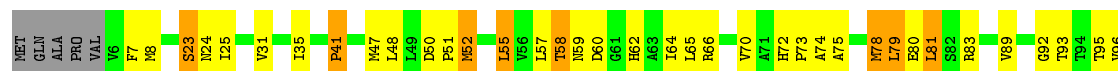




• Molecule 7: T-complex protein 1 subunit alpha

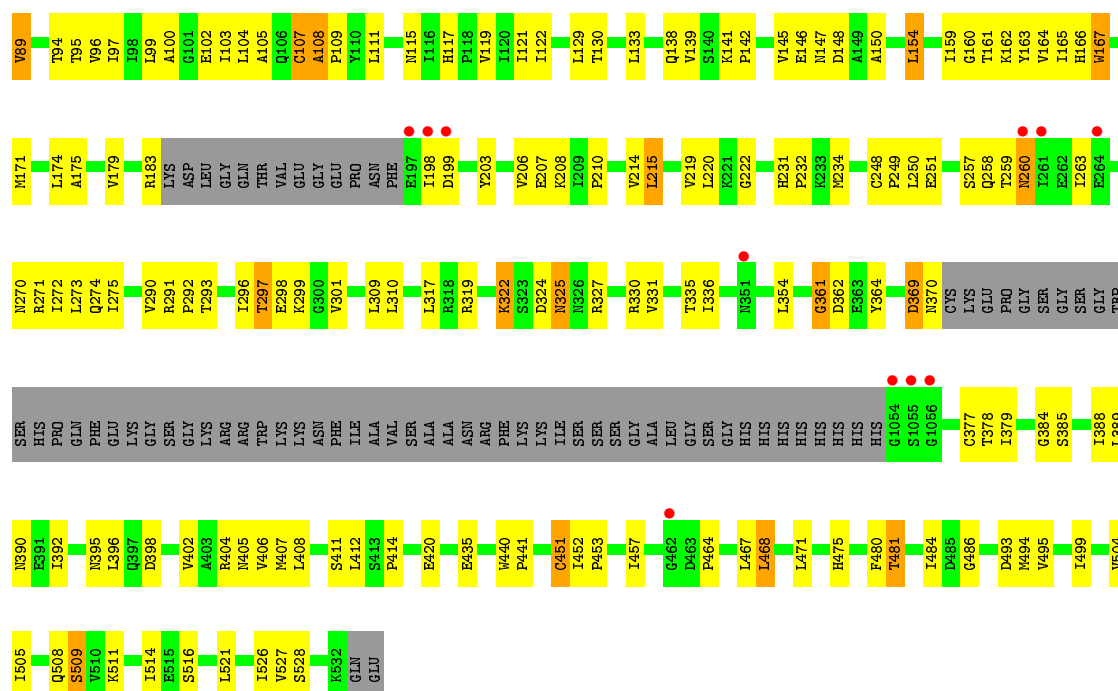


• Molecule 8: T-complex protein 1 subunit gamma

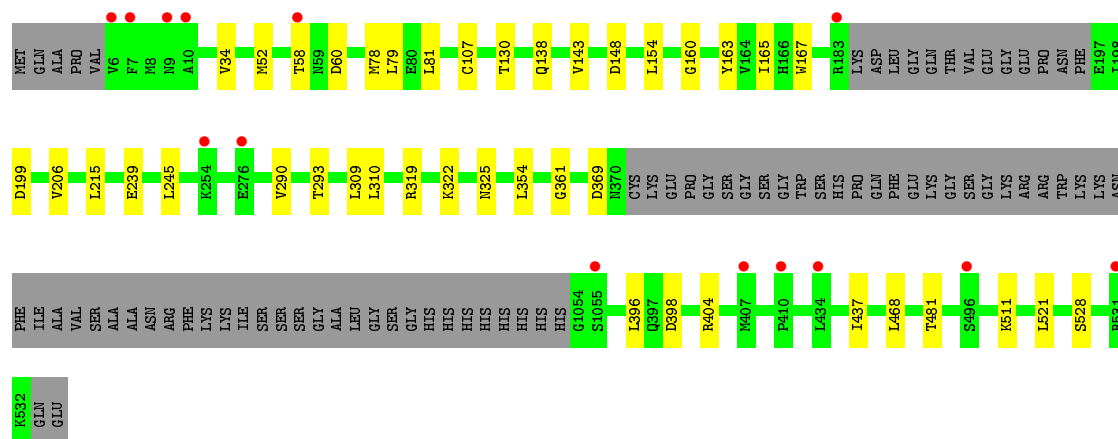
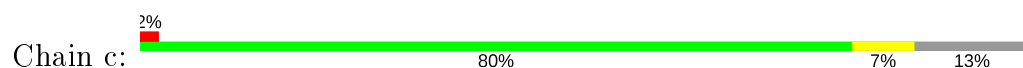


• Molecule 8: T-complex protein 1 subunit gamma

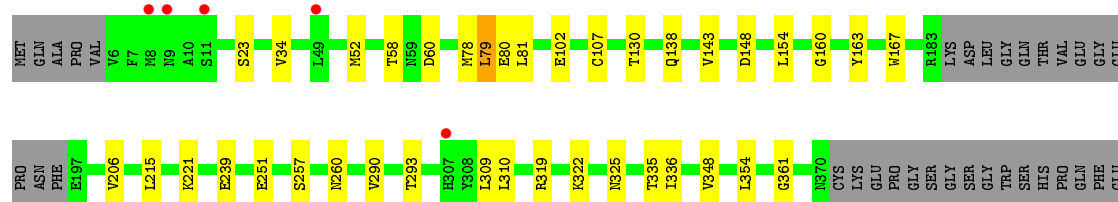
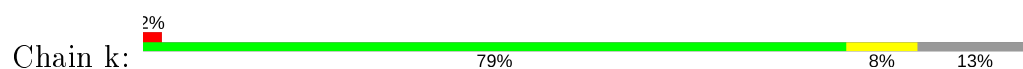


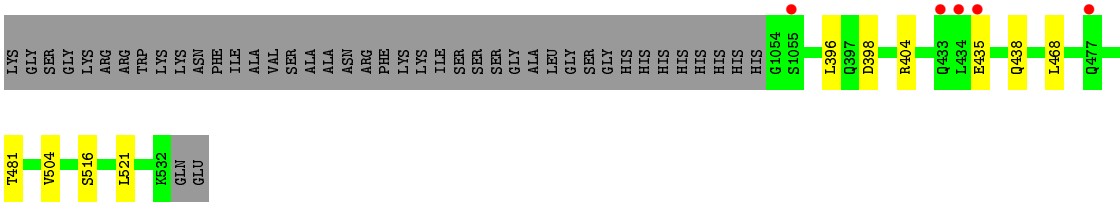


• Molecule 8: T-complex protein 1 subunit gamma



• Molecule 8: T-complex protein 1 subunit gamma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	30.00 – 3.80 30.01 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (30.00-3.80) 91.6 (30.01-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.257 , 0.305 0.276 , 0.314	Depositor DCC
$R_{free}$ test set	10463 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.0	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 70.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	120080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	F	0.35	0/3886	0.55	0/5318
1	N	0.34	0/3886	0.53	0/5318
1	f	0.34	0/3886	0.52	1/5318 (0.0%)
1	n	0.35	0/3886	0.54	0/5318
2	H	0.35	0/3661	0.55	0/5005
2	P	0.36	0/3661	0.54	0/5005
2	h	0.35	0/3661	0.52	0/5005
2	p	0.36	0/3661	0.54	0/5005
3	G	0.36	0/3803	0.53	0/5194
3	O	0.36	0/3803	0.51	0/5194
3	g	0.37	0/3803	0.53	0/5194
3	o	0.38	0/3803	0.53	0/5194
4	E	0.34	0/3849	0.52	0/5252
4	M	0.34	0/3849	0.52	0/5252
4	e	0.36	0/3849	0.51	0/5252
4	m	0.36	0/3849	0.53	0/5252
5	B	0.36	0/3726	0.56	0/5077
5	J	0.35	0/3726	0.54	0/5077
5	b	0.35	0/3726	0.54	0/5077
5	j	0.40	1/3726 (0.0%)	0.55	0/5077
6	D	0.36	0/3723	0.56	0/5089
6	L	0.34	0/3723	0.52	0/5089
6	d	0.35	0/3723	0.53	0/5089
6	l	0.36	0/3723	0.54	0/5089
7	A	0.36	0/3805	0.54	0/5196
7	I	0.35	0/3805	0.53	0/5196
7	a	0.35	0/3805	0.53	0/5196
7	i	0.35	0/3805	0.53	0/5196
8	C	0.38	0/3657	0.57	0/5003
8	K	0.35	0/3657	0.55	0/5003
8	c	0.35	0/3657	0.55	0/5003
8	k	0.34	0/3657	0.56	1/5003 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
All	All	0.36	1/120440 (0.0%)	0.54	2/164536 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
6	d	0	1
6	l	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	j	452	SER	CB-OG	7.94	1.52	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	k	79	LEU	CA-CB-CG	5.19	127.24	115.30
1	f	434	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	194	VAL	Peptide
6	d	243	PRO	Peptide
6	l	243	PRO	Peptide

## 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	F	3836	0	3618	149	0
1	N	3836	0	3618	133	0
1	f	3836	0	3618	0	0
1	n	3836	0	3618	0	0
2	H	3619	0	3425	139	0
2	P	3619	0	3425	137	0
2	h	3619	0	3425	0	0
2	p	3619	0	3425	0	0
3	G	3752	0	3581	169	0
3	O	3752	0	3581	151	0
3	g	3752	0	3581	0	0
3	o	3752	0	3581	0	0
4	E	3798	0	3576	140	0
4	M	3798	0	3576	136	0
4	e	3798	0	3576	0	0
4	m	3798	0	3576	0	0
5	B	3689	0	3546	176	0
5	J	3689	0	3546	167	0
5	b	3689	0	3546	0	0
5	j	3689	0	3546	0	0
6	D	3685	0	3540	165	0
6	L	3685	0	3540	143	0
6	d	3685	0	3540	0	0
6	l	3685	0	3540	0	0
7	A	3770	0	3626	163	0
7	I	3770	0	3626	156	0
7	a	3770	0	3626	0	0
7	i	3770	0	3626	0	0
8	C	3615	0	3455	168	0
8	K	3615	0	3455	147	0
8	c	3615	0	3455	0	0
8	k	3615	0	3455	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	1	0	0	0	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
9	a	1	0	0	0	0
9	b	1	0	0	0	0
9	c	1	0	0	0	0
9	d	1	0	0	0	0
9	e	1	0	0	0	0
9	f	1	0	0	0	0
9	g	1	0	0	0	0
9	h	1	0	0	0	0
9	i	1	0	0	0	0
9	j	1	0	0	0	0
9	k	1	0	0	0	0
9	l	1	0	0	0	0
9	m	1	0	0	0	0
9	n	1	0	0	0	0
9	o	1	0	0	0	0
9	p	1	0	0	0	0
10	A	27	0	12	1	0
10	B	27	0	12	3	0
10	C	27	0	12	5	0
10	D	27	0	12	1	0
10	E	27	0	12	1	0
10	F	27	0	12	0	0
10	G	27	0	12	0	0
10	H	27	0	12	0	0
10	I	27	0	12	1	0
10	J	27	0	12	2	0
10	K	27	0	12	1	0
10	L	27	0	12	0	0
10	M	27	0	12	1	0
10	N	27	0	12	0	0
10	O	27	0	12	0	0
10	P	27	0	12	0	0
10	a	27	0	12	0	0
10	b	27	0	12	0	0
10	c	27	0	12	0	0
10	d	27	0	12	0	0
10	e	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	f	27	0	12	0	0
10	g	27	0	12	0	0
10	h	27	0	12	0	0
10	i	27	0	12	0	0
10	j	27	0	12	0	0
10	k	27	0	12	0	0
10	l	27	0	12	0	0
10	m	27	0	12	0	0
10	n	27	0	12	0	0
10	o	27	0	12	0	0
10	p	27	0	12	0	0
11	A	4	0	0	0	0
11	B	4	0	0	2	0
11	C	4	0	0	2	0
11	D	4	0	0	1	0
11	E	4	0	0	1	0
11	F	4	0	0	0	0
11	G	4	0	0	1	0
11	H	4	0	0	0	0
11	I	4	0	0	0	0
11	J	4	0	0	1	0
11	K	4	0	0	1	0
11	L	4	0	0	0	0
11	M	4	0	0	1	0
11	N	4	0	0	0	0
11	O	4	0	0	1	0
11	P	4	0	0	0	0
11	a	4	0	0	0	0
11	b	4	0	0	0	0
11	c	4	0	0	0	0
11	d	4	0	0	0	0
11	e	4	0	0	0	0
11	f	4	0	0	0	0
11	g	4	0	0	0	0
11	h	4	0	0	0	0
11	i	4	0	0	0	0
11	j	4	0	0	0	0
11	k	4	0	0	0	0
11	l	4	0	0	0	0
11	m	4	0	0	0	0
11	n	4	0	0	0	0
11	o	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	p	4	0	0	0	0
All	All	120080	0	113852	2215	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 9.

All (2215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:GLN:HE21	2:H:544:ILE:HD11	1.02	1.15
3:G:107:GLU:HG2	3:G:448:VAL:HG21	1.24	1.11
3:G:147:ILE:HD11	3:G:409:ILE:HB	1.67	1.11
7:I:26:ARG:HG3	7:I:26:ARG:HH11	1.20	1.09
6:D:520:ARG:HH21	6:D:520:ARG:HG3	1.41	1.08
3:O:107:GLU:HG2	3:O:448:VAL:HG21	1.31	1.07
7:A:26:ARG:HH11	7:A:26:ARG:HG3	1.18	1.06
6:L:353:ILE:HG22	6:L:354:ASP:H	1.89	1.04
2:H:27:GLN:NE2	2:H:544:ILE:HD11	1.72	1.03
6:L:520:ARG:HH21	6:L:520:ARG:HG3	1.20	1.03
5:B:290:ILE:HG12	5:B:307:GLU:HB3	1.60	1.02
4:M:219:VAL:HG11	4:M:431:ARG:HB2	1.49	1.02
1:N:97:LEU:O	1:N:101:LEU:HB2	1.65	1.02
5:B:232:LEU:HB2	5:B:281:ILE:HD13	1.66	1.01
6:D:165:GLN:HG3	7:A:130:ARG:HD3	1.43	1.01
4:E:219:VAL:HG11	4:E:431:ARG:HB2	1.61	1.01
5:J:290:ILE:HG12	5:J:307:GLU:HB3	1.44	0.99
8:K:103:ILE:O	8:K:107:CYS:HB3	1.62	0.98
5:J:239:ASP:HA	5:J:291:TYR:HB2	1.57	0.95
6:D:138:MET:HB2	6:D:478:LEU:HD13	1.45	0.95
8:K:59:ASN:HB3	8:K:162:LYS:HG2	1.47	0.95
2:P:62:ILE:HD11	3:O:81:LYS:HD3	1.72	0.94
1:F:97:LEU:O	1:F:101:LEU:HB2	1.71	0.92
3:O:218:VAL:HG21	3:O:326:VAL:HA	1.53	0.92
5:J:183:ARG:HH11	5:J:365:CYS:HB3	1.50	0.92
6:L:165:GLN:HG3	7:I:130:ARG:HD3	1.66	0.92
8:C:103:ILE:O	8:C:107:CYS:HB3	1.73	0.91
6:L:448:GLU:OE2	6:L:466:VAL:HG11	1.95	0.91
6:L:138:MET:HB2	6:L:478:LEU:HD13	1.52	0.90
2:P:333:CYS:SG	2:P:340:PRO:HD3	3.02	0.90
8:C:65:LEU:HB3	8:C:79:LEU:HD13	1.51	0.89
2:H:27:GLN:HA	2:H:31:SER:HB2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:SER:HB3	2:H:266:LEU:O	1.73	0.89
8:K:481:THR:HG22	8:K:494:MET:HB2	1.54	0.89
7:A:256:MET:HB3	7:A:260:VAL:HB	1.52	0.88
1:F:195:GLU:HG3	1:F:327:ARG:NH1	2.13	0.88
5:J:219:GLY:O	5:J:220:ASN:HB2	1.71	0.87
3:G:218:VAL:HG21	3:G:326:VAL:HA	1.54	0.87
3:G:88:ARG:HG2	3:G:88:ARG:HH11	1.37	0.87
4:M:51:ILE:HD13	4:M:134:LEU:HB2	1.57	0.87
5:B:239:ASP:HA	5:B:291:TYR:HB2	1.66	0.86
2:H:27:GLN:HE21	2:H:544:ILE:CD1	1.87	0.86
1:N:75:LEU:HD12	8:K:55:LEU:HD23	1.75	0.86
5:J:413:LYS:HA	5:J:464:TYR:HE1	1.40	0.86
3:O:147:ILE:HD11	3:O:409:ILE:HB	1.56	0.86
8:C:198:ILE:HG21	8:C:408:LEU:HD21	1.57	0.85
6:L:127:ALA:HA	6:L:440:TRP:HE1	1.59	0.85
7:A:55:ASP:HB2	7:A:59:ASP:O	1.91	0.85
5:B:219:GLY:O	5:B:220:ASN:HB2	1.76	0.85
6:L:432:MET:SD	6:L:440:TRP:HZ3	2.43	0.85
3:O:107:GLU:CG	3:O:448:VAL:HG21	2.07	0.84
7:I:12:THR:HB	7:I:14:PHE:CE2	2.12	0.84
5:B:413:LYS:HA	5:B:464:TYR:HE1	1.66	0.84
6:L:448:GLU:CD	6:L:470:ARG:HH22	1.94	0.84
5:J:232:LEU:HB2	5:J:281:ILE:HD13	1.66	0.84
3:O:189:LEU:HD11	3:O:195:ASP:O	1.86	0.84
8:C:59:ASN:HB3	8:C:162:LYS:HG2	1.70	0.84
1:F:195:GLU:HG3	1:F:327:ARG:HH11	1.75	0.84
3:O:135:LEU:HD23	3:O:424:LEU:HD23	1.61	0.83
4:E:107:LEU:HG	4:E:544:LEU:HD13	1.59	0.83
7:A:12:THR:HB	7:A:14:PHE:CE2	2.35	0.83
5:B:183:ARG:HH11	5:B:365:CYS:HB3	1.61	0.83
7:A:256:MET:HG2	8:C:257:SER:HB2	1.78	0.83
5:J:183:ARG:HH22	5:J:211:GLY:H	1.39	0.83
4:M:72:LYS:HB2	4:M:90:ILE:HD12	1.59	0.82
1:N:251:PHE:HB3	8:K:263:ILE:HB	1.61	0.82
6:D:448:GLU:OE2	6:D:466:VAL:HG11	1.79	0.82
7:A:16:GLY:O	7:A:548:ASP:N	2.11	0.82
4:E:115:ILE:HD13	4:E:533:GLY:HA2	1.60	0.82
3:O:86:ILE:HD11	3:O:510:ALA:HA	1.62	0.82
3:O:297:LEU:HB3	3:O:298:PRO:HD2	1.58	0.82
7:A:55:ASP:O	7:A:56:ASP:HB3	1.78	0.82
3:G:297:LEU:HB3	3:G:298:PRO:HD2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:26:ARG:CG	7:A:26:ARG:HH11	1.92	0.82
5:B:441:PRO:HA	5:B:444:LEU:HD12	2.05	0.82
3:O:107:GLU:HG2	3:O:448:VAL:CG2	2.09	0.82
8:C:453:PRO:O	8:C:457:ILE:HG12	2.14	0.82
6:L:353:ILE:HG22	6:L:354:ASP:N	2.24	0.81
7:I:129:PHE:HB3	7:I:532:LEU:HD11	1.62	0.81
6:L:35:ILE:HA	6:L:46:LYS:NZ	2.22	0.81
8:C:481:THR:HG22	8:C:494:MET:HB2	1.63	0.81
6:D:25:ILE:HG23	6:D:104:LEU:HB3	1.62	0.81
6:L:71:LEU:HD21	7:I:15:LEU:HB2	1.69	0.81
3:G:107:GLU:CG	3:G:448:VAL:HG21	2.09	0.80
6:D:127:ALA:HA	6:D:440:TRP:HE1	1.46	0.80
5:J:291:TYR:HB3	5:J:294:PRO:HD2	1.63	0.80
7:I:94:ILE:HD13	7:I:523:SER:HA	1.64	0.80
5:J:279:PHE:HB3	5:J:281:ILE:HD12	2.10	0.80
7:A:212:SER:HB2	8:C:511:LYS:HE3	2.00	0.80
5:J:183:ARG:NH1	5:J:365:CYS:HB3	2.23	0.80
3:G:86:ILE:HD11	3:G:510:ALA:HA	1.64	0.79
7:I:256:MET:HB3	7:I:260:VAL:HB	1.65	0.79
5:J:285:ILE:HG22	5:J:306:ILE:HB	1.76	0.79
2:H:62:ILE:HD11	3:G:81:LYS:HD3	1.72	0.78
7:I:103:ILE:HG22	7:I:457:ILE:HG21	1.71	0.78
6:D:244:PRO:HD3	6:D:270:TYR:CE2	2.32	0.78
8:C:162:LYS:HB2	8:C:395:ASN:OD1	1.92	0.78
5:B:285:ILE:HD12	5:B:317:LEU:HD13	1.66	0.78
3:G:280:GLU:O	3:G:284:GLN:HB2	1.82	0.78
2:P:225:GLY:HA2	2:P:335:VAL:HG21	1.66	0.78
5:J:46:LEU:HD11	5:J:63:ILE:HA	1.66	0.77
1:N:439:LYS:O	1:N:442:THR:HG22	2.23	0.77
5:J:285:ILE:HD12	5:J:317:LEU:HD13	1.80	0.77
3:G:107:GLU:HG2	3:G:448:VAL:CG2	2.10	0.77
1:N:254:SER:HB3	2:P:266:LEU:O	1.89	0.77
5:J:301:LEU:HD23	5:J:303:ILE:HD11	2.27	0.77
5:B:46:LEU:HD11	5:B:63:ILE:HA	1.67	0.77
8:C:50:ASP:HB2	8:C:51:PRO:HD3	1.66	0.77
1:F:251:PHE:HB3	8:C:263:ILE:HB	1.64	0.77
2:H:225:GLY:HA2	2:H:335:VAL:HG21	1.68	0.77
5:B:285:ILE:HG22	5:B:306:ILE:HB	1.76	0.76
3:O:37:GLN:HG3	3:O:103:ILE:HA	1.96	0.76
6:D:210:ILE:HD12	6:D:214:VAL:HG22	1.67	0.76
7:I:458:ILE:HB	7:I:459:PRO:HD3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:291:TYR:HB3	5:B:294:PRO:HD2	1.67	0.76
1:F:93:THR:O	1:F:97:LEU:HB2	1.85	0.76
7:A:17:GLY:HA2	7:A:546:THR:O	1.86	0.76
4:M:73:ILE:HD11	5:J:72:PRO:HB2	1.65	0.76
7:A:129:PHE:HB3	7:A:532:LEU:HD11	1.67	0.76
5:B:183:ARG:HH22	5:B:210:GLU:HA	1.50	0.76
6:L:237:ILE:HD11	6:L:286:LEU:HD22	1.67	0.76
2:H:284:ILE:HD11	2:H:308:LEU:HB3	1.81	0.75
6:L:288:ILE:HD13	6:L:297:VAL:HG21	1.67	0.75
7:I:16:GLY:O	7:I:548:ASP:N	2.19	0.75
6:L:35:ILE:HD11	6:L:65:LEU:HD21	1.83	0.75
4:E:180:LEU:HD22	4:E:430:VAL:HG13	2.09	0.75
7:A:262:ILE:HG21	8:C:259:THR:HG23	1.68	0.75
4:M:115:ILE:HD13	4:M:533:GLY:HA2	1.77	0.75
5:B:80:ILE:HD12	5:B:504:ALA:HB2	1.68	0.75
8:K:162:LYS:HB2	8:K:395:ASN:OD1	1.87	0.75
8:K:89:VAL:HG11	8:K:505:ILE:CG1	3.04	0.75
7:I:262:ILE:HG21	8:K:259:THR:HG23	1.90	0.74
4:E:192:ILE:HD11	4:E:415:ILE:HG23	2.45	0.74
6:D:288:ILE:HD13	6:D:297:VAL:HG21	1.68	0.74
7:I:165:SER:O	7:I:166:SER:HB3	1.86	0.74
5:B:95:VAL:HG22	5:B:497:VAL:HA	2.02	0.74
4:E:211:VAL:HG12	4:E:402:LYS:O	1.87	0.74
2:H:78:VAL:HB	3:G:11:VAL:O	1.88	0.74
3:G:478:TRP:CE3	3:G:492:PHE:HB2	2.22	0.74
6:L:420:GLU:HB2	6:L:473:HIS:CE1	2.23	0.74
5:B:231:ILE:HD12	5:B:321:THR:HG21	1.71	0.74
5:B:409:MET:HG3	5:B:459:LEU:HD21	2.16	0.74
4:E:64:SER:HB2	4:E:72:LYS:NZ	2.20	0.74
5:J:490:SER:HB3	5:J:493:LEU:HB2	2.25	0.73
6:L:274:ILE:O	6:L:278:ILE:HG12	1.88	0.73
6:D:274:ILE:O	6:D:278:ILE:HG12	1.92	0.73
7:A:50:ASP:OD1	7:A:64:ASN:HB2	1.89	0.73
8:K:111:LEU:HD22	8:K:440:TRP:HB3	1.84	0.73
1:N:253:TYR:CE1	1:N:259:ARG:HG3	2.43	0.73
3:G:204:ILE:HD13	3:G:362:TYR:CE2	2.67	0.73
7:I:26:ARG:HH11	7:I:26:ARG:CG	2.00	0.73
5:B:183:ARG:NH2	5:B:210:GLU:HA	2.03	0.73
8:C:24:ASN:HD22	8:C:74:ALA:HB2	1.54	0.73
7:A:304:ASP:HA	7:A:307:LEU:HD12	1.71	0.73
8:C:353:GLY:HA3	8:C:370:ASN:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:77:HIS:CE1	3:O:79:ALA:HB3	2.24	0.73
2:P:240:SER:HA	2:P:245:HIS:NE2	2.04	0.73
3:O:204:ILE:HD12	3:O:205:PRO:HD2	1.74	0.72
2:H:65:THR:HG22	2:H:67:ASP:H	1.54	0.72
1:N:195:GLU:HG3	1:N:327:ARG:NH1	2.04	0.72
7:A:94:ILE:HD13	7:A:523:SER:HA	1.70	0.72
5:B:183:ARG:NH1	5:B:365:CYS:HB3	2.31	0.72
7:I:55:ASP:HB2	7:I:59:ASP:O	2.15	0.72
6:L:353:ILE:CG2	6:L:354:ASP:H	2.42	0.72
3:G:242:LEU:HD22	3:G:244:LEU:HG	1.71	0.72
4:E:51:ILE:HD13	4:E:134:LEU:HB2	1.93	0.72
3:G:189:LEU:HD11	3:G:195:ASP:O	2.14	0.72
8:C:208:LYS:HE3	8:C:390:ASN:OD1	1.89	0.72
3:O:446:LEU:HD21	3:O:507:LEU:HD21	1.69	0.72
8:C:31:VAL:HG11	8:C:78:MET:HG2	1.71	0.71
4:E:387:THR:HB	5:B:86:ASP:O	2.32	0.71
8:K:89:VAL:HG11	8:K:505:ILE:HG12	2.49	0.71
3:G:446:LEU:HD21	3:G:507:LEU:HD21	1.97	0.71
7:A:458:ILE:HB	7:A:459:PRO:HD3	1.73	0.71
5:J:373:THR:HG22	5:J:375:GLN:H	1.73	0.71
5:B:413:LYS:HA	5:B:464:TYR:CE1	2.44	0.71
5:J:413:LYS:HA	5:J:464:TYR:CE1	2.25	0.71
8:K:121:ILE:HG23	8:K:441:PRO:HB3	1.93	0.71
8:K:50:ASP:HB2	8:K:51:PRO:HD3	1.72	0.71
7:I:63:THR:HA	7:I:397:GLU:HG3	1.91	0.71
3:O:88:ARG:HG2	3:O:88:ARG:HH11	2.03	0.70
6:L:520:ARG:HH21	6:L:520:ARG:CG	2.03	0.70
7:I:86:LEU:HD21	7:I:101:VAL:HG12	1.73	0.70
7:A:26:ARG:NH1	7:A:26:ARG:HG3	2.00	0.70
6:D:353:ILE:HG22	6:D:354:ASP:N	2.06	0.70
6:D:35:ILE:HA	6:D:46:LYS:NZ	2.08	0.70
4:M:411:SER:HB3	5:J:503:GLU:OE1	2.26	0.70
6:D:237:ILE:HD11	6:D:286:LEU:HD22	1.72	0.70
4:M:494:THR:O	4:M:498:LEU:HB2	1.92	0.70
1:N:103:ARG:O	1:N:107:ARG:HD2	1.92	0.70
1:N:159:LEU:HA	1:N:167:THR:HG21	1.82	0.70
3:O:280:GLU:O	3:O:284:GLN:HB2	1.98	0.70
6:D:448:GLU:CD	6:D:470:ARG:HH22	1.95	0.70
2:H:240:SER:HA	2:H:245:HIS:NE2	2.07	0.70
4:M:328:ASP:OD2	5:J:245:ILE:HD11	2.51	0.70
7:A:104:ILE:HG12	7:A:458:ILE:HD11	1.87	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:424:CYS:SG	7:A:500:TYR:HB2	2.31	0.70
8:C:50:ASP:HB2	8:C:51:PRO:CD	2.22	0.70
1:F:253:TYR:CE1	1:F:259:ARG:HG3	2.27	0.70
7:I:63:THR:HG23	7:I:397:GLU:HG2	1.79	0.70
6:D:244:PRO:HD3	6:D:270:TYR:HE2	1.70	0.69
3:G:147:ILE:HD13	3:G:157:LEU:HD11	1.74	0.69
3:G:388:GLU:O	3:G:392:SER:HB2	2.26	0.69
3:O:245:ASN:HB3	3:O:336:SER:HA	1.74	0.69
6:D:130:ARG:O	6:D:134:ILE:HG13	1.93	0.69
1:F:181:VAL:HG22	1:F:193:MET:CB	2.22	0.69
6:D:74:VAL:HG13	6:D:518:ILE:HD12	1.72	0.69
3:O:264:VAL:HG23	4:M:294:GLU:OE2	2.33	0.69
1:F:159:LEU:HA	1:F:167:THR:HG21	1.75	0.69
7:A:462:LEU:HB3	7:A:504:LEU:HD11	1.75	0.69
1:N:93:THR:O	1:N:97:LEU:HB2	1.99	0.69
7:I:28:GLN:HE21	7:I:77:HIS:HE1	1.55	0.69
5:B:440:LEU:HB3	5:B:441:PRO:HD3	1.98	0.69
6:D:125:GLN:HE21	6:D:513:GLU:HG2	2.02	0.69
7:I:179:MET:HE1	7:I:385:ILE:HG23	1.74	0.69
6:D:214:VAL:HG23	6:D:376:SER:HB3	1.79	0.69
2:P:27:GLN:HE21	2:P:544:ILE:HD11	2.38	0.69
5:B:132:LEU:HD21	5:B:495:ARG:HG3	2.23	0.69
6:D:238:GLN:HB2	6:D:334:ALA:HA	1.75	0.69
4:E:96:LEU:HD13	4:E:101:ALA:HB1	1.74	0.69
7:A:103:ILE:HG22	7:A:457:ILE:HG21	1.91	0.68
8:K:47:MET:HG3	8:K:57:LEU:HB3	1.75	0.68
6:D:520:ARG:CG	6:D:520:ARG:HH21	2.07	0.68
1:N:181:VAL:HG22	1:N:193:MET:CB	2.23	0.68
3:G:153:SER:HB3	3:G:156:GLU:CB	2.36	0.68
2:H:333:CYS:SG	2:H:340:PRO:HD3	2.84	0.68
3:G:163:ARG:HG2	3:G:179:VAL:HG21	1.75	0.68
6:L:244:PRO:HD3	6:L:270:TYR:CE2	2.31	0.68
3:O:167:SER:O	3:O:168:SER:HB3	2.02	0.68
5:B:132:LEU:CD2	5:B:495:ARG:HG3	2.40	0.68
5:J:80:ILE:HD12	5:J:504:ALA:HB2	1.81	0.68
6:L:138:MET:SD	6:L:478:LEU:HD22	2.52	0.68
4:E:29:PHE:H	4:E:29:PHE:HD2	1.48	0.68
6:L:163:VAL:HG23	6:L:204:ILE:HG21	1.96	0.68
7:A:501:GLY:HA3	7:A:512:GLU:HG2	1.93	0.67
3:G:419:GLU:HB2	3:G:472:HIS:HE1	1.60	0.67
6:D:253:ILE:CG2	7:A:263:ASN:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:432:MET:SD	6:D:440:TRP:HZ3	2.17	0.67
6:D:35:ILE:HD11	6:D:65:LEU:HD21	2.30	0.67
5:J:279:PHE:HB3	5:J:281:ILE:CD1	2.55	0.67
1:N:178:VAL:HG22	1:N:399:LEU:HD23	1.74	0.67
2:P:509:VAL:CG1	2:P:510:LYS:N	2.61	0.67
6:D:353:ILE:CG2	6:D:354:ASP:H	2.08	0.67
4:E:211:VAL:HB	4:E:223:LEU:HD23	1.87	0.67
3:G:147:ILE:HD13	3:G:157:LEU:CD1	2.25	0.67
3:G:88:ARG:NH1	3:G:88:ARG:HG2	2.09	0.67
6:L:138:MET:SD	6:L:478:LEU:CD2	3.09	0.67
4:M:98:ASN:HD22	4:M:101:ALA:H	1.42	0.67
7:A:251:LEU:HD23	7:A:285:VAL:HG22	1.97	0.67
1:F:248:ASN:HB2	8:C:260:ASN:HB3	1.75	0.67
2:P:26:GLY:O	2:P:31:SER:HB2	1.94	0.67
1:F:79:ALA:HB2	1:F:523:ILE:HD12	1.76	0.67
6:L:238:GLN:HB2	6:L:334:ALA:HA	1.75	0.67
5:J:231:ILE:HD12	5:J:321:THR:HG21	1.76	0.67
4:M:73:ILE:HG22	5:J:511:VAL:HG13	1.77	0.67
8:C:162:LYS:O	8:C:164:VAL:N	2.28	0.66
8:C:219:VAL:HG22	8:C:379:ILE:HG12	1.76	0.66
3:G:55:THR:HG22	3:G:56:SER:H	1.59	0.66
3:G:245:ASN:HB3	3:G:336:SER:HA	1.77	0.66
7:I:55:ASP:O	7:I:56:ASP:HB3	2.01	0.66
4:M:40:ARG:NH1	4:M:42:HIS:ND1	2.94	0.66
3:O:77:HIS:HE1	3:O:79:ALA:HB3	1.59	0.66
2:P:509:VAL:CG1	2:P:510:LYS:H	2.15	0.66
6:D:479:ASN:HB2	6:D:491:ASN:OD1	1.95	0.66
8:C:414:PRO:CB	8:C:481:THR:HG23	2.25	0.66
7:I:41:LYS:HE2	7:I:103:ILE:HG23	1.78	0.66
3:O:221:LYS:HA	3:O:362:TYR:CZ	2.34	0.66
2:P:27:GLN:HA	2:P:31:SER:HB2	2.11	0.66
3:G:45:GLY:HA3	3:G:453:LEU:HD22	1.88	0.66
6:L:397:ALA:O	6:L:400:VAL:HG22	1.95	0.66
6:D:38:SER:HB2	6:D:46:LYS:HE3	1.78	0.66
7:A:53:LEU:HD23	8:C:527:VAL:HB	2.00	0.66
7:I:17:GLY:HA2	7:I:546:THR:O	1.95	0.66
4:M:107:LEU:HG	4:M:544:LEU:HD13	2.13	0.66
4:M:61:ILE:HD11	4:M:91:LEU:HD21	1.77	0.66
3:O:362:TYR:CE1	3:O:377:LEU:HD21	2.31	0.66
1:N:248:ASN:HB2	8:K:260:ASN:HB3	1.84	0.66
1:N:79:ALA:HB2	1:N:523:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:165:SER:O	7:A:166:SER:HB3	1.96	0.65
8:C:208:LYS:HD2	8:C:389:LEU:HB3	2.01	0.65
6:D:421:ILE:HG22	6:D:447:LEU:HD13	1.76	0.65
3:G:204:ILE:HD12	3:G:205:PRO:HD2	1.78	0.65
7:I:26:ARG:HG3	7:I:26:ARG:NH1	2.00	0.65
1:N:325:MET:HE3	1:N:336:ALA:HB1	1.79	0.65
3:O:282:LEU:HD21	3:O:306:PHE:HB3	2.06	0.65
1:F:75:LEU:HD12	8:C:55:LEU:HD23	1.78	0.65
8:K:50:ASP:HB2	8:K:51:PRO:CD	2.26	0.65
4:M:211:VAL:HB	4:M:223:LEU:HD23	1.76	0.65
7:A:109:LEU:HD11	7:A:538:ILE:HG21	1.79	0.65
7:A:190:GLN:HA	7:A:195:GLU:O	2.11	0.65
8:C:167:TRP:CE3	8:C:214:VAL:HB	2.31	0.65
4:E:144:ILE:HD11	4:E:550:LYS:HA	1.78	0.65
7:I:458:ILE:O	7:I:462:LEU:HG	2.05	0.65
6:L:214:VAL:HG23	6:L:376:SER:HB3	1.77	0.65
6:L:448:GLU:OE1	6:L:470:ARG:NH2	2.37	0.65
6:L:35:ILE:HA	6:L:46:LYS:HZ3	1.85	0.65
3:O:352:PHE:CD1	3:O:365:PHE:HB3	2.32	0.65
7:A:63:THR:HA	7:A:397:GLU:HG3	1.79	0.65
5:B:109:LEU:HB3	5:B:115:ILE:HD12	1.78	0.65
5:B:179:ASN:O	5:B:183:ARG:HB2	1.97	0.65
6:D:71:LEU:HD21	7:A:15:LEU:HB2	1.77	0.65
4:E:147:ALA:HB1	4:E:546:ARG:HG3	1.78	0.65
3:O:478:TRP:CE3	3:O:492:PHE:HB2	2.32	0.65
3:G:158:LEU:HB3	3:G:400:VAL:HG13	1.78	0.65
5:J:287:ARG:HG3	5:J:310:ASP:HA	1.79	0.65
10:K:1102:ADP:O3B	11:K:1103:BEF:F2	2.05	0.65
6:L:411:ILE:HD11	6:L:501:VAL:HA	1.78	0.65
4:M:413:LYS:H	5:J:79:ASN:ND2	2.02	0.65
3:O:147:ILE:HD13	3:O:157:LEU:HD11	1.85	0.65
3:G:352:PHE:CD1	3:G:365:PHE:HB3	2.32	0.65
5:J:233:ILE:HG12	5:J:285:ILE:HD11	1.78	0.65
2:P:509:VAL:HG12	2:P:510:LYS:N	2.14	0.65
6:D:520:ARG:NH2	6:D:520:ARG:HG3	2.16	0.64
2:H:24:ALA:O	2:H:28:ILE:N	2.29	0.64
5:J:181:ILE:HD11	5:J:388:LEU:HA	1.79	0.64
5:J:472:LEU:HB3	5:J:474:LEU:HD13	1.89	0.64
8:K:385:SER:HB3	8:K:388:ILE:HG12	1.93	0.64
4:E:292:VAL:HG21	5:B:260:GLN:HB3	1.78	0.64
1:F:326:GLU:HG2	8:C:232:PRO:HB3	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:250:ASN:HB3	7:A:300:LYS:HB3	1.79	0.64
6:D:353:ILE:CG2	6:D:354:ASP:N	2.61	0.64
3:O:206:GLY:HA2	4:M:110:SER:HB3	2.04	0.64
1:F:130:MET:HE1	1:F:514:ARG:CG	2.45	0.64
8:K:108:ALA:HB3	8:K:109:PRO:HD3	1.79	0.64
6:L:35:ILE:HA	6:L:46:LYS:HZ1	1.86	0.64
1:N:492:ASP:HB2	1:N:499:CYS:HB3	1.79	0.64
2:P:182:VAL:HG22	2:P:401:ILE:HG13	1.87	0.64
6:D:138:MET:SD	6:D:478:LEU:HD22	2.37	0.64
4:E:494:THR:O	4:E:498:LEU:HB2	1.98	0.64
4:E:73:ILE:HD11	5:B:72:PRO:HB2	1.96	0.64
1:F:509:SER:HB2	1:F:512:VAL:HG23	1.90	0.64
8:K:24:ASN:HD22	8:K:74:ALA:HB2	1.78	0.64
6:D:420:GLU:HB2	6:D:473:HIS:CE1	2.38	0.64
3:G:220:PHE:C	3:G:222:LYS:H	1.99	0.64
7:I:75:VAL:HG21	7:I:84:VAL:HG21	1.79	0.64
5:J:39:PRO:HD2	5:J:474:LEU:HD23	1.80	0.64
8:K:162:LYS:O	8:K:164:VAL:N	2.35	0.64
6:L:448:GLU:CD	6:L:470:ARG:NH2	2.80	0.64
5:B:59:ASP:HB3	5:B:62:THR:OG1	1.97	0.64
4:E:73:ILE:HG23	5:B:514:ILE:HG12	1.79	0.64
3:G:323:MET:HA	3:G:326:VAL:HG12	1.79	0.64
3:G:37:GLN:HG3	3:G:103:ILE:HA	1.80	0.64
1:N:251:PHE:CB	8:K:263:ILE:HB	2.28	0.64
7:A:199:PRO:HB2	7:A:202:ALA:HB2	1.80	0.64
3:G:282:LEU:HD21	3:G:306:PHE:HB3	1.79	0.64
5:J:183:ARG:NH2	5:J:210:GLU:HA	2.12	0.64
4:M:412:ASN:HB2	5:J:80:ILE:HG12	1.80	0.64
2:H:509:VAL:CG1	2:H:510:LYS:N	2.61	0.63
8:K:161:THR:HG22	8:K:162:LYS:HG3	1.79	0.63
1:F:535:ARG:NH1	2:P:6:PRO:HB2	2.13	0.63
6:D:502:LEU:HA	6:D:505:THR:HB	1.81	0.63
2:H:420:LEU:HD11	2:H:521:LEU:HD12	1.79	0.63
6:D:224:GLY:HA3	6:D:306:SER:OG	2.15	0.63
1:F:153:VAL:HG11	1:F:405:VAL:HG21	1.80	0.63
1:F:130:MET:HE1	1:F:514:ARG:HG2	1.90	0.63
1:N:221:HIS:HD2	1:N:223:ASP:H	1.47	0.63
1:F:221:HIS:HD2	1:F:223:ASP:H	1.44	0.63
6:L:242:SER:HB3	6:L:243:PRO:CD	2.38	0.63
2:P:24:ALA:O	2:P:28:ILE:N	2.21	0.63
7:A:63:THR:HG23	7:A:397:GLU:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:460:ASP:O	3:O:464:ILE:HG12	2.26	0.63
7:A:75:VAL:HG21	7:A:84:VAL:HG21	1.92	0.63
8:C:121:ILE:HG23	8:C:441:PRO:HB3	1.93	0.63
6:D:31:VAL:HG21	6:D:75:ALA:HB1	1.85	0.63
1:F:173:ILE:HG23	1:F:209:PHE:HB2	2.07	0.63
3:G:204:ILE:HD13	3:G:362:TYR:HE2	2.00	0.63
5:B:441:PRO:HB3	5:B:472:LEU:HD11	1.81	0.63
4:E:412:ASN:HB3	4:E:415:ILE:HD12	1.80	0.63
4:E:168:ILE:HD11	4:E:439:VAL:HG13	1.80	0.63
1:F:325:MET:HE3	1:F:336:ALA:HB1	2.06	0.63
5:J:59:ASP:HB3	5:J:62:THR:OG1	2.20	0.63
4:E:73:ILE:CG2	5:B:514:ILE:HG12	2.29	0.63
6:D:138:MET:SD	6:D:478:LEU:CD2	2.87	0.63
4:M:412:ASN:HB3	4:M:415:ILE:CD1	2.29	0.63
7:A:28:GLN:HE21	7:A:77:HIS:HE1	1.56	0.62
8:C:421:MET:HG2	8:C:453:PRO:HG2	2.10	0.62
1:N:163:ASP:HB2	1:N:166:LEU:HB3	1.81	0.62
5:J:293:TYR:HB3	5:J:294:PRO:HD3	1.80	0.62
8:K:324:ASP:HA	8:K:327:ARG:NH2	2.25	0.62
5:J:441:PRO:HA	5:J:444:LEU:HD12	1.81	0.62
4:M:60:ILE:O	4:M:72:LYS:HE2	2.08	0.62
8:C:183:ARG:HD3	8:C:407:MET:HE3	2.08	0.62
7:I:160:ALA:O	7:I:164:MET:HG2	2.00	0.62
6:L:162:ILE:HB	7:I:540:ARG:HD3	1.82	0.62
4:M:228:GLY:HA3	4:M:420:GLU:OE2	2.13	0.62
3:O:74:ASP:O	4:M:32:VAL:HA	2.14	0.62
5:B:238:LEU:HD13	5:B:290:ILE:HG23	1.81	0.62
5:B:317:LEU:HA	5:B:320:VAL:HG12	1.98	0.62
8:C:111:LEU:HD22	8:C:440:TRP:HB3	1.92	0.62
3:G:26:ILE:O	3:G:30:ILE:HD12	2.00	0.62
7:I:198:TYR:CE2	7:I:413:LEU:HB3	2.35	0.62
3:O:419:GLU:HB2	3:O:472:HIS:HE1	1.63	0.62
5:B:82:LYS:NZ	5:B:86:ASP:OD2	2.32	0.62
6:L:42:LYS:HE2	6:L:484:VAL:HG13	1.80	0.62
6:D:50:THR:HG22	6:D:52:ARG:H	1.65	0.62
8:C:81:LEU:CD1	8:C:516:SER:HB2	2.30	0.62
6:D:242:SER:HB3	6:D:243:PRO:CD	2.29	0.62
1:F:87:THR:CG2	1:F:512:VAL:HG22	2.35	0.62
4:E:64:SER:HB2	4:E:72:LYS:HZ3	1.76	0.62
8:K:481:THR:HG21	8:K:495:VAL:HG23	2.15	0.62
6:L:239:PHE:HB3	6:L:334:ALA:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:458:ILE:O	7:A:462:LEU:HG	2.15	0.61
3:G:326:VAL:HG23	3:G:365:PHE:HE1	1.65	0.61
6:D:220:ILE:HG21	6:D:302:LEU:HD21	1.84	0.61
6:L:502:LEU:HA	6:L:505:THR:HB	2.22	0.61
4:M:86:ASP:HB3	4:M:89:THR:OG1	2.53	0.61
8:C:167:TRP:HE3	8:C:215:LEU:HD13	1.86	0.61
4:E:412:ASN:HB3	4:E:415:ILE:CD1	2.29	0.61
4:E:60:ILE:O	4:E:72:LYS:HE2	2.00	0.61
1:F:225:PRO:HG2	1:F:315:LEU:HB2	1.82	0.61
4:M:245:LEU:HD11	4:M:354:ILE:HD11	2.28	0.61
1:N:56:THR:HB	1:N:61:VAL:HG11	1.82	0.61
8:C:159:ILE:O	8:C:161:THR:N	2.37	0.61
5:J:184:LEU:HD11	5:J:192:HIS:HB2	1.81	0.61
3:O:26:ILE:O	3:O:30:ILE:HD12	2.18	0.61
2:P:43:LEU:HG	2:P:462:THR:CG2	2.38	0.61
8:C:183:ARG:HD3	8:C:407:MET:CE	2.56	0.61
3:O:20:SER:HB2	3:O:25:GLN:NE2	2.18	0.61
1:F:7:ASN:ND2	1:F:10:ALA:HB2	2.70	0.61
5:J:183:ARG:HH22	5:J:211:GLY:N	2.05	0.61
7:A:501:GLY:CA	7:A:512:GLU:HG2	2.48	0.61
6:D:35:ILE:HA	6:D:46:LYS:HZ3	1.64	0.61
4:E:507:ILE:HG22	4:E:509:ASN:H	1.67	0.61
5:J:405:GLY:O	5:J:408:GLU:HG2	2.37	0.61
6:L:244:PRO:HD3	6:L:270:TYR:HE2	1.75	0.61
4:M:240:ILE:HD13	4:M:244:ILE:HD11	2.73	0.61
5:B:184:LEU:HD11	5:B:192:HIS:HB2	1.83	0.61
7:I:304:ASP:HA	7:I:307:LEU:HD12	1.81	0.61
1:F:111:GLU:HG2	1:N:467:LEU:HD13	2.43	0.61
2:H:428:ILE:HD11	2:H:460:PRO:HG3	1.83	0.61
6:L:89:ALA:HA	6:L:403:CYS:SG	2.40	0.61
3:O:242:LEU:HD22	3:O:244:LEU:HG	1.82	0.61
1:N:251:PHE:HZ	2:P:259:THR:HB	1.85	0.61
1:F:251:PHE:CB	8:C:263:ILE:HB	2.31	0.60
3:G:221:LYS:HA	3:G:362:TYR:CZ	2.49	0.60
1:N:47:VAL:HB	2:P:546:MET:HG2	1.83	0.60
8:C:353:GLY:HA3	8:C:370:ASN:CB	2.31	0.60
7:I:126:ILE:HG13	7:I:539:LEU:HD23	1.82	0.60
5:B:476:ASN:HB3	5:B:478:THR:HG22	1.83	0.60
1:F:269:PHE:HA	8:C:270:ASN:HD21	1.65	0.60
8:C:62:HIS:O	8:C:66:ARG:HB2	2.01	0.60
6:D:181:ILE:HD11	6:D:193:ASP:HB3	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:164:VAL:CG1	8:K:171:MET:HG3	2.31	0.60
8:K:41:PRO:HG2	8:K:486:GLY:HA3	1.82	0.60
8:C:108:ALA:HB3	8:C:109:PRO:HD3	1.83	0.60
6:D:165:GLN:HG3	7:A:130:ARG:CD	2.39	0.60
4:E:32:VAL:HG11	7:I:4:LEU:HD21	1.83	0.60
4:M:327:PHE:CD2	4:M:344:ARG:HD3	2.62	0.60
8:C:414:PRO:HB2	8:C:481:THR:HG23	1.82	0.60
4:E:457:GLU:O	4:E:461:GLN:HG2	2.22	0.60
1:F:124:ILE:HD11	1:F:434:LEU:HD11	1.81	0.60
2:H:291:ILE:HD13	2:H:347:PRO:HG3	1.82	0.60
7:A:86:LEU:HD21	7:A:101:VAL:HG12	1.82	0.60
6:L:59:ASN:HB3	6:L:161:LYS:HG2	2.20	0.60
4:M:448:VAL:HG21	4:M:498:LEU:HD22	1.83	0.60
1:N:450:ALA:O	1:N:453:VAL:HG22	2.13	0.60
6:D:135:LEU:HA	6:D:138:MET:HG2	1.94	0.60
1:F:458:LEU:HD22	1:F:493:LEU:HD11	1.82	0.60
4:M:275:PRO:HD3	4:M:325:TRP:HE3	1.66	0.60
1:F:296:ILE:HG12	1:F:317:LEU:HD23	1.83	0.60
7:I:538:ILE:HA	7:I:541:ILE:HD12	1.91	0.60
8:K:59:ASN:CB	8:K:162:LYS:HG2	2.28	0.60
5:B:232:LEU:HB2	5:B:281:ILE:CD1	2.34	0.60
5:B:508:LEU:O	5:B:511:VAL:HB	2.02	0.60
6:L:74:VAL:HG13	6:L:518:ILE:HD12	1.84	0.60
4:E:327:PHE:CE2	4:E:342:ALA:HB1	2.37	0.59
1:F:337:GLN:CG	1:F:347:ILE:HG21	2.35	0.59
5:J:192:HIS:CD2	5:J:319:LEU:HD12	2.37	0.59
3:O:464:ILE:O	3:O:468:LEU:HB2	2.02	0.59
3:G:215:ILE:HG22	3:G:217:GLY:H	1.67	0.59
3:G:204:ILE:HG23	3:G:379:ARG:HD3	1.99	0.59
1:N:153:VAL:HG11	1:N:405:VAL:HG21	1.87	0.59
1:N:19:LEU:O	1:N:23:VAL:HG23	2.02	0.59
6:D:162:ILE:HB	7:A:540:ARG:HD3	1.84	0.59
5:B:181:ILE:HD11	5:B:388:LEU:HA	1.84	0.59
2:H:25:ASP:C	2:H:27:GLN:H	2.03	0.59
5:J:14:ARG:HG2	5:J:15:ALA:H	1.67	0.59
3:O:449:ILE:O	3:O:453:LEU:HG	2.03	0.59
2:H:478:LEU:HD22	2:H:499:VAL:HG23	2.10	0.59
7:I:17:GLY:CA	7:I:546:THR:O	2.57	0.59
6:D:125:GLN:HE21	6:D:513:GLU:HA	1.66	0.59
4:E:273:THR:HG23	4:E:324:GLN:OE1	2.01	0.59
7:I:83:LEU:HD23	7:I:102:VAL:HG13	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:190:GLN:HA	7:I:195:GLU:O	2.35	0.59
5:B:162:SER:HA	5:B:167:SER:OG	2.02	0.59
2:H:154:ASN:HB3	2:H:190:LEU:HD13	1.99	0.59
2:H:299:ILE:HD12	2:H:313:LEU:HD21	2.11	0.59
2:H:498:GLY:O	2:H:509:VAL:HG13	2.03	0.59
4:M:287:LEU:HD12	5:J:248:THR:HG22	1.96	0.59
4:M:64:SER:HB2	4:M:72:LYS:NZ	2.18	0.59
8:C:146:GLU:OE2	8:C:183:ARG:NH1	2.34	0.59
6:D:89:ALA:HA	6:D:403:CYS:SG	2.42	0.59
3:G:220:PHE:HD2	3:G:363:ASN:HB2	1.67	0.59
7:I:173:SER:O	7:I:177:SER:HB2	2.06	0.59
7:A:159:ILE:HD13	7:A:412:THR:HG21	1.85	0.59
7:I:188:LYS:HG2	7:I:198:TYR:CE1	2.37	0.59
3:O:20:SER:HB2	3:O:25:GLN:HE21	1.68	0.59
7:I:97:GLY:O	7:I:101:VAL:HG23	2.12	0.59
6:L:220:ILE:HG21	6:L:302:LEU:HD21	2.01	0.59
8:C:119:VAL:HA	8:C:122:ILE:HD12	1.84	0.59
8:C:385:SER:HB3	8:C:388:ILE:HG12	1.85	0.59
4:E:98:ASN:HD22	4:E:101:ALA:H	1.51	0.59
2:H:123:SER:HB3	2:H:126:GLU:HG3	1.84	0.59
8:K:402:VAL:HA	8:K:405:ASN:HD22	1.99	0.59
8:C:125:LEU:HD22	8:C:445:VAL:CG2	2.33	0.58
1:F:439:LYS:O	1:F:442:THR:HG22	2.02	0.58
10:J:602:ADP:O3B	11:J:603:BEF:F3	2.10	0.58
3:O:268:GLN:HA	3:O:271:VAL:HG12	1.85	0.58
7:A:89:GLN:HA	7:A:92:ARG:HD3	2.02	0.58
5:B:505:ALA:O	5:B:509:LEU:HB2	2.03	0.58
6:D:234:ILE:H	6:D:345:ASP:HB3	1.69	0.58
2:H:27:GLN:CA	2:H:31:SER:HB2	2.31	0.58
6:L:503:VAL:O	6:L:507:ALA:HB2	2.22	0.58
1:N:337:GLN:CG	1:N:347:ILE:HG21	2.33	0.58
3:G:352:PHE:HD1	3:G:365:PHE:HB3	1.68	0.58
2:H:186:VAL:HG11	2:H:408:VAL:HG11	1.84	0.58
7:I:104:ILE:HG12	7:I:458:ILE:HD11	1.85	0.58
8:K:142:PRO:HA	8:K:411:SER:HA	1.84	0.58
1:N:171:THR:HB	1:N:172:PRO:HD3	1.85	0.58
2:H:509:VAL:HG12	2:H:510:LYS:N	2.19	0.58
5:J:317:LEU:HA	5:J:320:VAL:HG12	1.98	0.58
5:B:406:CYS:O	5:B:410:VAL:HG23	2.05	0.58
7:I:54:VAL:HG12	7:I:56:ASP:H	1.69	0.58
4:M:219:VAL:CG1	4:M:431:ARG:HB2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:73:ILE:HG23	5:J:514:ILE:HG12	2.07	0.58
2:P:33:ALA:HA	2:P:36:ARG:HD3	1.87	0.58
7:A:17:GLY:CA	7:A:546:THR:O	2.56	0.58
6:D:397:ALA:O	6:D:400:VAL:HG22	2.04	0.58
3:G:77:HIS:CE1	3:G:79:ALA:HB3	2.43	0.58
2:H:322:LYS:O	2:H:323:VAL:HB	2.15	0.58
7:I:63:THR:HG22	7:I:64:ASN:N	2.36	0.58
3:O:153:SER:HB3	3:O:156:GLU:CB	2.34	0.58
8:C:81:LEU:HD13	8:C:516:SER:HB2	1.86	0.58
2:H:39:HIS:O	2:H:43:LEU:HB2	2.04	0.58
6:L:177:SER:OG	6:L:375:VAL:HG11	2.03	0.58
4:E:141:ILE:HD11	6:L:463:ILE:HD12	1.94	0.58
2:P:284:ILE:HD11	2:P:308:LEU:HB3	1.88	0.58
2:P:388:GLY:HA3	2:P:394:LEU:HD21	2.16	0.58
5:B:194:GLN:HB2	5:B:316:ARG:NH1	2.18	0.58
5:B:490:SER:HB3	5:B:493:LEU:HB2	1.84	0.58
5:J:109:LEU:HB3	5:J:115:ILE:HD12	1.86	0.58
1:N:26:ALA:HB3	1:N:102:LEU:HD12	1.86	0.58
3:G:167:SER:O	3:G:168:SER:HB3	2.04	0.58
5:J:232:LEU:HB2	5:J:281:ILE:CD1	2.34	0.58
8:K:89:VAL:HG11	8:K:505:ILE:HG13	2.76	0.58
1:N:242:TYR:CZ	2:P:260:GLU:HB3	2.39	0.58
2:H:512:ILE:HG23	2:H:517:ILE:HB	1.95	0.58
5:J:197:LYS:NZ	5:J:378:ASP:OD1	2.78	0.58
3:O:163:ARG:HG2	3:O:179:VAL:HG21	1.91	0.58
3:O:326:VAL:HG23	3:O:365:PHE:HE1	1.69	0.58
5:B:155:HIS:CB	5:B:488:VAL:HG22	2.56	0.57
1:F:210:ILE:HD13	1:F:214:VAL:HG21	1.84	0.57
8:K:159:ILE:O	8:K:161:THR:N	2.33	0.57
7:A:160:ALA:O	7:A:164:MET:HG2	2.27	0.57
5:J:184:LEU:HD11	5:J:192:HIS:CB	2.34	0.57
8:K:105:ALA:O	8:K:109:PRO:HD2	2.28	0.57
2:P:65:THR:HG22	2:P:67:ASP:H	1.71	0.57
7:A:247:LEU:HD11	7:A:288:ILE:HD13	1.87	0.57
4:M:29:PHE:HD2	4:M:29:PHE:H	1.53	0.57
6:D:244:PRO:CD	6:D:270:TYR:CE2	2.95	0.57
6:D:72:HIS:CD2	6:D:74:VAL:HB	2.55	0.57
4:M:180:LEU:HD22	4:M:430:VAL:HG13	1.89	0.57
4:M:275:PRO:HD3	4:M:325:TRP:CE3	2.39	0.57
5:B:301:LEU:HD23	5:B:303:ILE:HD11	1.86	0.57
5:B:46:LEU:HD21	5:B:63:ILE:HG23	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:208:LYS:HB3	8:C:389:LEU:HD13	1.99	0.57
8:C:198:ILE:CG2	8:C:408:LEU:HD21	2.48	0.57
7:A:209:HIS:HE1	8:C:83:ARG:HH21	1.52	0.57
3:G:232:GLN:HG2	3:G:308:ALA:HA	1.86	0.57
5:J:439:GLN:O	5:J:443:ILE:HG13	2.33	0.57
6:L:125:GLN:HE21	6:L:513:GLU:HA	2.07	0.57
2:P:215:GLY:H	3:O:505:ASN:HD21	1.68	0.57
8:C:402:VAL:HA	8:C:405:ASN:ND2	2.35	0.57
8:C:444:ALA:HA	8:C:447:ASP:HB2	1.87	0.57
4:E:40:ARG:NH1	4:E:42:HIS:ND1	2.52	0.57
4:E:72:LYS:HG3	5:B:513:ASN:HB3	1.87	0.57
5:J:183:ARG:HH22	5:J:210:GLU:HA	1.68	0.57
8:K:65:LEU:HB3	8:K:79:LEU:HD13	1.92	0.57
3:O:94:VAL:HG11	3:O:502:VAL:HG22	1.91	0.57
6:D:203:THR:HA	7:A:533:GLU:OE2	2.04	0.57
5:B:194:GLN:HB2	5:B:316:ARG:HH12	1.69	0.57
5:B:233:ILE:HG12	5:B:285:ILE:HD11	1.86	0.57
6:D:353:ILE:HG22	6:D:354:ASP:H	1.68	0.57
6:L:514:CYS:O	6:L:518:ILE:HG12	2.34	0.57
4:M:412:ASN:HB3	4:M:415:ILE:HD12	1.87	0.57
7:I:251:LEU:HD23	7:I:285:VAL:HG22	1.95	0.57
8:K:174:LEU:HD22	8:K:219:VAL:HG23	1.85	0.57
7:I:462:LEU:HB3	7:I:504:LEU:HD11	1.87	0.56
7:I:535:CYS:O	7:I:539:LEU:HB2	2.05	0.56
5:B:293:TYR:HB3	5:B:294:PRO:HD3	1.86	0.56
8:C:402:VAL:HA	8:C:405:ASN:HD22	1.80	0.56
5:J:98:LEU:HB2	5:J:440:LEU:HD11	1.87	0.56
8:K:107:CYS:SG	8:K:108:ALA:N	3.12	0.56
4:M:507:ILE:HG22	4:M:509:ASN:H	1.70	0.56
2:P:56:VAL:HB	3:O:525:THR:HG23	1.90	0.56
4:E:413:LYS:H	5:B:79:ASN:ND2	2.15	0.56
6:L:234:ILE:HB	6:L:345:ASP:HB3	1.85	0.56
5:B:373:THR:HG22	5:B:375:GLN:H	1.94	0.56
8:C:167:TRP:CE3	8:C:215:LEU:HD13	2.72	0.56
8:C:174:LEU:HD22	8:C:219:VAL:HG23	2.55	0.56
1:F:262:LEU:HA	1:F:265:SER:HB2	1.86	0.56
7:I:250:ASN:HB3	7:I:300:LYS:HB3	1.86	0.56
8:K:81:LEU:HD13	8:K:516:SER:HB2	1.87	0.56
6:L:171:ALA:HB3	6:L:172:PRO:HD3	1.91	0.56
4:M:72:LYS:HG3	5:J:513:ASN:HB3	2.01	0.56
4:E:74:LEU:HD13	4:E:93:GLN:HG3	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:135:LEU:HD23	3:G:424:LEU:HD23	1.87	0.56
2:H:247:VAL:HG22	2:H:298:CYS:HB3	1.87	0.56
5:J:255:THR:CG2	6:L:263:ILE:HA	2.35	0.56
7:A:141:ASN:HA	7:A:144:LEU:HD12	1.87	0.56
4:E:412:ASN:ND2	4:E:414:MET:SD	2.72	0.56
8:K:102:GLU:OE1	8:K:451:CYS:HB2	2.06	0.56
6:L:195:ARG:HD3	6:L:323:PHE:CZ	2.41	0.56
6:L:432:MET:SD	6:L:440:TRP:CZ3	3.33	0.56
3:O:189:LEU:HD13	3:O:199:ILE:HG23	2.05	0.56
7:I:50:ASP:OD1	7:I:64:ASN:HB2	2.06	0.56
2:P:478:LEU:HD22	2:P:499:VAL:HG23	2.31	0.56
2:P:65:THR:HG21	2:P:70:THR:HB	1.97	0.56
8:C:164:VAL:CG1	8:C:171:MET:HG3	2.42	0.56
6:D:239:PHE:HB3	6:D:334:ALA:O	2.05	0.56
6:D:451:PRO:HB3	6:D:482:ILE:HD11	1.86	0.56
6:D:76:ARG:HH11	6:D:76:ARG:HG2	1.70	0.56
2:H:509:VAL:CG1	2:H:510:LYS:H	2.18	0.56
8:C:41:PRO:HG2	8:C:486:GLY:HA3	2.07	0.56
4:E:115:ILE:HD11	4:E:536:GLN:HB3	1.89	0.56
3:G:173:ASN:HD21	4:E:148:ASN:HA	1.71	0.56
2:H:54:ILE:HD11	3:G:78:PRO:HB2	1.88	0.56
7:I:89:GLN:HA	7:I:92:ARG:HD3	1.88	0.56
5:J:441:PRO:HB3	5:J:472:LEU:HD11	2.27	0.56
5:B:293:TYR:HB3	5:B:294:PRO:CD	2.36	0.56
7:A:71:SER:HB2	7:A:88:GLN:NE2	2.22	0.56
4:E:220:ASP:HB3	4:E:223:LEU:HB2	2.52	0.56
2:H:310:LEU:O	2:H:314:ASN:HB2	2.06	0.56
6:L:224:GLY:HA3	6:L:306:SER:OG	2.05	0.56
7:A:39:VAL:HG11	7:A:73:LEU:HD11	2.02	0.55
1:F:370:ASN:H	1:F:370:ASN:HD22	1.53	0.55
2:H:311:HIS:CD2	3:G:336:SER:H	2.48	0.55
7:I:55:ASP:CB	7:I:59:ASP:O	2.86	0.55
3:O:224:PHE:CD2	3:O:225:SER:N	2.91	0.55
3:O:337:THR:HG22	3:O:339:SER:H	1.71	0.55
2:P:232:PRO:HG3	2:P:369:THR:OG1	2.33	0.55
2:P:43:LEU:HG	2:P:462:THR:HG22	1.88	0.55
7:A:4:LEU:HD21	4:M:32:VAL:HG11	1.99	0.55
7:A:41:LYS:HE2	7:A:103:ILE:HG23	2.43	0.55
6:D:367:ARG:O	6:D:368:ASN:CB	2.58	0.55
4:E:448:VAL:HG21	4:E:498:LEU:HD22	2.01	0.55
1:F:171:THR:HB	1:F:172:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:ILE:HD12	1:F:510:TYR:HA	1.88	0.55
2:H:33:ALA:HA	2:H:36:ARG:HD3	1.89	0.55
8:K:464:PRO:O	8:K:468:LEU:HB2	2.31	0.55
3:O:411:ALA:HB2	3:O:478:TRP:CD2	2.42	0.55
5:B:230:LYS:O	5:B:281:ILE:HG23	2.14	0.55
8:C:250:LEU:HD12	8:C:301:VAL:HG22	1.89	0.55
8:C:324:ASP:OD1	8:C:327:ARG:NH2	2.39	0.55
6:D:35:ILE:HD12	6:D:97:VAL:HG11	2.36	0.55
7:I:228:VAL:HG12	7:I:233:MET:SD	2.60	0.55
4:M:544:LEU:O	4:M:548:ILE:HG12	2.34	0.55
5:B:127:ALA:HB2	5:B:430:VAL:HG13	1.88	0.55
8:C:167:TRP:N	8:C:167:TRP:CD1	2.74	0.55
8:C:297:THR:HG22	8:C:299:LYS:H	1.80	0.55
6:D:143:SER:HB2	6:D:146:ASP:HB2	1.89	0.55
2:H:27:GLN:HE22	2:H:81:ALA:HB2	1.71	0.55
5:J:471:GLY:HA3	5:J:482:MET:CG	2.52	0.55
4:M:84:THR:HG22	4:M:418:GLU:OE1	2.08	0.55
7:A:28:GLN:HE21	7:A:77:HIS:CE1	2.30	0.55
5:B:152:ASP:OD1	5:B:400:THR:HG21	2.07	0.55
8:C:369:ASP:HB3	8:C:370:ASN:HD22	2.00	0.55
4:E:67:PRO:HA	4:E:190:SER:HA	1.88	0.55
4:E:322:ILE:HG23	4:E:346:VAL:HG21	1.88	0.55
3:G:7:THR:O	3:G:8:PRO:O	2.26	0.55
7:I:199:PRO:HB2	7:I:202:ALA:HB2	1.89	0.55
7:I:53:LEU:HD23	8:K:527:VAL:HB	1.89	0.55
4:M:464:ILE:H	4:M:464:ILE:HD12	1.71	0.55
8:C:324:ASP:HA	8:C:327:ARG:NH2	2.25	0.55
7:A:394:SER:HB2	8:C:519:LEU:HD22	2.16	0.55
3:G:221:LYS:HA	3:G:362:TYR:CE1	2.57	0.55
2:H:111:LEU:HD11	2:H:538:VAL:HG21	2.03	0.55
7:I:281:VAL:O	7:I:285:VAL:HG23	2.30	0.55
8:K:96:VAL:HG22	8:K:509:SER:HA	2.05	0.55
6:L:138:MET:SD	6:L:478:LEU:HD21	2.80	0.55
6:L:295:ASP:O	6:L:296:ALA:HB3	2.07	0.55
1:N:203:SER:O	1:N:206:ASP:HB2	2.17	0.55
1:N:368:THR:HG22	1:N:369:GLU:H	1.97	0.55
3:O:174:ASN:ND2	4:M:546:ARG:HH22	2.04	0.55
7:A:523:SER:O	7:A:527:SER:HB2	2.07	0.55
5:B:165:ILE:HG12	6:D:520:ARG:NH2	2.70	0.55
5:J:179:ASN:O	5:J:183:ARG:HB2	2.08	0.55
3:O:319:SER:HB3	3:O:322:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:13:GLU:O	5:B:18:ALA:HB2	2.06	0.55
5:B:503:GLU:O	5:B:507:VAL:HG23	2.15	0.55
3:G:167:SER:O	3:G:168:SER:CB	2.58	0.55
3:G:383:GLU:HA	3:G:386:ILE:HD12	1.89	0.55
3:G:411:ALA:HB2	3:G:478:TRP:CD2	2.41	0.55
7:I:252:GLN:HA	7:I:303:ASP:HB2	1.97	0.55
7:I:417:ASN:HB3	7:I:521:THR:HB	1.90	0.55
8:K:457:ILE:HD11	8:K:484:ILE:HG12	1.89	0.55
1:N:337:GLN:HG2	1:N:347:ILE:HG21	1.89	0.55
1:F:248:ASN:HD22	8:C:260:ASN:HB3	1.72	0.55
3:G:200:GLY:HA3	3:G:325:ARG:CZ	2.67	0.55
3:G:198:LEU:HB3	3:G:373:THR:OG1	2.27	0.55
5:J:74:ALA:O	5:J:78:VAL:HG23	2.34	0.55
6:L:237:ILE:HG22	6:L:239:PHE:H	1.72	0.55
7:A:83:LEU:HD23	7:A:102:VAL:HG13	2.09	0.54
5:B:183:ARG:HH22	5:B:211:GLY:H	1.64	0.54
5:B:281:ILE:HG22	5:B:283:THR:H	1.72	0.54
1:F:153:VAL:HG11	1:F:405:VAL:CG2	2.36	0.54
7:I:99:THR:O	7:I:103:ILE:HG13	2.13	0.54
8:K:322:LYS:HD3	8:K:322:LYS:H	1.71	0.54
1:N:430:ASN:HD21	1:N:441:LYS:CB	2.20	0.54
1:N:458:LEU:HD22	1:N:493:LEU:HD11	1.88	0.54
1:N:56:THR:HG22	1:N:58:ASP:H	1.72	0.54
3:O:352:PHE:HD1	3:O:365:PHE:HB3	1.70	0.54
3:O:133:VAL:HB	3:O:511:THR:HG21	1.88	0.54
7:A:333:THR:HG22	7:A:377:THR:HG22	1.89	0.54
8:C:401:ALA:O	8:C:404:ARG:HG3	2.25	0.54
4:E:423:LEU:O	4:E:427:LEU:N	2.39	0.54
1:F:178:VAL:HG22	1:F:399:LEU:HD23	1.98	0.54
2:H:227:VAL:HG13	2:H:368:VAL:CG1	2.37	0.54
8:K:369:ASP:HB3	8:K:370:ASN:HD22	1.88	0.54
1:N:296:ILE:HA	1:N:317:LEU:HB3	1.88	0.54
2:P:428:ILE:HD11	2:P:460:PRO:HG3	1.98	0.54
8:C:322:LYS:H	8:C:322:LYS:HD3	1.88	0.54
4:M:269:LEU:H	4:M:375:GLY:H	1.54	0.54
7:A:415:SER:OG	7:A:522:ILE:HD11	2.07	0.54
8:C:161:THR:HG22	8:C:162:LYS:HG3	1.88	0.54
8:C:414:PRO:HB3	8:C:481:THR:HG23	1.89	0.54
1:F:103:ARG:O	1:F:107:ARG:HD2	2.17	0.54
8:K:222:GLY:HA2	8:K:331:VAL:HG11	2.07	0.54
1:N:326:GLU:HG2	8:K:232:PRO:HB3	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:63:THR:HG22	7:A:64:ASN:N	2.23	0.54
6:L:181:ILE:HD11	6:L:193:ASP:HB3	1.90	0.54
4:M:457:GLU:O	4:M:461:GLN:HG2	2.17	0.54
3:O:242:LEU:HD21	3:O:341:ILE:HD13	1.90	0.54
2:P:109:GLU:HG2	2:P:458:VAL:CG2	2.37	0.54
5:B:374:ASP:HB2	6:D:80:GLU:OE1	2.39	0.54
3:G:261:VAL:HG21	3:G:270:ILE:HD13	2.04	0.54
2:H:48:PRO:HB3	2:H:172:TYR:CD1	2.42	0.54
2:H:65:THR:HG21	2:H:70:THR:HB	1.94	0.54
1:N:269:PHE:HA	8:K:270:ASN:HD21	1.98	0.54
6:L:31:VAL:HG21	6:L:75:ALA:HB1	2.13	0.54
1:N:459:VAL:HG22	1:N:491:VAL:HG11	1.89	0.54
3:O:249:GLU:O	3:O:278:ILE:HG21	2.74	0.54
2:P:123:SER:HB3	2:P:126:GLU:HG3	1.88	0.54
2:P:509:VAL:HG13	2:P:510:LYS:H	1.79	0.54
5:B:412:SER:O	5:B:416:ASP:HB2	2.07	0.54
10:B:602:ADP:O3B	11:B:603:BEF:F2	2.54	0.54
8:C:122:ILE:HG23	8:C:518:CYS:HB3	1.89	0.54
6:D:436:GLN:HA	6:D:439:ILE:HD12	1.88	0.54
2:H:79:HIS:HD2	2:H:81:ALA:H	1.56	0.54
5:J:22:ALA:HA	5:J:73:ALA:CB	2.38	0.54
7:I:212:SER:HB2	8:K:511:LYS:HE3	2.04	0.54
3:O:220:PHE:C	3:O:222:LYS:H	2.11	0.54
3:O:385:VAL:O	3:O:389:VAL:HG23	2.08	0.54
5:B:121:ILE:HG12	5:B:506:GLU:HG2	1.90	0.54
10:D:602:ADP:O3B	11:D:603:BEF:F2	2.24	0.54
3:G:113:LYS:O	3:G:117:GLU:HG2	2.08	0.54
3:G:323:MET:O	3:G:326:VAL:HG12	2.07	0.54
4:M:251:HIS:CE1	5:J:325:VAL:HB	2.43	0.54
8:K:219:VAL:HG22	8:K:379:ILE:HG12	1.90	0.54
3:O:158:LEU:HB3	3:O:400:VAL:HG13	1.98	0.54
5:B:472:LEU:HB3	5:B:474:LEU:HD13	1.91	0.54
5:B:132:LEU:HD23	5:B:495:ARG:HG3	1.89	0.54
10:C:1102:ADP:O3B	11:C:1103:BEF:F2	2.15	0.54
8:C:223:VAL:HA	8:C:378:THR:OG1	2.08	0.54
4:E:161:LEU:HD11	4:E:440:VAL:HG11	2.14	0.54
7:A:228:VAL:HG12	7:A:233:MET:SD	2.48	0.54
4:E:291:SER:HB3	4:E:294:GLU:HB2	2.21	0.54
5:J:69:LEU:O	5:J:75:LYS:HE3	2.08	0.54
2:P:329:LEU:O	2:P:333:CYS:HB2	2.39	0.54
7:A:26:ARG:CG	7:A:26:ARG:NH1	2.58	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:451:SER:O	4:E:455:SER:HB2	2.15	0.53
4:E:544:LEU:O	4:E:548:ILE:HG12	2.24	0.53
7:I:141:ASN:HA	7:I:144:LEU:HD12	2.02	0.53
6:L:253:ILE:CG2	7:I:263:ASN:HB2	2.38	0.53
8:C:222:GLY:HA2	8:C:331:VAL:HG11	2.04	0.53
1:N:189:LEU:HD22	8:K:364:TYR:HE1	1.73	0.53
4:M:67:PRO:HA	4:M:190:SER:HA	1.90	0.53
3:O:297:LEU:HB3	3:O:298:PRO:CD	2.34	0.53
3:G:297:LEU:HB3	3:G:298:PRO:CD	2.35	0.53
7:I:39:VAL:HG11	7:I:73:LEU:HD11	1.97	0.53
8:K:324:ASP:HA	8:K:327:ARG:HH21	1.87	0.53
8:K:198:ILE:HG21	8:K:408:LEU:HD21	1.89	0.53
4:M:253:GLN:HE21	5:J:325:VAL:HG23	1.72	0.53
4:M:52:LEU:HA	4:M:55:ARG:HB2	1.99	0.53
1:N:521:THR:O	1:N:525:SER:HB3	2.09	0.53
3:O:113:LYS:O	3:O:117:GLU:HG2	2.24	0.53
3:O:249:GLU:HG2	3:O:250:LEU:H	1.72	0.53
2:P:247:VAL:HG22	2:P:298:CYS:HB3	2.14	0.53
8:K:133:LEU:HD21	8:K:511:LYS:HD2	2.21	0.53
3:O:323:MET:HA	3:O:326:VAL:HG12	1.94	0.53
5:B:155:HIS:HB2	5:B:488:VAL:HG22	2.32	0.53
8:C:324:ASP:HA	8:C:327:ARG:HH21	1.76	0.53
6:D:432:MET:HG3	6:D:440:TRP:CZ3	2.61	0.53
8:K:102:GLU:HA	8:K:105:ALA:HB3	1.97	0.53
7:I:73:LEU:HB3	8:K:8:MET:HE1	2.25	0.53
1:N:509:SER:HB2	1:N:512:VAL:HG23	1.91	0.53
3:O:220:PHE:HE1	3:O:322:ASP:HB3	1.74	0.53
3:O:86:ILE:HD11	3:O:510:ALA:CA	2.37	0.53
2:P:390:THR:HG21	3:O:82:THR:HG23	2.02	0.53
5:B:194:GLN:HE21	5:B:196:ILE:HD11	1.74	0.53
6:D:260:MET:SD	7:A:273:ILE:HG23	2.75	0.53
1:F:192:HIS:NE2	1:F:326:GLU:HB2	2.32	0.53
1:F:87:THR:HG21	1:F:512:VAL:HA	1.90	0.53
2:H:43:LEU:HG	2:H:462:THR:HG22	1.94	0.53
7:I:180:VAL:HG13	7:I:406:LEU:HD23	2.27	0.53
5:J:239:ASP:OD1	5:J:291:TYR:HD1	2.29	0.53
3:O:221:LYS:HA	3:O:362:TYR:CE1	2.45	0.53
6:D:305:LEU:HD12	6:D:310:ILE:HD12	1.91	0.53
4:E:86:ASP:O	4:E:90:ILE:HG12	2.07	0.53
5:J:413:LYS:HG3	5:J:464:TYR:HD1	2.10	0.53
1:N:465:ASP:HB3	1:N:468:ASP:HB2	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:48:PRO:HB3	2:P:172:TYR:CD1	2.65	0.53
2:P:512:ILE:HG23	2:P:517:ILE:HB	2.13	0.53
7:A:143:VAL:O	7:A:143:VAL:HG12	2.07	0.53
5:B:48:SER:HA	6:D:527:SER:O	2.08	0.53
8:C:457:ILE:HG21	8:C:464:PRO:HA	1.89	0.53
1:F:163:ASP:HB2	1:F:166:LEU:HB3	1.93	0.53
5:J:95:VAL:O	5:J:99:SER:HB2	2.09	0.53
4:M:329:ASP:OD2	5:J:235:ASN:HB3	2.36	0.53
1:N:204:PRO:HB3	1:N:391:THR:HG21	2.02	0.53
2:P:291:ILE:HD13	2:P:347:PRO:HG3	1.89	0.53
7:A:477:LEU:HD11	7:A:502:LEU:HD13	1.90	0.53
6:D:171:ALA:HB3	6:D:172:PRO:HD3	1.91	0.53
6:D:253:ILE:HG21	7:A:263:ASN:HB2	1.91	0.53
4:E:102:LYS:O	4:E:105:VAL:HB	2.09	0.53
3:G:282:LEU:HD21	3:G:306:PHE:CB	2.39	0.53
3:G:319:SER:HB3	3:G:322:ASP:HB2	1.91	0.53
7:I:12:THR:HB	7:I:14:PHE:HE2	1.70	0.53
7:I:368:ASP:O	7:I:369:ASP:HB2	2.09	0.53
4:M:73:ILE:CG2	5:J:511:VAL:HG13	2.39	0.53
1:N:192:HIS:NE2	1:N:326:GLU:HB2	2.33	0.53
2:P:21:TYR:CD2	2:P:21:TYR:N	2.86	0.53
2:P:322:LYS:O	2:P:323:VAL:HB	2.08	0.53
7:A:52:MET:CE	8:C:73:PRO:HB2	2.39	0.53
1:F:203:SER:O	1:F:206:ASP:HB2	2.08	0.53
3:G:163:ARG:NH2	3:G:176:ASP:OD1	2.42	0.53
7:A:188:LYS:HG2	7:A:198:TYR:CE1	2.43	0.52
4:E:85:ASN:HB3	4:E:191:LYS:HG2	1.90	0.52
4:E:440:VAL:HG12	4:E:441:TYR:H	1.93	0.52
1:F:424:ARG:HH21	1:F:477:LEU:HD22	1.74	0.52
7:I:63:THR:HA	7:I:397:GLU:CG	2.56	0.52
2:P:327:PHE:CG	2:P:328:GLU:N	2.77	0.52
7:A:173:SER:O	7:A:177:SER:HB2	2.11	0.52
8:C:203:TYR:HE1	8:C:330:ARG:HE	1.62	0.52
8:C:79:LEU:C	8:C:81:LEU:H	2.12	0.52
4:E:207:ALA:HB1	4:E:224:ILE:HD12	1.90	0.52
4:E:324:GLN:HB2	4:E:351:LEU:HD11	1.92	0.52
1:F:492:ASP:HB2	1:F:499:CYS:HB3	1.91	0.52
7:I:144:LEU:CD2	7:I:419:VAL:HG22	2.40	0.52
5:J:254:SER:O	5:J:256:ALA:N	2.44	0.52
1:N:439:LYS:O	1:N:442:THR:CG2	2.64	0.52
2:P:25:ASP:C	2:P:27:GLN:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:322:LYS:HG3	2:P:323:VAL:HG23	2.16	0.52
8:C:65:LEU:HD11	8:C:97:ILE:HD13	1.90	0.52
2:H:43:LEU:HA	2:H:105:ILE:HD11	2.41	0.52
7:I:256:MET:HG2	8:K:257:SER:HB2	1.90	0.52
6:L:162:ILE:HG13	6:L:162:ILE:O	2.19	0.52
4:M:298:LEU:HD21	5:J:248:THR:HG21	2.18	0.52
1:N:221:HIS:CD2	1:N:223:ASP:H	2.32	0.52
2:P:92:GLN:OE1	2:P:103:VAL:HG23	2.16	0.52
2:P:27:GLN:HG3	2:P:541:ILE:HB	2.16	0.52
5:B:181:ILE:HD13	5:B:391:LEU:CB	2.40	0.52
8:C:47:MET:HG3	8:C:57:LEU:HB3	2.06	0.52
2:H:243:LYS:HA	2:H:245:HIS:CE1	2.44	0.52
2:H:478:LEU:HD22	2:H:499:VAL:CG2	2.66	0.52
7:I:63:THR:HG22	7:I:65:ASP:H	1.93	0.52
4:M:385:PHE:O	4:M:409:ARG:NH2	2.42	0.52
3:O:167:SER:O	3:O:168:SER:CB	2.57	0.52
1:F:518:THR:HG21	8:C:213:ASP:HB3	2.09	0.52
3:G:409:ILE:HD13	3:G:497:TRP:HE3	1.74	0.52
3:G:478:TRP:HE3	3:G:492:PHE:HB2	1.70	0.52
4:M:72:LYS:HB2	4:M:90:ILE:CD1	2.37	0.52
1:N:303:PRO:HA	1:N:306:LEU:HD12	2.01	0.52
3:O:147:ILE:HD13	3:O:157:LEU:CD1	2.39	0.52
3:O:83:LEU:O	3:O:86:ILE:HG22	2.09	0.52
7:A:248:ASP:HB3	7:A:339:SER:HA	1.97	0.52
6:D:35:ILE:HA	6:D:46:LYS:HZ1	1.84	0.52
1:F:337:GLN:HG2	1:F:347:ILE:HG21	1.92	0.52
3:G:224:PHE:CD2	3:G:225:SER:N	2.77	0.52
1:F:251:PHE:HZ	2:H:259:THR:HB	1.74	0.52
7:I:458:ILE:HD12	7:I:458:ILE:H	1.80	0.52
7:I:255:ARG:HA	8:K:257:SER:HA	1.91	0.52
1:N:130:MET:HE1	1:N:514:ARG:HG2	1.91	0.52
3:O:191:ARG:O	3:O:192:ASN:C	2.58	0.52
7:A:179:MET:HE1	7:A:385:ILE:HG23	1.92	0.52
5:B:438:ARG:O	5:B:441:PRO:HD2	2.09	0.52
6:D:35:ILE:CG2	6:D:94:THR:HG23	2.40	0.52
4:E:269:LEU:H	4:E:375:GLY:H	1.56	0.52
3:G:246:VAL:HA	3:G:297:LEU:HD12	1.90	0.52
2:H:85:LEU:HD22	2:H:534:ALA:HB1	2.09	0.52
3:O:462:ILE:O	3:O:466:ASN:HB2	2.11	0.52
6:D:175:VAL:HA	6:D:401:ILE:HD13	1.95	0.52
1:F:133:LEU:HD11	1:F:412:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:329:LEU:O	2:H:333:CYS:HB2	2.16	0.52
7:I:165:SER:O	7:I:166:SER:CB	2.57	0.52
4:M:144:ILE:HD11	4:M:550:LYS:HA	2.01	0.52
1:N:142:ASN:HD22	1:N:409:LYS:HA	1.75	0.52
3:O:44:LEU:HD22	3:O:103:ILE:HD13	1.91	0.52
7:A:256:MET:HE3	7:A:260:VAL:HG11	1.92	0.52
7:A:417:ASN:HB3	7:A:521:THR:HB	1.92	0.52
6:D:125:GLN:NE2	6:D:513:GLU:HG2	2.49	0.52
5:J:374:ASP:HB2	6:L:80:GLU:OE1	2.32	0.52
5:J:373:THR:HB	5:J:376:THR:OG1	2.10	0.52
5:J:440:LEU:HB3	5:J:441:PRO:HD3	2.28	0.52
5:J:455:LEU:HD22	5:J:472:LEU:HD23	1.97	0.52
4:M:115:ILE:HG22	4:M:117:ASP:H	1.74	0.52
1:N:130:MET:HE1	1:N:514:ARG:CG	2.40	0.52
2:P:245:HIS:H	2:P:245:HIS:HD1	1.85	0.52
5:B:444:LEU:HB3	5:B:474:LEU:HD21	1.92	0.52
6:D:432:MET:HG3	6:D:440:TRP:CE3	2.46	0.52
1:F:233:VAL:N	1:F:349:GLY:O	2.42	0.52
3:G:51:ILE:HB	3:G:69:ILE:HD12	1.92	0.52
8:K:119:VAL:HA	8:K:122:ILE:HD12	1.96	0.52
6:L:254:VAL:HB	7:I:262:ILE:HD13	2.00	0.52
6:L:520:ARG:NH2	6:L:520:ARG:HG3	2.01	0.52
1:N:255:SER:HB3	1:N:258:GLN:HB2	1.90	0.52
6:D:163:VAL:HG23	6:D:204:ILE:HG21	1.99	0.51
1:F:303:PRO:HA	1:F:306:LEU:HD12	1.91	0.51
3:G:298:PRO:HB3	3:G:317:ARG:CZ	2.66	0.51
2:H:85:LEU:CD2	2:H:534:ALA:HB1	2.58	0.51
7:I:247:LEU:HD11	7:I:288:ILE:HD13	1.92	0.51
5:J:22:ALA:HA	5:J:73:ALA:HB2	1.92	0.51
6:L:367:ARG:O	6:L:368:ASN:CB	2.57	0.51
5:B:408:GLU:HG3	5:B:441:PRO:HD3	2.35	0.51
6:D:254:VAL:HB	7:A:262:ILE:HD13	2.05	0.51
4:E:428:CYS:O	4:E:431:ARG:HG3	2.23	0.51
1:F:327:ARG:O	1:F:331:VAL:HG23	2.10	0.51
8:K:48:LEU:HD11	8:K:64:ILE:HA	1.92	0.51
6:L:234:ILE:HD12	6:L:345:ASP:OD2	2.11	0.51
6:L:432:MET:HG3	6:L:440:TRP:CE3	2.55	0.51
3:O:215:ILE:HG23	3:O:366:GLN:HB3	2.05	0.51
7:A:132:ALA:HB2	7:A:448:ILE:HG23	1.90	0.51
5:B:409:MET:HB3	5:B:463:ILE:HD13	1.91	0.51
6:D:335:ASP:OD1	6:D:336:ILE:N	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:336:ILE:C	6:D:338:LEU:H	2.12	0.51
6:D:45:ASP:OD1	6:D:59:ASN:HB2	2.10	0.51
4:E:115:ILE:HG23	4:E:432:ASN:ND2	2.28	0.51
4:E:64:SER:HB2	4:E:72:LYS:HZ2	1.96	0.51
2:H:182:VAL:O	2:H:186:VAL:HG23	2.11	0.51
8:K:452:ILE:HB	8:K:453:PRO:HD3	2.12	0.51
6:L:25:ILE:HG23	6:L:104:LEU:HB3	1.91	0.51
4:M:115:ILE:HG23	4:M:432:ASN:ND2	2.26	0.51
2:P:55:ILE:HD11	2:P:71:MET:HG3	1.91	0.51
7:A:71:SER:HB2	7:A:88:GLN:HE22	1.76	0.51
5:B:14:ARG:HG2	5:B:15:ALA:H	1.76	0.51
6:D:411:ILE:HD11	6:D:501:VAL:HA	1.92	0.51
4:M:73:ILE:CG2	5:J:514:ILE:HG12	2.60	0.51
6:L:444:ALA:HA	6:L:447:LEU:HD12	2.10	0.51
6:L:479:ASN:HB2	6:L:491:ASN:OD1	2.24	0.51
7:A:15:LEU:C	7:A:17:GLY:N	2.62	0.51
7:A:521:THR:HG23	7:A:522:ILE:HG13	2.12	0.51
5:B:39:PRO:HG3	10:B:602:ADP:C5	2.45	0.51
3:G:173:ASN:ND2	4:E:148:ASN:HA	2.25	0.51
1:F:221:HIS:HB3	1:F:224:MET:HG3	2.01	0.51
1:F:274:LEU:O	1:F:278:ILE:HG13	2.24	0.51
8:K:183:ARG:HD3	8:K:407:MET:CE	2.84	0.51
6:L:151:VAL:HA	6:L:175:VAL:HG21	2.00	0.51
4:M:327:PHE:H	4:M:344:ARG:HD2	1.92	0.51
3:O:88:ARG:NH1	3:O:88:ARG:HG2	2.60	0.51
1:F:465:ASP:HB3	1:F:468:ASP:HB2	1.98	0.51
1:F:97:LEU:HD11	1:F:451:LEU:HD23	1.92	0.51
2:H:26:GLY:O	2:H:31:SER:HB2	2.42	0.51
3:G:120:ILE:HD11	7:I:471:SER:HB2	1.93	0.51
7:I:63:THR:HG22	7:I:64:ASN:H	1.99	0.51
5:J:412:SER:O	5:J:416:ASP:HB2	2.11	0.51
2:P:186:VAL:HG11	2:P:408:VAL:HG11	1.93	0.51
5:B:234:ALA:HA	5:B:326:VAL:O	2.11	0.51
5:B:279:PHE:HB3	5:B:281:ILE:HD12	2.16	0.51
5:B:301:LEU:HD23	5:B:303:ILE:CD1	2.41	0.51
5:B:43:ASP:OD2	6:D:520:ARG:NH2	2.74	0.51
4:E:251:HIS:HE1	4:E:253:GLN:HG2	1.75	0.51
10:E:602:ADP:O3B	11:E:603:BEF:F2	2.18	0.51
1:F:87:THR:HG22	1:F:89:ASP:H	1.85	0.51
3:G:301:ASP:O	3:G:305:GLN:HG2	2.18	0.51
2:H:77:ILE:HD13	2:H:86:VAL:HG21	1.97	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:13:LEU:HD13	1:N:21:VAL:HG21	1.98	0.51
1:N:133:LEU:HD11	1:N:412:ILE:CD1	2.61	0.51
3:O:215:ILE:HG22	3:O:217:GLY:H	1.75	0.51
3:O:204:ILE:HG23	3:O:379:ARG:HD3	1.95	0.51
7:A:252:GLN:HA	7:A:303:ASP:HB2	1.93	0.51
4:E:412:ASN:HB2	5:B:80:ILE:HG12	2.11	0.51
6:D:444:ALA:HA	6:D:447:LEU:HD12	1.93	0.51
7:I:431:ILE:HB	7:I:485:GLN:HE22	1.75	0.51
5:J:153:LEU:HD22	5:J:391:LEU:HG	2.39	0.51
8:K:361:GLY:O	8:K:362:ASP:HB2	2.18	0.51
6:L:506:SER:O	6:L:510:LEU:HG	2.30	0.51
1:N:534:LEU:HD12	8:K:48:LEU:CD2	2.41	0.51
7:A:538:ILE:HA	7:A:541:ILE:HD12	1.95	0.51
7:A:70:LEU:HB3	7:A:84:VAL:HG13	1.93	0.51
5:B:281:ILE:HD11	5:B:337:LEU:HD11	2.27	0.51
8:C:105:ALA:O	8:C:109:PRO:HD2	2.11	0.51
8:C:41:PRO:HG3	10:C:1102:ADP:C6	2.63	0.51
6:D:419:ILE:HD13	6:D:469:LEU:HG	1.93	0.51
6:D:516:LYS:O	6:D:520:ARG:HG2	2.11	0.51
4:E:52:LEU:HA	4:E:55:ARG:HB2	1.93	0.51
3:G:45:GLY:CA	3:G:453:LEU:HD22	2.64	0.51
8:K:208:LYS:HB3	8:K:389:LEU:HD13	2.04	0.51
6:L:291:SER:CB	6:L:296:ALA:HA	2.53	0.51
3:O:198:LEU:O	3:O:373:THR:HG23	2.20	0.51
2:P:79:HIS:HD2	2:P:81:ALA:H	1.95	0.51
7:A:477:LEU:HD11	7:A:502:LEU:HD22	2.55	0.51
5:B:239:ASP:OD1	5:B:291:TYR:HD1	1.94	0.51
6:D:220:ILE:HD12	6:D:302:LEU:HD11	2.34	0.51
3:G:166:MET:HE3	3:G:396:ALA:HB2	1.92	0.51
2:H:109:GLU:HG2	2:H:458:VAL:CG2	2.61	0.51
7:I:523:SER:O	7:I:527:SER:HB2	2.16	0.51
5:J:88:VAL:O	5:J:389:SER:HB3	2.33	0.51
6:L:89:ALA:O	6:L:399:CYS:HB3	2.10	0.51
2:P:267:LEU:HD13	2:P:273:MET:HG2	1.93	0.51
7:A:198:TYR:CE2	7:A:413:LEU:HB3	2.49	0.50
7:A:55:ASP:O	7:A:56:ASP:CB	2.56	0.50
1:F:296:ILE:HA	1:F:317:LEU:HB3	1.92	0.50
1:F:509:SER:HB2	1:F:512:VAL:CG2	2.46	0.50
3:G:44:LEU:HD22	3:G:103:ILE:HD13	1.93	0.50
2:H:123:SER:HB3	2:H:126:GLU:CG	2.41	0.50
2:H:43:LEU:HG	2:H:462:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:409:MET:HB3	5:J:463:ILE:HD13	1.96	0.50
1:N:98:VAL:HG13	1:N:524:ALA:HB2	1.93	0.50
5:B:184:LEU:HD11	5:B:192:HIS:CB	2.41	0.50
1:F:55:LEU:HD11	2:H:541:ILE:CD1	2.41	0.50
5:J:155:HIS:CB	5:J:488:VAL:HG22	2.40	0.50
6:L:130:ARG:O	6:L:134:ILE:HG13	2.12	0.50
4:M:88:ALA:O	4:M:92:SER:HB2	2.28	0.50
3:O:282:LEU:HD11	3:O:306:PHE:HB2	1.93	0.50
2:P:267:LEU:HB2	3:O:259:VAL:HG22	1.93	0.50
5:B:440:LEU:HB3	5:B:441:PRO:CD	2.63	0.50
4:E:385:PHE:O	4:E:409:ARG:NH2	2.45	0.50
1:F:46:LEU:HD23	2:H:545:ILE:HB	1.94	0.50
3:G:51:ILE:HG12	4:E:553:ASN:HB3	1.93	0.50
6:L:46:LYS:HB2	6:L:64:ILE:HD12	1.93	0.50
8:C:65:LEU:HD22	8:C:79:LEU:HB2	1.94	0.50
4:E:333:HIS:CE1	5:B:326:VAL:HG13	2.46	0.50
1:F:217:HIS:NE2	1:F:320:ALA:HA	2.29	0.50
3:G:3:PHE:N	3:G:3:PHE:CD2	2.89	0.50
2:H:227:VAL:HG13	2:H:368:VAL:HG11	1.93	0.50
5:J:380:ALA:O	5:J:384:LEU:HB2	2.11	0.50
5:B:162:SER:O	5:B:163:SER:HB3	2.11	0.50
5:B:346:ILE:HG22	5:B:347:MET:H	1.76	0.50
6:D:198:LYS:HE2	6:D:391:GLU:OE1	2.23	0.50
1:F:458:LEU:HB3	1:F:493:LEU:HD21	2.08	0.50
3:G:157:LEU:O	3:G:161:CYS:HB2	2.12	0.50
3:G:337:THR:HG22	3:G:339:SER:H	1.78	0.50
2:H:210:VAL:O	2:H:385:ILE:HA	2.11	0.50
8:K:453:PRO:O	8:K:457:ILE:HG12	2.12	0.50
4:M:211:VAL:HG12	4:M:402:LYS:O	2.11	0.50
1:N:198:GLN:HB2	1:N:388:LEU:HD13	1.94	0.50
3:O:482:VAL:HG22	3:O:491:ASN:HD21	2.14	0.50
8:C:48:LEU:HD11	8:C:64:ILE:HA	1.94	0.50
6:D:257:TYR:HA	6:D:260:MET:HE2	2.07	0.50
4:E:287:LEU:HD12	5:B:248:THR:HG22	1.94	0.50
7:I:139:PHE:CE2	7:I:143:VAL:HG21	2.47	0.50
7:I:52:MET:HG3	7:I:62:VAL:HG22	2.27	0.50
8:K:203:TYR:HE1	8:K:330:ARG:HE	1.59	0.50
8:K:70:VAL:HG11	8:K:75:ALA:CB	2.47	0.50
1:N:58:ASP:HA	1:N:161:LYS:HE2	1.93	0.50
7:A:17:GLY:HA3	7:A:546:THR:O	2.48	0.50
7:A:62:VAL:O	7:A:397:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:255:THR:CG2	6:D:263:ILE:HA	2.44	0.50
5:B:193:ILE:HA	5:B:365:CYS:O	2.11	0.50
5:B:44:LYS:HD3	6:D:523:ASP:HB3	2.02	0.50
5:J:476:ASN:HB3	5:J:478:THR:HG22	1.94	0.50
1:N:23:VAL:HG13	1:N:102:LEU:HB3	1.93	0.50
2:P:310:LEU:O	2:P:314:ASN:HB2	2.13	0.50
3:G:98:THR:OG1	11:G:603:BEF:F2	2.49	0.50
1:F:252:PHE:HD1	2:H:264:THR:HB	1.76	0.50
4:M:64:SER:HB2	4:M:72:LYS:HZ2	1.76	0.50
4:E:438:ARG:HH21	4:E:531:PHE:HE2	2.16	0.50
3:G:449:ILE:O	3:G:453:LEU:HG	2.12	0.50
2:H:311:HIS:HB2	3:G:336:SER:HB2	2.28	0.50
4:M:151:ASP:OD2	4:M:546:ARG:HD3	2.12	0.50
4:E:251:HIS:CE1	4:E:253:GLN:HG2	2.46	0.49
2:H:109:GLU:HG2	2:H:458:VAL:HG21	2.27	0.49
5:J:279:PHE:HE1	5:J:335:CYS:SG	2.60	0.49
8:C:160:GLY:HA2	8:C:165:ILE:HG12	1.93	0.49
2:H:135:ARG:HB2	2:H:532:THR:HG21	1.93	0.49
7:I:86:LEU:HD13	7:I:534:ALA:HB2	1.93	0.49
5:J:58:ASN:O	5:J:59:ASP:C	2.62	0.49
8:K:231:HIS:HB3	8:K:234:MET:HG3	1.93	0.49
8:K:62:HIS:O	8:K:66:ARG:HB2	2.12	0.49
7:A:12:THR:CB	7:A:14:PHE:CE2	3.06	0.49
7:A:437:ALA:HB1	7:A:445:GLN:HG3	2.01	0.49
5:B:214:LEU:HD11	5:B:317:LEU:HD11	2.10	0.49
8:C:78:MET:O	8:C:81:LEU:HB3	2.12	0.49
6:D:46:LYS:HB2	6:D:64:ILE:HD12	1.93	0.49
1:F:440:THR:O	1:F:444:ILE:HD12	2.11	0.49
2:H:444:LEU:HD12	2:H:444:LEU:H	1.77	0.49
7:I:228:VAL:HG23	7:I:363:GLN:OE1	2.29	0.49
5:J:103:LEU:HD21	5:J:505:ALA:HA	2.13	0.49
1:N:6:LEU:HB3	8:K:70:VAL:HG13	1.93	0.49
6:L:244:PRO:CD	6:L:270:TYR:CE2	3.00	0.49
4:M:242:GLY:HA3	4:M:395:ILE:O	2.25	0.49
1:N:245:THR:HG21	8:K:272:ILE:HD12	2.16	0.49
1:N:296:ILE:HG12	1:N:317:LEU:HD23	2.00	0.49
3:O:383:GLU:HA	3:O:386:ILE:HD12	2.25	0.49
5:B:254:SER:O	5:B:256:ALA:N	2.49	0.49
1:F:199:MET:HG3	1:F:379:LEU:HD21	2.64	0.49
1:F:87:THR:HG21	1:F:512:VAL:HG22	2.16	0.49
1:F:242:TYR:CZ	2:H:260:GLU:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:55:ASP:O	7:I:56:ASP:CB	2.66	0.49
1:N:87:THR:CG2	1:N:512:VAL:HG22	2.43	0.49
2:P:332:LEU:O	2:P:335:VAL:HG12	2.51	0.49
1:F:119:THR:HG23	1:F:525:SER:OG	2.35	0.49
8:K:167:TRP:CE3	8:K:214:VAL:HB	2.55	0.49
2:P:111:LEU:HD11	2:P:538:VAL:HG21	1.93	0.49
2:P:498:GLY:O	2:P:509:VAL:HG13	2.21	0.49
5:B:156:ILE:HD13	5:B:488:VAL:HG23	1.95	0.49
5:B:238:LEU:HB2	5:B:289:LEU:O	2.13	0.49
6:D:72:HIS:HD2	6:D:74:VAL:HB	2.01	0.49
5:J:255:THR:HG22	6:L:263:ILE:HA	1.93	0.49
5:J:192:HIS:HD2	5:J:319:LEU:HD12	1.75	0.49
5:J:45:LEU:HD23	6:L:524:ILE:HG12	1.93	0.49
4:M:168:ILE:HD11	4:M:439:VAL:HG13	1.97	0.49
3:O:90:GLN:HE21	3:O:97:GLY:HA3	1.85	0.49
7:A:267:PRO:HB3	8:C:272:ILE:HG23	1.94	0.49
8:C:355:PHE:HD2	8:C:368:LEU:CD1	2.26	0.49
8:C:204:VAL:HA	8:C:377:CYS:O	2.16	0.49
2:H:80:PRO:O	2:H:84:VAL:HG23	2.13	0.49
4:M:91:LEU:HD11	4:M:123:VAL:HG21	2.18	0.49
1:N:93:THR:HG23	1:N:454:ILE:HD11	1.95	0.49
5:B:27:ILE:HG12	5:B:104:ARG:HG2	1.94	0.49
4:E:251:HIS:CE1	5:B:325:VAL:HB	2.62	0.49
8:C:139:VAL:HG12	8:C:480:PHE:CD1	2.48	0.49
6:D:138:MET:HB2	6:D:478:LEU:CD1	2.32	0.49
4:E:269:LEU:CD1	4:E:358:THR:HG21	2.42	0.49
4:E:385:PHE:HD2	4:E:390:ASP:O	1.95	0.49
1:F:221:HIS:CD2	1:F:223:ASP:H	2.28	0.49
3:G:242:LEU:HD21	3:G:341:ILE:HD13	1.95	0.49
2:H:254:LEU:HB2	2:H:305:VAL:HG22	1.95	0.49
5:J:346:ILE:HG22	5:J:347:MET:N	2.28	0.49
8:K:175:ALA:O	8:K:179:VAL:HG23	2.26	0.49
6:L:150:LEU:HD23	6:L:179:LEU:HD11	1.94	0.49
7:A:100:SER:O	7:A:104:ILE:HG13	2.22	0.49
7:A:97:GLY:O	7:A:101:VAL:HG23	2.20	0.49
7:A:126:ILE:HG13	7:A:539:LEU:HD23	2.63	0.49
5:B:377:LEU:O	5:B:378:ASP:C	2.51	0.49
4:E:234:ILE:HA	4:E:409:ARG:O	2.13	0.49
4:E:511:GLY:O	4:E:520:ASN:HB3	2.11	0.49
1:F:133:LEU:HD11	1:F:412:ILE:HD11	1.95	0.49
1:F:35:THR:HG22	1:F:42:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:215:ILE:HD13	3:G:219:ALA:HB2	1.95	0.49
3:G:462:ILE:O	3:G:466:ASN:HB2	2.13	0.49
2:H:182:VAL:HG22	2:H:401:ILE:HG13	1.95	0.49
2:H:322:LYS:C	2:H:324:PRO:HD2	2.32	0.49
7:I:179:MET:HE3	7:I:218:LEU:HB2	1.94	0.49
2:P:209:VAL:HG11	2:P:398:GLU:HG3	2.07	0.49
7:A:77:HIS:CD2	7:A:79:ALA:H	2.31	0.49
5:B:56:VAL:HG23	5:B:375:GLN:HG2	1.93	0.49
1:F:6:LEU:HB3	8:C:70:VAL:HG13	1.99	0.49
6:D:42:LYS:HE2	6:D:484:VAL:HG13	1.94	0.49
7:I:26:ARG:NH1	7:I:26:ARG:CG	2.65	0.49
8:K:129:LEU:HD13	8:K:514:ILE:HD12	1.95	0.49
8:K:297:THR:HG22	8:K:299:LYS:H	2.17	0.49
4:M:320:VAL:HG22	4:M:341:PRO:HB2	2.05	0.49
1:N:221:HIS:HB3	1:N:224:MET:HG3	1.95	0.49
2:P:284:ILE:CD1	2:P:308:LEU:HB3	2.66	0.49
2:P:135:ARG:HB2	2:P:532:THR:HG21	1.98	0.49
8:C:269:TRP:NE1	8:C:273:LEU:HD22	2.28	0.48
1:F:534:LEU:HB2	8:C:48:LEU:HD23	1.94	0.48
6:D:199:LYS:O	6:D:380:ARG:NH1	2.46	0.48
1:F:234:LEU:HD11	1:F:343:LEU:HD11	2.56	0.48
1:F:459:VAL:HG22	1:F:491:VAL:HG11	2.01	0.48
3:G:362:TYR:CE1	3:G:377:LEU:HD21	2.56	0.48
7:I:28:GLN:HE21	7:I:77:HIS:CE1	2.34	0.48
1:N:133:LEU:HD11	1:N:412:ILE:HD11	2.15	0.48
3:O:157:LEU:O	3:O:161:CYS:HB2	2.14	0.48
2:P:413:LYS:CB	2:P:414:PRO:HD3	2.43	0.48
2:P:43:LEU:HG	2:P:462:THR:HG21	2.10	0.48
5:B:293:TYR:HA	6:D:334:ALA:HB1	1.98	0.48
7:A:211:LYS:H	8:C:508:GLN:HE22	1.61	0.48
1:F:111:GLU:CG	1:N:467:LEU:HD13	3.05	0.48
4:M:160:LYS:HG3	4:M:453:ALA:HB1	1.95	0.48
3:O:55:THR:HG22	3:O:56:SER:H	1.78	0.48
6:D:271:LEU:HD23	6:D:301:ALA:HB2	1.97	0.48
4:E:143:PRO:O	4:E:549:LEU:HD23	2.61	0.48
8:K:183:ARG:HD3	8:K:407:MET:HE3	2.64	0.48
4:M:254:MET:SD	4:M:341:PRO:HA	2.76	0.48
1:N:146:ASP:HB3	1:N:149:PHE:HB3	1.94	0.48
1:N:455:PRO:O	1:N:459:VAL:HG23	2.19	0.48
3:O:113:LYS:HB3	3:O:114:PRO:HD3	1.95	0.48
3:O:381:GLY:HA2	4:M:540:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:27:GLN:HA	2:P:31:SER:CB	2.60	0.48
5:B:95:VAL:O	5:B:99:SER:HB2	2.13	0.48
1:F:189:LEU:HA	8:C:359:MET:SD	2.57	0.48
2:H:142:LEU:HA	2:H:145:MET:HG3	2.20	0.48
2:H:27:GLN:HA	2:H:31:SER:CB	2.35	0.48
7:A:165:SER:O	7:A:166:SER:CB	2.61	0.48
6:D:295:ASP:O	6:D:296:ALA:HB3	2.14	0.48
6:D:421:ILE:CG2	6:D:447:LEU:HD13	2.43	0.48
1:F:107:ARG:HG3	1:N:107:ARG:CZ	2.43	0.48
3:G:139:LYS:O	3:G:143:LEU:HB2	2.13	0.48
2:H:509:VAL:HG13	2:H:510:LYS:H	1.77	0.48
5:J:121:ILE:HG12	5:J:506:GLU:HG2	2.50	0.48
6:L:203:THR:HG22	6:L:205:ASP:H	1.88	0.48
6:L:271:LEU:HD23	6:L:301:ALA:HB2	1.94	0.48
2:P:27:GLN:HE21	2:P:544:ILE:HG12	1.79	0.48
4:E:275:PRO:HD3	4:E:325:TRP:HE3	1.77	0.48
2:H:92:GLN:HG3	2:H:526:PHE:HB3	2.01	0.48
5:J:327:SER:O	5:J:329:PHE:N	2.47	0.48
5:J:33:VAL:HB	5:J:93:THR:HG23	1.96	0.48
1:N:248:ASN:HD22	8:K:260:ASN:HB3	1.79	0.48
1:N:452:LEU:HD22	1:N:470:LEU:HD21	1.94	0.48
5:B:157:ALA:HB2	5:B:391:LEU:HD11	1.95	0.48
8:C:173:GLU:O	8:C:177:ASP:HB2	2.14	0.48
6:D:465:VAL:O	6:D:469:LEU:HB2	2.24	0.48
7:I:501:GLY:CA	7:I:512:GLU:HG2	2.51	0.48
8:K:324:ASP:OD1	8:K:327:ARG:NH2	2.63	0.48
8:K:7:PHE:CG	8:K:8:MET:N	2.88	0.48
2:P:154:ASN:HB3	2:P:190:LEU:HD13	2.05	0.48
5:B:45:LEU:HD13	5:B:56:VAL:HG22	1.95	0.48
5:B:155:HIS:HB3	5:B:488:VAL:HG22	1.95	0.48
8:C:471:LEU:O	8:C:475:HIS:HB2	2.19	0.48
4:E:269:LEU:HD13	4:E:322:ILE:HD12	2.07	0.48
4:E:29:PHE:CD2	4:E:29:PHE:N	2.83	0.48
1:F:13:LEU:HD13	1:F:21:VAL:HG21	1.96	0.48
6:L:465:VAL:O	6:L:469:LEU:HB2	2.13	0.48
7:A:269:GLN:HA	7:A:272:GLN:HB2	2.04	0.48
7:A:228:VAL:HG22	7:A:372:ILE:HD11	1.96	0.48
5:B:231:ILE:HG12	5:B:283:THR:HB	2.14	0.48
7:A:209:HIS:CE1	8:C:83:ARG:HH21	2.30	0.48
4:E:335:LEU:HD23	4:E:342:ALA:HB2	2.17	0.48
7:I:181:VAL:O	7:I:185:LEU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:17:GLY:HA3	7:I:546:THR:O	2.44	0.48
5:J:459:LEU:HD13	5:J:472:LEU:HG	2.16	0.48
8:K:220:LEU:O	8:K:222:GLY:N	2.70	0.48
8:K:291:ARG:N	8:K:292:PRO:HD3	2.29	0.48
8:K:79:LEU:C	8:K:81:LEU:H	2.22	0.48
6:L:420:GLU:HB2	6:L:473:HIS:HE1	1.73	0.48
6:D:138:MET:SD	6:D:478:LEU:HD21	2.54	0.48
3:G:202:LYS:HE2	3:G:221:LYS:H	2.04	0.48
3:G:20:SER:HB2	3:G:25:GLN:NE2	2.44	0.48
7:I:248:ASP:HB3	7:I:339:SER:HA	1.95	0.48
5:J:279:PHE:CE2	5:J:332:PRO:HG3	2.48	0.48
6:L:96:VAL:HG23	6:L:507:ALA:O	2.38	0.48
8:C:102:GLU:HA	8:C:105:ALA:HB3	1.95	0.47
8:C:142:PRO:HA	8:C:411:SER:HA	1.98	0.47
8:C:57:LEU:O	8:C:57:LEU:HG	2.14	0.47
1:F:56:THR:HG22	1:F:58:ASP:H	1.87	0.47
3:G:282:LEU:HD11	3:G:306:PHE:HB2	1.96	0.47
4:M:273:THR:O	4:M:273:THR:HG22	2.13	0.47
1:N:28:GLY:O	1:N:32:VAL:HG23	2.22	0.47
3:O:301:ASP:O	3:O:305:GLN:HG2	2.21	0.47
3:O:51:ILE:HG12	4:M:553:ASN:HB3	2.13	0.47
7:A:164:MET:CE	7:A:164:MET:HA	2.44	0.47
8:C:35:ILE:HB	8:C:97:ILE:HD11	1.96	0.47
1:F:450:ALA:O	1:F:453:VAL:HG22	2.14	0.47
3:G:202:LYS:HB3	3:G:377:LEU:HD23	2.30	0.47
5:J:459:LEU:HG	5:J:463:ILE:HD12	2.13	0.47
8:K:164:VAL:O	8:K:164:VAL:HG12	2.14	0.47
1:N:100:GLU:OE1	1:N:103:ARG:NH1	2.47	0.47
1:N:418:PHE:HE2	1:N:517:ILE:HD11	1.79	0.47
7:A:210:GLY:O	7:A:388:ARG:HB3	2.25	0.47
7:I:121:HIS:CE1	7:I:123:THR:HG1	3.65	0.47
5:J:190:LEU:HD12	5:J:190:LEU:N	2.47	0.47
4:E:322:ILE:HG21	4:E:354:ILE:HD13	2.29	0.47
3:G:107:GLU:CD	3:G:448:VAL:HG21	2.59	0.47
3:G:220:PHE:HE1	3:G:322:ASP:HB3	1.79	0.47
3:G:226:TYR:O	3:G:227:ALA:C	2.75	0.47
3:G:25:GLN:HG2	3:G:521:ASP:C	2.38	0.47
5:J:215:ALA:HA	5:J:353:PHE:HD1	2.29	0.47
8:K:145:VAL:HG12	8:K:406:VAL:HG12	1.95	0.47
6:L:149:GLN:HE21	6:L:410:LEU:HD23	1.79	0.47
2:P:182:VAL:O	2:P:186:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:94:ILE:CD1	7:A:523:SER:HA	2.42	0.47
7:A:52:MET:HE3	8:C:73:PRO:HB2	1.96	0.47
5:B:34:LYS:HD2	5:B:443:ILE:HD13	1.96	0.47
6:D:124:PHE:O	6:D:127:ALA:HB3	2.17	0.47
6:D:320:GLU:O	6:D:324:LEU:HB2	2.21	0.47
4:E:61:ILE:HD11	4:E:91:LEU:HD21	1.96	0.47
2:H:27:GLN:HA	2:H:31:SER:HB3	2.60	0.47
2:H:27:GLN:HG3	2:H:541:ILE:HB	1.97	0.47
5:J:320:VAL:O	5:J:359:CYS:HB3	2.14	0.47
6:D:195:ARG:HD3	6:D:323:PHE:CZ	2.51	0.47
6:D:432:MET:SD	6:D:440:TRP:CZ3	3.04	0.47
4:E:115:ILE:HG22	4:E:117:ASP:H	1.84	0.47
4:E:541:ALA:O	4:E:545:CYS:HB2	2.29	0.47
3:G:326:VAL:HG23	3:G:365:PHE:CE1	2.49	0.47
2:H:267:LEU:HD13	2:H:273:MET:HG2	1.96	0.47
3:O:173:ASN:HB2	4:M:546:ARG:NH1	2.29	0.47
6:D:149:GLN:HE21	6:D:410:LEU:HD23	1.97	0.47
6:D:78:LEU:HD22	6:D:97:VAL:HG13	1.96	0.47
4:E:151:ASP:OD2	4:E:546:ARG:HD3	2.15	0.47
4:E:281:PRO:HD2	4:E:285:HIS:CE1	2.49	0.47
3:G:356:GLN:HB2	3:G:361:ARG:CZ	2.45	0.47
2:H:54:ILE:CD1	3:G:78:PRO:HB2	2.44	0.47
5:J:194:GLN:HE21	5:J:196:ILE:HD11	1.79	0.47
8:K:167:TRP:HE3	8:K:215:LEU:HD13	1.89	0.47
8:K:21:GLN:O	8:K:25:ILE:HD12	2.15	0.47
4:M:322:ILE:HG23	4:M:346:VAL:HG21	1.95	0.47
2:H:6:PRO:HB2	1:N:535:ARG:HH12	2.07	0.47
3:O:107:GLU:CD	3:O:448:VAL:HG21	2.45	0.47
2:P:109:GLU:HG2	2:P:458:VAL:HG21	1.96	0.47
7:A:47:VAL:HG12	8:C:117:HIS:NE2	2.30	0.47
5:B:15:ALA:HB1	5:B:19:ARG:HH12	1.80	0.47
1:F:454:ILE:H	1:F:454:ILE:HD12	1.79	0.47
3:G:20:SER:HB2	3:G:25:GLN:HE21	1.92	0.47
3:G:30:ILE:HG13	3:G:109:MET:HB3	2.24	0.47
5:J:14:ARG:HG2	5:J:15:ALA:N	2.28	0.47
8:K:457:ILE:HG21	8:K:464:PRO:HA	2.18	0.47
4:M:125:LEU:HD22	4:M:129:LEU:HD13	2.03	0.47
4:M:207:ALA:HB1	4:M:224:ILE:HD12	1.97	0.47
1:N:30:GLN:HB2	1:N:96:CYS:HA	1.97	0.47
1:N:75:LEU:HD12	8:K:55:LEU:CD2	2.45	0.47
2:P:111:LEU:HD21	2:P:538:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:38:LEU:O	2:P:41:MET:HB3	2.66	0.47
7:A:403:HIS:O	7:A:407:SER:HB2	2.23	0.47
5:B:102:LEU:HD21	5:B:433:PHE:CD2	2.50	0.47
8:C:102:GLU:OE1	8:C:451:CYS:HB2	2.19	0.47
8:C:361:GLY:O	8:C:362:ASP:HB2	2.13	0.47
4:E:41:GLN:HB2	4:E:554:VAL:HB	1.96	0.47
1:F:326:GLU:HG2	8:C:232:PRO:HG3	1.97	0.47
1:F:56:THR:HB	1:F:61:VAL:HG11	1.97	0.47
7:I:118:ASN:O	7:I:119:LYS:HG2	2.26	0.47
7:I:210:GLY:O	7:I:388:ARG:HB3	2.26	0.47
5:J:444:LEU:HB3	5:J:474:LEU:HD21	2.05	0.47
5:J:155:HIS:HB3	5:J:488:VAL:HG22	1.96	0.47
7:I:211:LYS:H	8:K:508:GLN:HE22	1.60	0.47
8:K:65:LEU:HD11	8:K:97:ILE:HD13	1.96	0.47
6:L:69:ALA:O	7:I:14:PHE:HA	2.14	0.47
4:M:32:VAL:HG12	4:M:35:GLN:HG3	2.04	0.47
1:N:26:ALA:CB	1:N:102:LEU:HD12	2.45	0.47
8:C:296:ILE:HG12	8:C:317:LEU:HB2	1.97	0.47
8:C:248:CYS:O	8:C:297:THR:CG2	2.63	0.47
4:E:32:VAL:HG12	4:E:35:GLN:HG3	1.97	0.47
1:F:149:PHE:HZ	1:F:411:ILE:HG21	1.80	0.47
7:I:159:ILE:HD13	7:I:412:THR:HG21	1.98	0.47
5:J:192:HIS:CD2	5:J:319:LEU:CD1	3.11	0.47
5:J:57:THR:HG23	5:J:382:ARG:HE	1.79	0.47
1:N:248:ASN:HB2	8:K:260:ASN:CB	2.45	0.47
1:N:334:GLY:HA3	1:N:347:ILE:O	2.15	0.47
3:O:478:TRP:HE3	3:O:492:PHE:HB2	1.80	0.47
2:P:111:LEU:HD21	2:P:538:VAL:CG2	2.60	0.47
2:P:254:LEU:HB2	2:P:305:VAL:HG22	1.97	0.47
2:P:424:GLY:HA2	2:P:427:GLU:HG2	2.31	0.47
2:P:92:GLN:HG3	2:P:526:PHE:HB3	2.10	0.47
7:A:143:VAL:O	7:A:143:VAL:CG1	2.62	0.47
7:A:458:ILE:H	7:A:458:ILE:HD12	2.00	0.47
8:C:298:GLU:HG3	8:C:325:ASN:OD1	2.14	0.47
4:E:271:ILE:HG23	4:E:351:LEU:HD22	1.97	0.47
1:F:248:ASN:HB2	8:C:260:ASN:CB	2.44	0.47
3:G:77:HIS:HE1	3:G:79:ALA:HB3	1.81	0.47
2:H:428:ILE:HD11	2:H:478:LEU:HD21	2.09	0.47
7:I:437:ALA:HB1	7:I:445:GLN:HG3	2.05	0.47
5:J:408:GLU:HG3	5:J:441:PRO:HD3	2.08	0.47
5:J:453:SER:O	5:J:457:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:287:LEU:HD23	6:L:313:VAL:HB	1.97	0.47
6:L:230:GLU:HG2	6:L:349:LEU:HD12	2.75	0.47
4:M:291:SER:HB3	4:M:294:GLU:HB2	1.95	0.47
4:M:451:SER:O	4:M:455:SER:HB2	2.15	0.47
4:M:73:ILE:HG21	5:J:511:VAL:HG11	1.97	0.47
1:N:269:PHE:HE1	8:K:274:GLN:HG3	1.80	0.47
1:N:104:GLN:HG3	1:N:450:ALA:HA	1.97	0.47
1:N:86:ILE:HD11	8:K:210:PRO:HG2	2.39	0.47
3:O:108:LEU:HB3	3:O:514:THR:HG21	2.11	0.47
2:P:123:SER:HB3	2:P:126:GLU:CG	2.45	0.47
2:P:411:LEU:HD12	2:P:417:GLY:HA3	2.21	0.47
5:B:463:ILE:HD11	5:B:470:SER:O	2.31	0.46
6:D:177:SER:OG	6:D:375:VAL:HG11	2.15	0.46
6:D:448:GLU:O	6:D:451:PRO:HD2	2.15	0.46
6:D:495:GLU:HG3	6:D:495:GLU:O	2.15	0.46
6:D:65:LEU:HD11	6:D:97:VAL:HG21	1.97	0.46
4:E:498:LEU:HD21	4:E:510:ILE:O	2.15	0.46
4:E:74:LEU:HD22	4:E:93:GLN:HB2	2.49	0.46
2:H:229:ASN:HA	2:H:368:VAL:HG22	1.96	0.46
6:L:47:MET:O	7:I:544:MET:HA	2.14	0.46
8:K:139:VAL:HG12	8:K:480:PHE:CD1	2.62	0.46
4:M:98:ASN:HD21	4:M:100:ILE:HB	1.80	0.46
4:M:271:ILE:HG23	4:M:351:LEU:HD22	1.96	0.46
2:P:31:SER:OG	2:P:81:ALA:CB	2.76	0.46
7:A:229:ALA:HB2	7:A:319:ARG:HG2	1.97	0.46
8:C:93:THR:OG1	11:C:1103:BEF:F2	2.56	0.46
6:D:102:ALA:CB	6:D:449:VAL:HG21	2.45	0.46
6:D:77:MET:O	6:D:81:VAL:HG23	2.21	0.46
4:E:81:ILE:HD11	5:B:75:LYS:HD2	1.97	0.46
3:G:267:TYR:O	3:G:270:ILE:HG12	2.15	0.46
3:G:268:GLN:HA	3:G:271:VAL:HG12	1.98	0.46
3:G:86:ILE:HD11	3:G:510:ALA:CA	2.40	0.46
2:H:388:GLY:HA3	2:H:394:LEU:HD21	2.03	0.46
7:I:460:LYS:O	7:I:464:VAL:HG23	2.27	0.46
8:K:219:VAL:HG13	8:K:377:CYS:SG	2.55	0.46
3:O:242:LEU:HD13	3:O:285:VAL:HG13	2.03	0.46
6:D:29:ARG:HH12	6:D:108:GLU:CD	2.40	0.46
4:E:51:ILE:HG12	4:E:130:LEU:HB3	2.03	0.46
3:G:108:LEU:HB3	3:G:514:THR:HG21	2.10	0.46
2:H:102:LEU:HD13	2:H:524:LYS:HE2	1.97	0.46
2:H:53:LYS:HD2	2:H:71:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:69:LEU:HD13	5:J:74:ALA:HB1	2.53	0.46
1:N:225:PRO:HG2	1:N:315:LEU:HB2	2.08	0.46
7:A:221:GLY:HA3	7:A:374:ILE:O	2.16	0.46
5:B:321:THR:HG22	5:B:339:GLU:N	2.31	0.46
8:C:58:THR:O	8:C:64:ILE:HD11	2.14	0.46
8:C:96:VAL:HG22	8:C:509:SER:HA	1.97	0.46
6:D:63:THR:HG21	6:D:392:ARG:CD	2.45	0.46
4:E:72:LYS:HB2	4:E:90:ILE:HD12	2.31	0.46
1:F:454:ILE:HB	1:F:455:PRO:HD3	2.02	0.46
3:G:179:VAL:C	3:G:181:MET:H	2.37	0.46
2:H:35:ILE:HD13	2:H:111:LEU:HD13	1.98	0.46
2:H:117:LEU:HB3	2:H:122:LEU:HD12	1.98	0.46
5:J:219:GLY:O	5:J:220:ASN:CB	2.54	0.46
5:J:279:PHE:CB	5:J:281:ILE:HD12	2.84	0.46
6:L:125:GLN:HE21	6:L:513:GLU:HG2	1.80	0.46
6:L:64:ILE:O	6:L:68:MET:HG2	2.37	0.46
4:M:86:ASP:O	4:M:90:ILE:HG12	2.41	0.46
7:A:15:LEU:O	7:A:17:GLY:N	2.49	0.46
5:B:183:ARG:HH22	5:B:211:GLY:N	2.28	0.46
5:B:255:THR:HG22	6:D:263:ILE:HA	1.97	0.46
5:B:31:ASP:HA	5:B:34:LYS:HG3	1.98	0.46
10:C:1102:ADP:H8	10:C:1102:ADP:H5'2	2.16	0.46
3:G:162:ALA:HB3	3:G:179:VAL:HG23	1.97	0.46
6:L:166:TYR:O	6:L:170:LEU:HB2	2.15	0.46
6:L:257:TYR:HA	6:L:260:MET:HE2	2.23	0.46
4:M:269:LEU:HD13	4:M:322:ILE:HD12	1.97	0.46
2:P:43:LEU:HA	2:P:105:ILE:HD11	1.98	0.46
2:P:245:HIS:ND1	2:P:245:HIS:N	2.80	0.46
4:E:269:LEU:H	4:E:375:GLY:N	2.13	0.46
1:F:217:HIS:HE2	1:F:320:ALA:HA	1.80	0.46
1:F:269:PHE:CG	8:C:273:LEU:HD23	2.51	0.46
7:I:95:GLY:HA3	7:I:407:SER:OG	2.41	0.46
7:I:77:HIS:CD2	7:I:79:ALA:HB3	2.64	0.46
6:L:398:LEU:HA	6:L:401:ILE:HD12	1.97	0.46
4:M:327:PHE:CE2	4:M:342:ALA:HB1	2.50	0.46
4:M:147:ALA:HB1	4:M:546:ARG:HG3	2.01	0.46
3:O:86:ILE:CD1	3:O:510:ALA:HA	2.40	0.46
3:O:83:LEU:HA	3:O:86:ILE:HG22	2.05	0.46
2:P:110:LEU:O	2:P:114:SER:HB2	2.14	0.46
2:P:27:GLN:NE2	2:P:544:ILE:HD11	2.90	0.46
7:A:54:VAL:HG12	7:A:56:ASP:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:494:GLU:C	6:D:496:HIS:H	2.19	0.46
3:G:264:VAL:O	3:G:267:TYR:HB2	2.15	0.46
3:G:449:ILE:HD12	3:G:449:ILE:H	1.80	0.46
2:H:25:ASP:C	2:H:27:GLN:N	2.68	0.46
7:I:101:VAL:HG22	7:I:527:SER:OG	2.30	0.46
5:J:409:MET:CB	5:J:463:ILE:HD13	2.51	0.46
2:P:428:ILE:HD11	2:P:478:LEU:HD21	1.98	0.46
2:P:85:LEU:CD2	2:P:534:ALA:HB1	2.46	0.46
1:F:177:ALA:O	1:F:181:VAL:HG23	2.18	0.46
3:G:327:ILE:HA	3:G:330:VAL:HG12	1.97	0.46
3:G:55:THR:HG22	3:G:56:SER:N	2.30	0.46
2:H:281:GLU:OE1	3:G:337:THR:HG21	2.16	0.46
2:H:512:ILE:CG2	2:H:517:ILE:O	2.67	0.46
6:L:30:SER:OG	7:I:11:ASP:HB3	2.31	0.46
7:I:77:HIS:HD2	7:I:79:ALA:HB3	1.95	0.46
6:L:500:PRO:HB2	6:L:503:VAL:HG23	2.19	0.46
6:L:78:LEU:HD22	6:L:97:VAL:HG13	2.28	0.46
7:A:198:TYR:CD2	7:A:198:TYR:N	2.84	0.46
7:A:281:VAL:O	7:A:285:VAL:HG23	2.21	0.46
7:A:52:MET:HG3	7:A:62:VAL:HG22	1.97	0.46
8:C:246:LEU:HD13	8:C:250:LEU:HD21	1.97	0.46
6:D:450:ILE:HB	6:D:451:PRO:HD3	1.98	0.46
4:E:168:ILE:HD11	4:E:439:VAL:CG1	2.44	0.46
4:E:224:ILE:HD13	4:E:404:VAL:HG12	2.05	0.46
7:I:488:LYS:CB	7:I:489:PRO:HD2	2.59	0.46
4:M:415:ILE:HD13	5:J:503:GLU:OE1	2.15	0.46
8:K:208:LYS:HE3	8:K:390:ASN:OD1	2.16	0.46
6:L:286:LEU:HD12	6:L:305:LEU:HD21	1.96	0.46
6:L:63:THR:HG21	6:L:392:ARG:HD3	1.98	0.46
4:M:323:CYS:HB3	4:M:327:PHE:CE1	2.56	0.46
1:N:195:GLU:HG3	1:N:327:ARG:HH11	1.77	0.46
3:O:288:THR:HG22	3:O:346:LEU:HD11	2.22	0.46
2:P:252:CYS:HB2	2:P:342:PRO:O	2.19	0.46
5:B:441:PRO:HB3	5:B:472:LEU:CD1	2.45	0.46
6:D:103:LEU:O	6:D:106:ALA:HB3	2.15	0.46
4:E:322:ILE:HD13	4:E:354:ILE:HD13	1.97	0.46
4:E:275:PRO:HD3	4:E:325:TRP:CE3	2.51	0.46
7:I:501:GLY:HA3	7:I:512:GLU:HG2	1.98	0.46
5:J:234:ALA:HA	5:J:326:VAL:O	2.17	0.46
5:J:321:THR:HG22	5:J:339:GLU:N	2.33	0.46
5:J:440:LEU:CB	5:J:441:PRO:HD3	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:147:ASN:HB3	8:K:150:ALA:HB3	1.98	0.46
6:L:469:LEU:O	6:L:473:HIS:HB2	2.16	0.46
4:M:98:ASN:ND2	4:M:101:ALA:H	2.12	0.46
1:F:251:PHE:HZ	2:H:259:THR:CB	2.37	0.45
3:G:249:GLU:O	3:G:278:ILE:HG21	2.30	0.45
2:H:155:ASP:O	2:H:159:LEU:HG	2.17	0.45
6:L:520:ARG:CG	6:L:520:ARG:NH2	2.71	0.45
4:M:240:ILE:HD12	4:M:244:ILE:HD11	1.98	0.45
3:O:368:CYS:HA	3:O:369:PRO:HD2	1.73	0.45
8:C:99:LEU:O	8:C:103:ILE:HG13	2.16	0.45
8:C:252:TYR:H	8:C:252:TYR:HD2	1.62	0.45
7:A:73:LEU:HB3	8:C:8:MET:HE1	2.18	0.45
3:G:243:SER:HB3	3:G:323:MET:CE	2.46	0.45
3:G:424:LEU:HB2	3:G:443:ALA:HB2	1.98	0.45
5:J:346:ILE:HG22	5:J:347:MET:H	1.83	0.45
8:K:167:TRP:N	8:K:167:TRP:CD1	2.86	0.45
8:K:298:GLU:HG3	8:K:325:ASN:OD1	2.17	0.45
8:K:198:ILE:CG2	8:K:408:LEU:HD21	2.84	0.45
6:L:103:LEU:HB3	6:L:515:VAL:HG21	2.11	0.45
6:L:236:LEU:HD12	6:L:287:LEU:HB2	2.08	0.45
1:N:509:SER:HB2	1:N:512:VAL:CG2	2.50	0.45
4:E:278:PRO:HA	4:E:279:PRO:HD3	1.92	0.45
1:F:301:ILE:CG1	1:F:318:ARG:HB3	2.46	0.45
3:G:40:LEU:HG	3:G:99:THR:HG23	2.12	0.45
2:H:21:TYR:CE1	3:G:10:ILE:HG13	2.51	0.45
5:J:443:ILE:HA	5:J:446:ASP:HB2	1.98	0.45
1:N:473:VAL:HG13	1:N:489:VAL:HG22	2.02	0.45
2:P:128:ILE:HG12	2:P:536:THR:HG23	2.19	0.45
2:P:79:HIS:HD2	2:P:81:ALA:N	2.41	0.45
5:B:320:VAL:O	5:B:359:CYS:HB3	2.61	0.45
5:B:181:ILE:HD13	5:B:391:LEU:HB3	1.99	0.45
4:E:327:PHE:H	4:E:344:ARG:HD2	1.80	0.45
4:E:481:MET:O	4:E:485:GLU:HB2	2.35	0.45
1:F:457:THR:HA	1:F:460:LYS:HB2	2.16	0.45
5:J:214:LEU:HD11	5:J:317:LEU:HD11	1.99	0.45
4:M:267:VAL:HB	4:M:377:CYS:HB2	2.15	0.45
1:N:281:LYS:O	1:N:285:CYS:HB2	2.17	0.45
1:N:57:LYS:O	1:N:57:LYS:HG2	2.25	0.45
7:A:250:ASN:HB3	7:A:300:LYS:CB	2.49	0.45
7:A:262:ILE:CG2	8:C:259:THR:HG23	2.54	0.45
8:C:23:SER:HB3	8:C:72:HIS:CE1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:162:ILE:O	6:D:162:ILE:CG1	2.64	0.45
6:D:237:ILE:HG23	6:D:239:PHE:CE2	2.68	0.45
1:F:30:GLN:HB2	1:F:96:CYS:HA	1.97	0.45
1:F:79:ALA:HB2	1:F:523:ILE:CD1	2.45	0.45
3:G:88:ARG:CG	3:G:88:ARG:NH1	2.79	0.45
7:I:466:ALA:O	7:I:467:ALA:HB3	2.17	0.45
5:J:213:ILE:HG22	5:J:353:PHE:HB3	1.98	0.45
4:M:413:LYS:H	5:J:79:ASN:HD21	1.65	0.45
1:N:102:LEU:HD11	1:N:527:LEU:HD13	1.98	0.45
1:N:153:VAL:HG11	1:N:405:VAL:CG2	2.46	0.45
1:N:327:ARG:O	1:N:331:VAL:HG23	2.16	0.45
3:O:166:MET:HE3	3:O:396:ALA:HB2	2.26	0.45
3:O:7:THR:O	3:O:8:PRO:O	2.38	0.45
1:N:252:PHE:HD1	2:P:264:THR:HB	1.95	0.45
8:C:25:ILE:HG21	8:C:109:PRO:HG3	2.33	0.45
4:E:232:GLY:H	5:B:87:GLU:HG3	1.81	0.45
4:E:492:ILE:H	4:E:492:ILE:HG13	1.46	0.45
7:I:366:PHE:HB3	7:I:388:ARG:NH1	2.32	0.45
5:J:234:ALA:C	5:J:286:ASN:HD22	2.20	0.45
5:J:255:THR:HG21	6:L:263:ILE:HA	1.98	0.45
6:L:198:LYS:HE2	6:L:391:GLU:OE1	2.57	0.45
4:M:324:GLN:HB2	4:M:351:LEU:HD11	2.11	0.45
1:N:119:THR:HG21	1:N:529:LEU:HD11	1.99	0.45
3:O:264:VAL:O	3:O:267:TYR:HB2	2.16	0.45
2:P:428:ILE:HA	2:P:431:ILE:HD12	2.22	0.45
5:B:181:ILE:HD13	5:B:391:LEU:HB2	1.98	0.45
3:G:147:ILE:HG22	3:G:152:SER:HB3	2.24	0.45
3:G:204:ILE:HB	3:G:362:TYR:OH	2.17	0.45
6:L:323:PHE:CD1	6:L:323:PHE:C	2.90	0.45
3:O:108:LEU:HD21	3:O:442:PHE:CE2	2.91	0.45
3:O:488:ILE:H	3:O:488:ILE:HG13	1.47	0.45
2:P:109:GLU:CG	2:P:458:VAL:HG21	2.46	0.45
2:P:238:SER:C	2:P:240:SER:N	2.79	0.45
7:A:422:GLY:HA2	10:A:602:ADP:N3	2.39	0.45
8:C:59:ASN:CB	8:C:162:LYS:HG2	2.44	0.45
4:E:73:ILE:HG22	5:B:511:VAL:HG13	2.31	0.45
1:F:324:ASN:ND2	1:F:327:ARG:HD2	2.32	0.45
1:F:370:ASN:H	1:F:370:ASN:ND2	2.14	0.45
1:F:45:MET:HB2	2:H:541:ILE:HD12	2.13	0.45
5:J:53:THR:HG22	5:J:54:CYS:N	2.32	0.45
2:P:39:HIS:ND1	2:P:108:GLY:HA3	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:323:VAL:O	2:P:324:PRO:C	2.66	0.45
7:A:335:ALA:HB2	7:A:356:GLY:N	2.59	0.45
5:B:192:HIS:CD2	5:B:319:LEU:CD1	3.00	0.45
8:C:154:LEU:HG	8:C:412:LEU:HD21	2.19	0.45
8:C:164:VAL:HG12	8:C:164:VAL:O	2.38	0.45
1:F:122:PHE:HD1	1:F:525:SER:HB2	1.82	0.45
3:G:348:THR:HG22	3:G:349:CYS:H	1.81	0.45
4:M:250:SER:HB3	4:M:332:ASN:OD1	2.17	0.45
3:O:465:LEU:HD12	3:O:469:ARG:HH21	1.82	0.45
2:P:22:SER:OG	2:P:23:ASN:N	2.68	0.45
5:B:14:ARG:HG3	5:B:513:ASN:ND2	2.48	0.45
8:C:118:PRO:O	8:C:122:ILE:HG13	2.17	0.45
6:D:162:ILE:HG13	6:D:162:ILE:O	2.23	0.45
6:D:469:LEU:O	6:D:473:HIS:HB2	2.17	0.45
4:E:323:CYS:HB3	4:E:327:PHE:CE1	2.52	0.45
4:E:363:VAL:HA	4:E:364:PRO:HD3	1.92	0.45
4:E:464:ILE:HD12	4:E:464:ILE:H	1.84	0.45
5:J:152:ASP:OD1	5:J:400:THR:HG21	2.16	0.45
7:I:52:MET:CE	8:K:73:PRO:HB2	2.46	0.45
2:P:238:SER:C	2:P:240:SER:H	2.27	0.45
2:P:32:ILE:HG13	2:P:111:LEU:HB3	1.99	0.45
8:C:198:ILE:CG2	8:C:199:ASP:N	2.80	0.44
4:E:450:MET:HB3	4:E:450:MET:HE2	1.84	0.44
2:H:323:VAL:O	2:H:324:PRO:C	2.56	0.44
7:I:336:THR:HB	7:I:354:TYR:CD2	2.83	0.44
7:I:68:THR:O	7:I:72:LEU:HG	2.17	0.44
8:K:414:PRO:HB3	8:K:481:THR:HG23	2.00	0.44
8:K:35:ILE:HB	8:K:97:ILE:HD11	2.20	0.44
4:M:41:GLN:HB2	4:M:554:VAL:HB	2.17	0.44
1:N:114:HIS:O	1:N:117:ILE:HB	2.17	0.44
2:H:6:PRO:HB2	1:N:535:ARG:NH1	2.38	0.44
3:O:226:TYR:O	3:O:227:ALA:C	2.55	0.44
3:O:416:THR:O	3:O:420:VAL:HG23	2.17	0.44
2:P:77:ILE:HD13	2:P:86:VAL:HG21	2.00	0.44
8:C:219:VAL:HG13	8:C:377:CYS:SG	2.64	0.44
1:F:39:PRO:HD3	1:F:160:THR:HG22	2.00	0.44
1:F:455:PRO:O	1:F:459:VAL:HG23	2.17	0.44
1:F:47:VAL:HG21	2:H:80:PRO:HG3	2.00	0.44
5:J:197:LYS:HB2	5:J:377:LEU:HD22	2.56	0.44
6:L:516:LYS:O	6:L:520:ARG:HG2	2.17	0.44
2:P:21:TYR:N	2:P:21:TYR:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:12:THR:HB	7:A:14:PHE:HE2	2.19	0.44
5:B:474:LEU:HD12	5:B:474:LEU:HA	1.85	0.44
10:B:602:ADP:O3B	11:B:603:BEF:F3	2.48	0.44
1:F:37:LEU:HD23	1:F:458:LEU:HG	1.98	0.44
1:F:452:LEU:HD22	1:F:470:LEU:HD21	1.99	0.44
1:F:465:ASP:HA	1:F:466:PRO:HD3	1.78	0.44
3:G:40:LEU:HD11	3:G:66:GLY:HA2	2.46	0.44
7:I:512:GLU:OE1	7:I:517:VAL:HG21	2.18	0.44
5:J:293:TYR:HB3	5:J:294:PRO:CD	2.49	0.44
4:M:211:VAL:HG11	4:M:224:ILE:CD1	2.63	0.44
4:M:319:ASP:O	4:M:341:PRO:HD2	2.31	0.44
3:O:232:GLN:NE2	3:O:304:THR:HG23	2.32	0.44
3:O:3:PHE:N	3:O:3:PHE:CD2	2.81	0.44
7:A:316:MET:O	7:A:316:MET:HG2	2.16	0.44
7:A:477:LEU:CD2	7:A:509:ILE:HG12	2.47	0.44
5:B:287:ARG:HG3	5:B:310:ASP:HA	1.98	0.44
5:B:88:VAL:O	5:B:389:SER:HB3	2.23	0.44
8:C:353:GLY:CA	8:C:370:ASN:HB2	2.43	0.44
1:N:196:ILE:HG21	1:N:392:LYS:HG3	2.08	0.44
1:N:87:THR:HG22	1:N:89:ASP:H	1.83	0.44
8:C:209:ILE:HA	8:C:210:PRO:HD2	1.78	0.44
4:E:115:ILE:CD1	4:E:536:GLN:HB3	2.48	0.44
3:G:74:ASP:O	4:E:32:VAL:HA	2.16	0.44
7:I:198:TYR:CD2	7:I:198:TYR:N	2.91	0.44
7:I:253:LYS:HE2	7:I:305:LEU:HD22	2.51	0.44
7:I:327:ARG:HH22	7:I:328:ARG:NH2	2.16	0.44
5:J:102:LEU:HD21	5:J:433:PHE:CD2	2.53	0.44
8:K:377:CYS:SG	8:K:378:THR:N	2.90	0.44
4:M:38:LYS:HG2	4:M:557:SER:HA	2.16	0.44
1:N:241:GLU:HA	1:N:302:ASP:HB2	2.11	0.44
2:P:42:CYS:SG	2:P:104:MET:HG2	2.57	0.44
7:A:103:ILE:HG22	7:A:457:ILE:CG2	2.65	0.44
7:A:338:VAL:HG21	7:A:350:PHE:HE1	2.03	0.44
7:A:366:PHE:HB3	7:A:388:ARG:NH1	2.33	0.44
5:B:346:ILE:HG22	5:B:347:MET:N	2.36	0.44
8:C:92:GLY:HA2	10:C:1102:ADP:O2B	2.24	0.44
7:A:255:ARG:HA	8:C:257:SER:HA	1.98	0.44
8:C:478:GLY:O	8:C:479:ASN:HB2	2.35	0.44
6:D:96:VAL:HG23	6:D:507:ALA:O	2.17	0.44
4:E:38:LYS:HG2	4:E:557:SER:HA	1.99	0.44
2:H:92:GLN:OE1	2:H:103:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:335:ALA:HB2	7:I:356:GLY:N	2.56	0.44
8:K:389:LEU:HA	8:K:392:ILE:HD12	1.99	0.44
1:N:534:LEU:HD12	8:K:48:LEU:HD23	1.99	0.44
4:M:428:CYS:O	4:M:431:ARG:HG3	2.17	0.44
3:O:179:VAL:HG13	3:O:180:LYS:N	2.32	0.44
2:P:233:GLU:HB2	2:P:320:VAL:HB	1.99	0.44
7:A:410:LYS:HD3	7:A:411:ARG:NE	2.54	0.44
7:A:53:LEU:HD11	7:A:69:ILE:HG23	1.99	0.44
5:B:58:ASN:O	5:B:59:ASP:C	2.56	0.44
5:B:33:VAL:HB	5:B:93:THR:HG23	2.00	0.44
8:C:291:ARG:N	8:C:292:PRO:HD3	2.33	0.44
6:D:420:GLU:HB2	6:D:473:HIS:HE1	1.81	0.44
4:E:324:GLN:HB2	4:E:351:LEU:CD1	2.53	0.44
4:E:84:THR:HG22	4:E:418:GLU:OE1	2.18	0.44
1:F:298:GLN:O	1:F:319:ARG:HA	2.17	0.44
3:G:242:LEU:HD13	3:G:285:VAL:HG13	2.17	0.44
7:I:236:ARG:HG3	7:I:362:VAL:HG22	2.18	0.44
5:J:193:ILE:HA	5:J:365:CYS:O	2.37	0.44
5:J:57:THR:HG21	5:J:62:THR:HB	2.00	0.44
5:J:46:LEU:HD21	5:J:63:ILE:HG23	2.03	0.44
4:M:387:THR:HB	5:J:86:ASP:O	2.17	0.44
8:K:257:SER:O	8:K:258:GLN:HG2	2.17	0.44
8:K:389:LEU:HD23	8:K:392:ILE:HD12	1.99	0.44
8:K:457:ILE:CD1	8:K:484:ILE:HG12	2.48	0.44
5:J:370:ARG:NH2	6:L:88:GLU:OE2	2.56	0.44
1:N:27:GLU:HG2	1:N:103:ARG:HE	1.83	0.44
3:O:220:PHE:C	3:O:222:LYS:N	2.70	0.44
2:P:341:LEU:HD23	2:P:342:PRO:HD2	2.26	0.44
2:P:78:VAL:HB	3:O:11:VAL:O	2.17	0.44
7:A:68:THR:O	7:A:72:LEU:HG	2.18	0.44
5:B:419:ALA:C	5:B:421:ASN:H	2.50	0.44
5:B:518:ARG:HA	5:B:519:PRO:HD2	1.85	0.44
6:D:161:LYS:O	6:D:163:VAL:N	2.50	0.44
4:E:320:VAL:HG22	4:E:341:PRO:HB2	2.00	0.44
3:G:348:THR:HG22	3:G:349:CYS:N	2.33	0.44
2:H:409:LYS:O	2:H:409:LYS:HD2	2.17	0.44
2:H:428:ILE:HA	2:H:431:ILE:HD12	2.03	0.44
5:J:32:LEU:O	5:J:44:LYS:HE3	2.29	0.44
5:B:119:THR:OG1	6:L:8:ASN:OD1	2.25	0.44
7:A:52:MET:HE1	8:C:73:PRO:HB2	2.15	0.44
4:E:388:THR:HG21	5:B:385:HIS:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:471:VAL:HG21	8:K:115:ASN:HD22	1.82	0.44
7:I:338:VAL:HG21	7:I:350:PHE:HE1	1.91	0.44
7:I:144:LEU:HD23	7:I:419:VAL:HG13	1.99	0.44
6:L:432:MET:HG3	6:L:440:TRP:HE3	1.96	0.44
4:M:324:GLN:HB2	4:M:351:LEU:CD1	2.53	0.44
4:M:381:TYR:CE1	4:M:394:ILE:HD12	2.63	0.44
2:P:147:VAL:O	2:P:419:LEU:HB2	2.29	0.44
1:N:253:TYR:O	2:P:265:VAL:HA	2.19	0.44
2:P:302:GLY:HA3	2:P:329:LEU:HD11	1.99	0.44
2:P:68:ALA:HA	2:P:71:MET:HE1	2.00	0.44
7:A:25:ILE:HG21	7:A:542:ASP:O	2.18	0.43
5:B:402:LEU:H	5:B:402:LEU:HD12	1.83	0.43
5:B:407:ALA:O	5:B:411:MET:HG3	2.17	0.43
5:B:426:LYS:O	5:B:430:VAL:HG23	2.33	0.43
8:C:485:ASP:HB2	8:C:492:VAL:HG21	1.98	0.43
6:D:242:SER:HB3	6:D:243:PRO:HD2	2.00	0.43
6:D:448:GLU:OE1	6:D:470:ARG:NH2	2.51	0.43
1:F:473:VAL:HG13	1:F:489:VAL:HG22	1.99	0.43
6:L:49:LYS:HD3	7:I:546:THR:HG23	1.99	0.43
8:K:271:ARG:O	8:K:275:ILE:HG13	2.16	0.43
8:K:81:LEU:CD1	8:K:516:SER:HB2	2.47	0.43
4:M:96:LEU:HD13	4:M:101:ALA:HB1	2.09	0.43
4:M:47:LYS:NZ	4:M:143:PRO:HG3	2.32	0.43
4:M:498:LEU:HD21	4:M:510:ILE:O	2.18	0.43
3:O:83:LEU:HB3	3:O:102:THR:HG23	2.00	0.43
2:P:305:VAL:HG11	2:P:310:LEU:HD12	2.00	0.43
8:C:425:VAL:HA	8:C:428:ALA:HB3	1.99	0.43
8:C:440:TRP:HB2	8:C:441:PRO:HD3	1.99	0.43
6:D:323:PHE:C	6:D:323:PHE:CD1	2.91	0.43
6:D:102:ALA:HB2	6:D:449:VAL:HG21	1.99	0.43
4:E:353:HIS:HB3	4:E:403:THR:HG21	1.99	0.43
7:I:266:ASP:HA	7:I:267:PRO:HD2	1.84	0.43
7:I:269:GLN:HA	7:I:272:GLN:HB2	2.00	0.43
7:I:53:LEU:HD11	7:I:69:ILE:HG23	2.00	0.43
5:J:162:SER:HA	5:J:167:SER:OG	2.18	0.43
8:K:78:MET:O	8:K:81:LEU:HB3	2.26	0.43
6:L:436:GLN:HA	6:L:439:ILE:HD12	1.99	0.43
6:L:72:HIS:HB2	7:I:13:LEU:HD12	1.99	0.43
4:M:158:ILE:HG13	4:M:159:SER:N	2.57	0.43
1:N:269:PHE:CG	8:K:273:LEU:HD23	2.67	0.43
1:N:30:GLN:HB2	1:N:96:CYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:311:HIS:CD2	3:O:336:SER:H	2.36	0.43
3:O:395:ASP:OD2	11:O:603:BEF:F2	2.63	0.43
2:P:8:ASN:HA	2:P:9:PRO:HD3	1.94	0.43
7:A:56:ASP:C	7:A:56:ASP:OD1	2.56	0.43
4:E:245:LEU:HD11	4:E:354:ILE:HD11	1.99	0.43
4:E:381:TYR:CE1	4:E:394:ILE:HD12	2.58	0.43
1:F:269:PHE:HE1	8:C:274:GLN:HG3	1.83	0.43
2:H:411:LEU:HD12	2:H:417:GLY:HA3	2.01	0.43
5:J:281:ILE:HG22	5:J:283:THR:H	1.83	0.43
2:H:121:GLY:HA3	8:K:464:PRO:HG2	2.13	0.43
1:N:101:LEU:HG	1:N:122:PHE:CE1	2.53	0.43
1:N:457:THR:HA	1:N:460:LYS:HB2	2.17	0.43
3:O:165:ALA:HB2	3:O:399:ILE:HD12	1.99	0.43
6:D:47:MET:O	7:A:544:MET:HA	2.18	0.43
5:B:203:LEU:N	6:D:513:GLU:OE2	2.51	0.43
1:F:418:PHE:HE2	1:F:517:ILE:HD11	1.86	0.43
1:F:84:ASP:HB2	1:F:91:THR:HG21	2.11	0.43
7:I:47:VAL:HG12	8:K:117:HIS:NE2	2.44	0.43
5:J:503:GLU:O	5:J:507:VAL:HG23	2.38	0.43
5:J:82:LYS:NZ	5:J:86:ASP:OD2	2.58	0.43
8:K:99:LEU:HG	8:K:452:ILE:HD11	1.98	0.43
6:L:158:LEU:O	6:L:160:SER:N	2.51	0.43
1:N:458:LEU:HB3	1:N:493:LEU:HD21	1.99	0.43
1:N:55:LEU:HD11	2:P:541:ILE:HD11	1.99	0.43
3:O:247:GLU:HB3	3:O:298:PRO:HD2	2.20	0.43
3:O:51:ILE:HB	3:O:69:ILE:HD12	2.06	0.43
2:P:280:GLU:O	2:P:284:ILE:HG12	2.54	0.43
8:C:100:ALA:O	8:C:104:LEU:HD12	2.27	0.43
5:B:370:ARG:NH2	6:D:88:GLU:OE2	2.68	0.43
4:E:322:ILE:CG2	4:E:346:VAL:HG21	2.48	0.43
1:F:22:ASN:HA	1:F:72:THR:HG21	2.13	0.43
1:F:277:ILE:HG13	1:F:340:VAL:HG11	2.01	0.43
1:F:459:VAL:HA	1:F:462:SER:HB3	1.99	0.43
1:F:70:SER:HB3	1:F:73:ALA:HB3	2.06	0.43
3:G:220:PHE:C	3:G:222:LYS:N	2.68	0.43
3:G:83:LEU:HA	3:G:86:ILE:HG22	2.10	0.43
2:H:189:VAL:HG11	2:H:206:SER:HB3	2.01	0.43
2:H:256:ILE:HG13	2:H:256:ILE:H	1.62	0.43
2:H:25:ASP:O	2:H:27:GLN:N	2.52	0.43
5:J:151:GLU:HA	5:J:154:ILE:HD12	2.01	0.43
5:J:181:ILE:HD13	5:J:391:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:138:MET:HB2	6:L:478:LEU:CD1	2.41	0.43
1:N:420:ILE:O	1:N:424:ARG:HG3	2.19	0.43
1:N:121:GLY:HA3	1:N:443:GLY:HA3	2.35	0.43
2:P:117:LEU:HD22	2:P:122:LEU:HD12	2.13	0.43
2:P:62:ILE:HG13	2:P:62:ILE:H	1.61	0.43
7:A:55:ASP:CB	7:A:59:ASP:O	2.62	0.43
1:F:342:ASP:HB3	8:C:307:HIS:CE1	2.53	0.43
8:C:502:PRO:HD2	8:C:505:ILE:HD12	2.02	0.43
6:D:500:PRO:HB2	6:D:503:VAL:HG23	2.01	0.43
6:D:520:ARG:CG	6:D:520:ARG:NH2	2.76	0.43
3:G:86:ILE:CD1	3:G:510:ALA:HA	2.45	0.43
2:H:387:ARG:HH22	3:G:93:GLU:CD	2.34	0.43
7:I:162:THR:HG23	7:I:517:VAL:HG13	2.47	0.43
7:I:333:THR:HA	7:I:377:THR:HG22	1.99	0.43
5:J:440:LEU:CB	5:J:441:PRO:CD	3.09	0.43
8:K:471:LEU:O	8:K:475:HIS:HB2	2.18	0.43
7:I:209:HIS:NE2	8:K:87:GLU:OE1	3.08	0.43
6:L:295:ASP:O	6:L:296:ALA:CB	2.67	0.43
6:L:320:GLU:O	6:L:324:LEU:HB2	2.19	0.43
3:O:342:LYS:C	3:O:344:GLU:H	2.22	0.43
3:O:45:GLY:HA3	3:O:453:LEU:HD22	2.04	0.43
7:A:522:ILE:H	7:A:522:ILE:HG13	1.69	0.43
7:A:411:ARG:HB3	7:A:522:ILE:HD12	2.43	0.43
7:A:56:ASP:OD1	7:A:57:ILE:N	2.52	0.43
6:D:409:GLY:C	6:D:501:VAL:HG23	2.45	0.43
2:H:79:HIS:HA	2:H:80:PRO:HD3	1.83	0.43
7:I:179:MET:CE	7:I:385:ILE:HG23	2.45	0.43
8:K:250:LEU:HD12	8:K:301:VAL:HG22	2.00	0.43
8:K:58:THR:O	8:K:64:ILE:HD11	2.25	0.43
6:L:242:SER:HB3	6:L:243:PRO:HD2	1.99	0.43
6:L:45:ASP:OD1	6:L:59:ASN:HB2	2.19	0.43
6:L:77:MET:O	6:L:81:VAL:HG23	2.44	0.43
4:M:412:ASN:OD1	4:M:415:ILE:HG13	2.21	0.43
3:O:209:MET:HG2	4:M:543:GLN:NE2	2.34	0.43
3:O:94:VAL:CG1	3:O:502:VAL:HG22	2.49	0.43
2:P:311:HIS:HB2	3:O:336:SER:HB2	2.27	0.43
7:A:121:HIS:CG	7:A:122:PRO:HD2	2.53	0.43
8:C:145:VAL:HG12	8:C:406:VAL:HG12	2.02	0.43
6:D:404:LEU:HD11	6:D:410:LEU:HD13	2.00	0.43
3:G:206:GLY:HA2	4:E:110:SER:HB3	2.01	0.43
4:E:269:LEU:HD12	4:E:358:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:91:LEU:HD11	4:E:123:VAL:HG21	2.04	0.43
1:F:255:SER:HB3	1:F:258:GLN:HB2	2.03	0.43
7:I:56:ASP:OD1	7:I:57:ILE:N	2.86	0.43
4:M:473:ALA:HA	4:M:476:LEU:HD12	2.01	0.43
1:N:251:PHE:HZ	2:P:259:THR:CB	2.43	0.43
3:O:162:ALA:O	3:O:166:MET:HG2	2.22	0.43
3:O:202:LYS:HB3	3:O:377:LEU:HD23	2.01	0.43
2:P:478:LEU:HD22	2:P:499:VAL:CG2	2.49	0.43
2:P:71:MET:HE2	2:P:72:LEU:HG	2.44	0.43
7:A:255:ARG:O	7:A:257:ALA:N	2.64	0.43
7:A:510:VAL:HG12	7:A:511:ASP:N	2.35	0.43
5:B:326:VAL:HG12	5:B:327:SER:O	2.19	0.43
2:H:122:LEU:HD22	2:H:126:GLU:HB3	2.00	0.43
2:H:424:GLY:HA2	2:H:427:GLU:HG2	2.23	0.43
8:K:154:LEU:HG	8:K:412:LEU:HD21	2.01	0.43
8:K:35:ILE:O	8:K:35:ILE:CG2	2.72	0.43
1:N:492:ASP:HB2	1:N:499:CYS:CB	2.48	0.43
2:P:322:LYS:O	2:P:324:PRO:HD3	2.71	0.43
7:A:63:THR:HG22	7:A:65:ASP:H	1.94	0.43
5:B:279:PHE:HB3	5:B:281:ILE:CD1	2.49	0.43
5:B:409:MET:HG3	5:B:459:LEU:CD2	2.80	0.43
8:C:457:ILE:HD13	8:C:484:ILE:HG21	2.01	0.43
6:D:64:ILE:O	6:D:68:MET:HG2	2.19	0.43
1:F:301:ILE:HG12	1:F:318:ARG:HB3	2.00	0.43
3:G:191:ARG:O	3:G:192:ASN:C	2.57	0.43
3:G:18:ASP:O	3:G:524:ILE:HA	2.19	0.43
2:H:63:ILE:HG21	2:H:74:GLU:HG3	1.99	0.43
5:J:56:VAL:HG23	5:J:375:GLN:HG2	2.02	0.43
4:M:74:LEU:HD13	4:M:93:GLN:HG3	2.01	0.43
6:D:253:ILE:HG22	7:A:263:ASN:HB2	2.01	0.42
7:A:53:LEU:HB3	8:C:530:VAL:HG21	2.01	0.42
5:B:220:ASN:HB3	5:B:221:ASN:H	1.59	0.42
6:D:225:GLY:N	6:D:226:PRO:HD3	2.34	0.42
1:F:278:ILE:HG13	1:F:278:ILE:H	1.67	0.42
1:F:57:LYS:HG2	1:F:57:LYS:O	2.19	0.42
3:G:218:VAL:HG12	3:G:219:ALA:H	1.83	0.42
3:G:322:ASP:HA	3:G:325:ARG:HB2	2.01	0.42
4:M:507:ILE:H	4:M:507:ILE:HG13	1.62	0.42
3:O:220:PHE:HD2	3:O:363:ASN:HB2	1.83	0.42
3:O:297:LEU:CB	3:O:298:PRO:HD2	2.40	0.42
2:P:39:HIS:O	2:P:43:LEU:HB2	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:73:LEU:HD22	8:C:8:MET:HE1	2.01	0.42
7:A:77:HIS:CD2	7:A:79:ALA:HB3	2.68	0.42
5:B:175:GLU:O	5:B:179:ASN:HB2	2.19	0.42
5:B:197:LYS:HB2	5:B:377:LEU:HD13	2.01	0.42
5:B:32:LEU:O	5:B:44:LYS:HE3	2.33	0.42
5:B:36:THR:HG23	5:B:58:ASN:CG	2.57	0.42
8:C:161:THR:HG21	10:C:1102:ADP:O2A	2.37	0.42
8:C:206:VAL:HG13	8:C:379:ILE:HB	2.01	0.42
3:G:263:HIS:HA	4:E:294:GLU:OE2	2.32	0.42
2:H:327:PHE:CG	2:H:328:GLU:N	2.86	0.42
7:I:126:ILE:HD11	7:I:539:LEU:HB3	2.01	0.42
7:I:12:THR:CB	7:I:14:PHE:CE2	2.96	0.42
7:I:422:GLY:O	7:I:502:LEU:HB3	2.19	0.42
8:K:248:CYS:O	8:K:297:THR:CG2	2.67	0.42
8:K:467:LEU:O	8:K:471:LEU:HB2	2.45	0.42
8:K:70:VAL:HG11	8:K:75:ALA:HB1	2.01	0.42
6:L:242:SER:O	6:L:244:PRO:HD3	2.23	0.42
6:L:409:GLY:C	6:L:501:VAL:HG23	2.55	0.42
10:M:602:ADP:O3B	11:M:603:BEF:F2	2.27	0.42
1:N:285:CYS:SG	1:N:293:PHE:HB2	2.74	0.42
1:N:202:LEU:O	1:N:383:SER:HB3	2.18	0.42
3:O:498:GLU:HA	3:O:499:PRO:HD3	1.90	0.42
5:B:239:ASP:CA	5:B:291:TYR:HB2	2.49	0.42
5:B:327:SER:O	5:B:329:PHE:N	2.53	0.42
5:B:390:VAL:CG1	5:B:493:LEU:HD12	2.73	0.42
6:D:398:LEU:HA	6:D:401:ILE:HD12	2.00	0.42
6:D:463:ILE:HD12	4:M:141:ILE:HD11	2.13	0.42
4:E:100:ILE:HG23	4:E:548:ILE:HD12	2.02	0.42
1:F:329:GLN:HG2	1:F:334:GLY:O	2.40	0.42
3:G:488:ILE:HG13	3:G:488:ILE:H	1.58	0.42
7:I:143:VAL:O	7:I:143:VAL:CG1	2.67	0.42
7:I:333:THR:HG22	7:I:377:THR:HG22	2.37	0.42
7:I:366:PHE:O	7:I:367:SER:C	2.58	0.42
3:G:120:ILE:HD13	7:I:469:ASP:OD2	2.28	0.42
8:K:494:MET:SD	8:K:499:ILE:HB	2.59	0.42
6:L:366:ILE:N	6:L:366:ILE:HD13	2.34	0.42
6:L:419:ILE:O	6:L:422:SER:HB3	2.35	0.42
1:F:467:LEU:HD13	1:N:111:GLU:HG2	2.11	0.42
4:E:357:SER:HA	4:E:401:THR:HB	2.02	0.42
1:F:202:LEU:O	1:F:383:SER:HB3	2.26	0.42
3:G:113:LYS:HB3	3:G:114:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:133:VAL:O	3:G:137:VAL:HG23	2.19	0.42
3:G:491:ASN:HD22	3:G:491:ASN:HA	1.73	0.42
7:I:359:ASP:HB2	7:I:376:GLY:HA3	2.09	0.42
5:J:314:VAL:HG11	5:J:325:VAL:HG13	2.20	0.42
8:K:322:LYS:H	8:K:322:LYS:CD	2.32	0.42
6:L:509:THR:O	6:L:513:GLU:HB2	2.20	0.42
4:M:269:LEU:CD1	4:M:358:THR:HG21	2.66	0.42
4:M:473:ALA:O	4:M:476:LEU:HB2	2.34	0.42
1:N:70:SER:HB3	1:N:73:ALA:HB3	2.01	0.42
2:P:54:ILE:O	2:P:54:ILE:HG23	2.32	0.42
7:A:63:THR:HG22	7:A:64:ASN:H	1.85	0.42
8:C:70:VAL:HG11	8:C:75:ALA:CB	2.59	0.42
8:C:8:MET:HB3	8:C:8:MET:HE3	2.30	0.42
6:D:59:ASN:HB3	6:D:161:LYS:HG2	2.02	0.42
4:E:329:ASP:OD2	5:B:235:ASN:HB3	2.42	0.42
4:E:71:ASP:OD1	4:E:85:ASN:HB2	2.31	0.42
1:F:204:PRO:HA	1:F:381:LYS:O	2.19	0.42
1:F:234:LEU:HD23	1:F:295:ILE:HG12	2.02	0.42
7:I:248:ASP:HA	7:I:299:THR:HB	2.03	0.42
5:J:220:ASN:HB3	5:J:221:ASN:H	1.64	0.42
5:J:47:GLN:O	6:L:527:SER:N	2.59	0.42
8:K:165:ILE:H	8:K:165:ILE:HG13	1.81	0.42
8:K:78:MET:HE2	8:K:81:LEU:HD22	2.35	0.42
6:L:198:LYS:HB3	6:L:387:ILE:HG21	2.09	0.42
5:B:155:HIS:HB2	5:B:488:VAL:CG2	2.88	0.42
8:C:140:SER:HA	8:C:414:PRO:HD3	2.02	0.42
7:A:256:MET:CG	8:C:257:SER:HB2	2.69	0.42
8:C:133:LEU:HD21	8:C:511:LYS:HD2	2.01	0.42
8:C:7:PHE:CG	8:C:8:MET:N	2.87	0.42
5:B:292:ASP:HB3	6:D:238:GLN:OE1	2.53	0.42
4:E:90:ILE:H	4:E:90:ILE:HG12	1.73	0.42
3:G:460:ASP:O	3:G:464:ILE:HG12	2.19	0.42
3:G:75:VAL:O	3:G:81:LYS:HE3	2.19	0.42
2:H:455:ALA:O	2:H:458:VAL:HG23	2.19	0.42
2:H:8:ASN:HA	2:H:9:PRO:HD3	1.86	0.42
7:I:120:ILE:HD13	7:I:120:ILE:HA	2.23	0.42
7:I:422:GLY:HA2	10:I:602:ADP:N3	2.34	0.42
7:I:510:VAL:HG12	7:I:511:ASP:N	2.35	0.42
5:J:141:ASP:HA	5:J:399:ARG:HA	2.00	0.42
5:J:80:ILE:HG22	5:J:95:VAL:HG11	2.16	0.42
8:K:336:ILE:H	8:K:336:ILE:HG13	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:440:TRP:HB2	8:K:441:PRO:HD3	2.03	0.42
4:M:201:ALA:C	4:M:203:MET:H	2.46	0.42
4:M:423:LEU:O	4:M:427:LEU:N	2.43	0.42
4:M:73:ILE:CG2	5:J:511:VAL:CG1	2.97	0.42
1:N:204:PRO:HA	1:N:381:LYS:O	2.19	0.42
3:O:86:ILE:HD12	3:O:513:ALA:CB	2.50	0.42
7:A:471:SER:HB2	3:O:120:ILE:HD11	2.01	0.42
4:E:72:LYS:HD2	4:E:72:LYS:N	2.37	0.42
1:F:100:GLU:HA	1:F:103:ARG:HB3	2.09	0.42
3:G:409:ILE:HD13	3:G:497:TRP:CE3	2.53	0.42
3:G:419:GLU:HB2	3:G:472:HIS:CE1	2.47	0.42
2:H:35:ILE:HD13	2:H:111:LEU:CD1	2.50	0.42
2:H:142:LEU:HG	2:H:430:LEU:HD21	2.61	0.42
2:H:56:VAL:HB	3:G:525:THR:HG23	2.08	0.42
5:J:95:VAL:HG22	5:J:497:VAL:HA	2.08	0.42
8:K:60:ASP:HB3	8:K:63:ALA:HB3	2.00	0.42
3:O:326:VAL:HG23	3:O:365:PHE:CE1	2.52	0.42
5:B:453:SER:O	5:B:457:SER:HB2	2.20	0.42
3:G:482:VAL:HG22	3:G:491:ASN:HD21	2.22	0.42
1:F:253:TYR:O	2:H:265:VAL:HA	2.26	0.42
7:I:269:GLN:HE21	7:I:269:GLN:HB2	1.66	0.42
5:J:351:GLN:HA	5:J:352:PRO:HD3	1.79	0.42
6:L:72:HIS:CD2	6:L:74:VAL:HB	2.64	0.42
4:M:278:PRO:HA	4:M:279:PRO:HD3	1.92	0.42
4:M:269:LEU:HG	4:M:375:GLY:O	2.50	0.42
1:N:215:LEU:HD22	1:N:217:HIS:HE1	1.85	0.42
1:N:87:THR:HG21	1:N:512:VAL:HA	2.02	0.42
2:P:299:ILE:HD12	2:P:313:LEU:HD21	2.07	0.42
5:B:165:ILE:HG12	6:D:520:ARG:HH22	2.76	0.42
5:B:228:ASN:N	5:B:341:ASP:O	2.46	0.42
1:F:518:THR:HG21	8:C:213:ASP:CB	2.65	0.42
6:D:99:LEU:O	6:D:103:LEU:HB2	2.20	0.42
3:G:424:LEU:HD13	3:G:442:PHE:HD1	1.87	0.42
2:H:234:GLY:O	2:H:235:HIS:CG	2.73	0.42
7:I:140:ILE:O	7:I:144:LEU:HG	2.19	0.42
7:I:65:ASP:HB3	7:I:68:THR:OG1	2.19	0.42
7:I:90:GLN:NE2	7:I:94:ILE:HD12	2.68	0.42
5:J:455:LEU:HD22	5:J:472:LEU:CD2	2.50	0.42
8:K:59:ASN:O	8:K:60:ASP:C	2.66	0.42
6:L:199:LYS:O	6:L:380:ARG:NH1	2.55	0.42
6:L:35:ILE:CG2	6:L:94:THR:HG23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:168:ILE:HD11	4:M:439:VAL:CG1	2.50	0.42
4:M:253:GLN:HB2	4:M:336:LEU:HD11	2.13	0.42
1:N:162:VAL:HB	1:N:166:LEU:HD23	2.34	0.42
2:P:25:ASP:C	2:P:27:GLN:N	2.73	0.42
7:A:67:ALA:HB1	7:A:88:GLN:HG3	2.01	0.42
5:B:471:GLY:HA3	5:B:482:MET:CG	2.50	0.42
8:C:252:TYR:CD2	8:C:252:TYR:N	2.88	0.42
6:D:200:VAL:HG13	6:D:387:ILE:HD11	2.00	0.42
6:D:420:GLU:HG2	6:D:478:LEU:HD11	2.02	0.42
1:F:173:ILE:HG12	1:F:209:PHE:HB2	2.37	0.42
2:H:152:ASP:HB3	2:H:155:ASP:HB2	2.27	0.42
2:H:348:THR:HA	2:H:349:PRO:HD3	1.98	0.42
7:I:337:LEU:HD23	7:I:337:LEU:HA	1.88	0.42
5:J:155:HIS:HB2	5:J:488:VAL:HG22	2.02	0.42
6:L:65:LEU:HD11	6:L:97:VAL:HG21	2.02	0.42
1:N:529:LEU:HB3	8:K:45:LEU:HD13	2.08	0.42
3:O:181:MET:HE2	3:O:214:PHE:HB2	2.19	0.42
2:P:35:ILE:HD11	2:P:81:ALA:O	2.87	0.42
4:E:292:VAL:CG2	5:B:260:GLN:HB3	2.47	0.41
5:B:409:MET:CG	5:B:459:LEU:HD21	2.79	0.41
8:C:52:MET:HG3	8:C:52:MET:H	1.66	0.41
6:D:384:ASN:HA	6:D:387:ILE:HD12	2.02	0.41
6:D:24:ASN:CG	6:D:74:VAL:HG21	2.83	0.41
1:F:173:ILE:HG22	1:F:378:ILE:HG12	2.01	0.41
1:F:459:VAL:HB	1:F:466:PRO:HA	2.02	0.41
3:G:158:LEU:HD21	3:G:404:LEU:HG	2.02	0.41
3:G:268:GLN:O	3:G:272:ASP:HB2	2.19	0.41
3:G:41:LYS:N	3:G:42:PRO:CD	2.83	0.41
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.88	0.41
7:I:189:THR:CG2	7:I:190:GLN:N	3.08	0.41
4:M:70:LEU:HB3	5:J:510:ARG:O	2.20	0.41
6:L:234:ILE:H	6:L:345:ASP:HB3	1.94	0.41
6:L:56:ILE:HD13	6:L:67:GLN:HG3	2.47	0.41
4:M:251:HIS:CE1	4:M:253:GLN:HG2	2.57	0.41
4:M:477:ASP:C	4:M:480:PRO:HD2	2.41	0.41
1:N:213:LEU:HD21	1:N:324:ASN:ND2	2.35	0.41
2:P:256:ILE:HG13	2:P:256:ILE:H	1.67	0.41
7:A:460:LYS:O	7:A:464:VAL:HG23	2.46	0.41
6:D:151:VAL:HA	6:D:175:VAL:HG21	2.18	0.41
1:F:204:PRO:HB3	1:F:391:THR:HG21	2.01	0.41
3:G:24:GLY:O	3:G:28:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:61:THR:HG23	3:G:384:GLN:HE22	2.25	0.41
7:I:12:THR:CB	7:I:14:PHE:HE2	2.33	0.41
5:J:239:ASP:CA	5:J:291:TYR:HB2	2.40	0.41
8:K:141:LYS:HA	8:K:142:PRO:HD2	1.96	0.41
8:K:198:ILE:CG2	8:K:199:ASP:N	2.97	0.41
4:M:324:GLN:HG2	4:M:325:TRP:CD1	2.84	0.41
4:M:353:HIS:HB3	4:M:403:THR:HG21	2.03	0.41
4:M:73:ILE:HG21	5:J:511:VAL:CG1	2.50	0.41
1:N:124:ILE:HD11	1:N:434:LEU:HD11	2.10	0.41
7:A:262:ILE:HB	8:C:259:THR:HA	2.10	0.41
7:A:458:ILE:HD12	7:A:458:ILE:N	2.64	0.41
4:E:483:LEU:O	4:E:487:SER:HB2	2.20	0.41
1:F:47:VAL:HG22	1:F:53:ILE:HG12	2.09	0.41
3:G:165:ALA:HB2	3:G:399:ILE:HD12	2.03	0.41
3:G:291:ASN:O	3:G:292:ILE:HG13	2.21	0.41
2:H:109:GLU:CG	2:H:458:VAL:HG21	2.72	0.41
4:M:411:SER:CB	5:J:503:GLU:OE1	3.11	0.41
8:K:121:ILE:HG12	8:K:441:PRO:HG3	2.14	0.41
8:C:198:ILE:CG2	8:C:199:ASP:H	2.33	0.41
1:F:119:THR:HG23	1:F:525:SER:HG	2.06	0.41
3:G:47:LEU:HD12	3:G:457:ALA:HB1	2.20	0.41
2:H:390:THR:C	2:H:392:ASN:H	2.23	0.41
8:K:100:ALA:O	8:K:104:LEU:HD12	2.21	0.41
8:K:72:HIS:HA	8:K:73:PRO:HD3	1.86	0.41
1:N:100:GLU:HA	1:N:103:ARG:HB3	2.08	0.41
2:P:142:LEU:HA	2:P:145:MET:HG3	2.30	0.41
2:P:41:MET:CE	3:O:524:ILE:HD11	2.50	0.41
5:B:89:GLY:HA3	5:B:389:SER:HB3	2.19	0.41
5:B:57:THR:HA	5:B:379:GLU:OE1	2.94	0.41
6:D:123:SER:HA	6:D:126:SER:HB2	2.02	0.41
6:D:355:SER:O	6:D:356:ASP:HB3	2.20	0.41
4:E:319:ASP:O	4:E:341:PRO:HD2	2.21	0.41
4:E:423:LEU:O	4:E:427:LEU:HB2	2.19	0.41
2:H:247:VAL:HG21	2:H:355:VAL:CG2	2.50	0.41
7:I:15:LEU:C	7:I:17:GLY:N	2.77	0.41
5:J:79:ASN:O	5:J:83:VAL:HG23	2.58	0.41
6:L:323:PHE:CZ	6:L:374:THR:HG21	2.56	0.41
6:L:495:GLU:HG3	6:L:495:GLU:O	2.20	0.41
4:M:29:PHE:CD2	4:M:29:PHE:N	2.90	0.41
3:O:334:ILE:H	3:O:334:ILE:HG13	1.98	0.41
2:P:178:LEU:HA	2:P:181:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:54:ILE:HD11	3:O:78:PRO:HB2	2.02	0.41
7:A:223:ALA:HA	7:A:373:LEU:HD12	2.01	0.41
7:A:226:CYS:SG	7:A:321:CYS:HB3	2.61	0.41
5:B:239:ASP:HA	5:B:291:TYR:CB	2.49	0.41
5:B:53:THR:HG22	5:B:54:CYS:N	2.46	0.41
8:C:269:TRP:O	8:C:272:ILE:HG13	2.20	0.41
6:D:395:HIS:O	6:D:399:CYS:HB2	2.20	0.41
6:D:89:ALA:HB1	6:D:503:VAL:HG22	2.02	0.41
1:F:162:VAL:HB	1:F:163:ASP:H	1.75	0.41
7:I:94:ILE:HG22	7:I:96:ASP:H	1.86	0.41
6:L:89:ALA:HB1	6:L:503:VAL:HG22	2.01	0.41
4:M:239:LEU:HD13	4:M:406:CYS:SG	2.60	0.41
3:O:419:GLU:HB2	3:O:472:HIS:CE1	2.51	0.41
7:A:337:LEU:HA	7:A:337:LEU:HD23	1.94	0.41
5:B:438:ARG:C	5:B:440:LEU:H	2.23	0.41
6:D:70:ILE:HD12	6:D:79:VAL:CG2	2.88	0.41
6:D:75:ALA:O	6:D:78:LEU:HB2	2.20	0.41
1:F:246:GLU:CB	8:C:252:TYR:HE1	2.34	0.41
3:G:327:ILE:HG21	3:G:334:ILE:HG13	2.03	0.41
3:G:381:GLY:HA2	4:E:540:LEU:HD22	2.02	0.41
2:H:21:TYR:N	2:H:21:TYR:CD2	2.88	0.41
7:I:246:CYS:HB3	7:I:337:LEU:HD23	2.24	0.41
3:O:418:MET:HG3	3:O:468:LEU:HD22	2.09	0.41
3:O:508:ASN:HA	3:O:508:ASN:HD22	1.64	0.41
8:C:81:LEU:HD11	8:C:516:SER:HB2	2.03	0.41
8:C:50:ASP:CB	8:C:51:PRO:CD	2.94	0.41
8:C:72:HIS:HA	8:C:73:PRO:HD3	1.96	0.41
4:E:335:LEU:HA	4:E:335:LEU:HD12	1.97	0.41
1:F:124:ILE:CG2	1:F:444:ILE:HD11	2.51	0.41
3:G:144:ALA:HB1	3:G:408:LEU:HG	2.20	0.41
2:H:341:LEU:HD23	2:H:342:PRO:HD2	2.02	0.41
5:J:39:PRO:HG3	10:J:602:ADP:C5	2.57	0.41
8:K:52:MET:H	8:K:52:MET:HG3	1.63	0.41
6:L:51:SER:O	7:I:549:PRO:HA	2.28	0.41
3:O:246:VAL:HA	3:O:297:LEU:HD12	2.03	0.41
3:O:108:LEU:HD21	3:O:442:PHE:HE2	2.64	0.41
1:F:535:ARG:HH12	2:P:6:PRO:HB2	1.82	0.41
2:H:238:SER:C	2:H:240:SER:H	2.29	0.41
2:H:209:VAL:HG11	2:H:398:GLU:HG3	2.03	0.41
2:H:111:LEU:HD21	2:H:535:ALA:O	2.21	0.41
5:J:127:ALA:HB2	5:J:430:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:84:GLN:HG2	5:J:91:GLY:O	2.59	0.41
8:K:248:CYS:HB2	8:K:249:PRO:HD2	2.03	0.41
8:K:296:ILE:HG12	8:K:317:LEU:HB2	2.02	0.41
3:O:177:PHE:HE2	3:O:212:SER:HB2	1.85	0.41
3:O:267:TYR:C	3:O:269:ALA:H	2.24	0.41
3:O:414:GLY:O	3:O:417:GLU:HG2	2.21	0.41
3:O:424:LEU:HD13	3:O:442:PHE:HD1	2.18	0.41
2:P:85:LEU:HD22	2:P:534:ALA:HB1	2.01	0.41
7:A:164:MET:HA	7:A:164:MET:HE2	2.02	0.41
3:G:358:GLY:HA3	3:G:379:ARG:HH22	1.84	0.41
5:J:276:ILE:O	5:J:279:PHE:HB2	2.21	0.41
8:K:146:GLU:OE2	8:K:183:ARG:NH1	2.97	0.41
6:L:124:PHE:O	6:L:127:ALA:HB3	2.21	0.41
1:N:178:VAL:HG21	1:N:402:VAL:HB	2.18	0.41
3:O:503:LYS:HD3	3:O:503:LYS:HA	2.11	0.41
2:P:19:ASN:HB3	2:P:21:TYR:CE2	2.81	0.41
5:B:237:THR:O	5:B:238:LEU:HG	2.21	0.41
5:B:409:MET:CB	5:B:463:ILE:HD13	2.51	0.41
6:D:372:ARG:HA	6:D:373:PRO:HD3	1.84	0.41
6:D:60:ASP:O	6:D:64:ILE:HG12	2.21	0.41
3:G:249:GLU:HG2	3:G:250:LEU:H	1.86	0.41
3:G:342:LYS:C	3:G:344:GLU:H	2.31	0.41
2:H:68:ALA:HA	2:H:71:MET:HE1	3.55	0.41
2:H:79:HIS:HD2	2:H:81:ALA:N	2.19	0.41
5:J:406:CYS:O	5:J:410:VAL:HG23	2.32	0.41
5:J:34:LYS:HD2	5:J:443:ILE:HD13	2.17	0.41
5:J:509:LEU:HA	5:J:509:LEU:HD12	2.12	0.41
8:K:70:VAL:HG11	8:K:75:ALA:HB3	2.15	0.41
1:N:521:THR:O	1:N:525:SER:CB	2.68	0.41
7:A:140:ILE:O	7:A:144:LEU:HG	2.39	0.40
7:A:301:GLY:HA2	7:A:320:ARG:HD2	2.14	0.40
7:A:95:GLY:HA3	7:A:407:SER:OG	2.21	0.40
5:B:192:HIS:CD2	5:B:319:LEU:HD12	2.56	0.40
4:E:415:ILE:HG12	5:B:507:VAL:HG21	2.03	0.40
8:C:322:LYS:HB2	8:C:322:LYS:HE2	1.86	0.40
8:C:521:LEU:HA	8:C:521:LEU:HD12	1.92	0.40
5:B:45:LEU:HD23	6:D:524:ILE:HG12	2.03	0.40
1:F:395:VAL:O	1:F:399:LEU:HB2	2.21	0.40
3:G:107:GLU:HG3	3:G:107:GLU:O	2.21	0.40
3:G:349:CYS:HB2	3:G:366:GLN:O	2.22	0.40
3:G:503:LYS:HA	3:G:503:LYS:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:284:ILE:CD1	2:H:308:LEU:HB3	2.56	0.40
2:H:426:THR:O	2:H:430:LEU:HG	2.20	0.40
4:M:232:GLY:H	5:J:87:GLU:HG3	1.86	0.40
6:L:443:PHE:CE1	6:L:447:LEU:HD11	2.56	0.40
6:L:76:ARG:HG2	6:L:76:ARG:HH11	2.39	0.40
4:M:193:VAL:O	4:M:195:LYS:N	2.67	0.40
4:M:492:ILE:H	4:M:492:ILE:HG13	1.61	0.40
1:F:107:ARG:CZ	1:N:107:ARG:HG3	2.70	0.40
3:O:179:VAL:C	3:O:181:MET:H	2.27	0.40
3:O:147:ILE:CD1	3:O:409:ILE:HB	2.44	0.40
3:O:86:ILE:HD12	3:O:513:ALA:HB2	2.03	0.40
2:P:55:ILE:HG12	3:O:524:ILE:HD12	2.02	0.40
7:A:118:ASN:HB3	7:A:119:LYS:H	1.71	0.40
5:B:276:ILE:O	5:B:279:PHE:HB2	2.21	0.40
5:B:293:TYR:CB	5:B:294:PRO:CD	2.98	0.40
8:C:165:ILE:H	8:C:165:ILE:HG13	1.81	0.40
8:C:166:HIS:HB2	8:C:167:TRP:CD1	2.56	0.40
6:D:109:ARG:NH2	6:D:442:GLU:OE1	2.64	0.40
4:E:144:ILE:CD1	4:E:550:LYS:HA	2.49	0.40
3:G:266:ASP:O	3:G:270:ILE:HG12	2.21	0.40
3:G:297:LEU:CB	3:G:298:PRO:HD2	2.43	0.40
3:G:352:PHE:CE1	3:G:365:PHE:CD2	3.18	0.40
1:F:42:THR:HB	2:H:542:ASP:OD1	2.21	0.40
2:H:31:SER:OG	2:H:81:ALA:HB3	2.20	0.40
4:M:104:LEU:HD23	4:M:107:LEU:HD12	2.03	0.40
4:M:256:LYS:O	4:M:381:TYR:HA	2.47	0.40
2:P:79:HIS:CE1	3:O:10:ILE:HD13	2.60	0.40
2:P:240:SER:HA	2:P:245:HIS:CE1	2.56	0.40
2:P:243:LYS:HA	2:P:245:HIS:CE1	2.64	0.40
2:P:394:LEU:HD23	2:P:397:ILE:HD11	2.03	0.40
5:B:245:ILE:H	5:B:245:ILE:HG13	1.59	0.40
5:B:29:VAL:HG13	5:B:64:LEU:HD21	2.03	0.40
1:F:142:ASN:O	1:F:145:ASN:ND2	2.54	0.40
1:F:253:TYR:CE1	1:F:259:ARG:CG	3.09	0.40
3:G:264:VAL:HG23	4:E:294:GLU:OE2	2.35	0.40
2:H:110:LEU:O	2:H:114:SER:HB2	2.54	0.40
7:I:99:THR:HG22	7:I:103:ILE:HD11	2.42	0.40
5:J:23:PHE:O	5:J:24:VAL:C	2.78	0.40
5:J:36:THR:HG23	5:J:58:ASN:OD1	2.22	0.40
6:L:237:ILE:HG23	6:L:239:PHE:CE2	2.66	0.40
6:L:237:ILE:HD11	6:L:286:LEU:HD13	2.13	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:82:SER:OG	6:L:93:THR:HB	2.35	0.40
4:M:534:LYS:O	4:M:538:ILE:HD12	2.42	0.40
1:N:162:VAL:HB	1:N:163:ASP:H	1.63	0.40
2:P:203:ASN:HD22	2:P:203:ASN:HA	1.66	0.40
2:P:19:ASN:HB3	2:P:21:TYR:HE2	2.22	0.40
2:P:294:MET:SD	2:P:349:PRO:HG3	2.61	0.40
2:P:79:HIS:ND1	3:O:10:ILE:HB	2.48	0.40
6:D:30:SER:OG	7:A:11:ASP:HB3	2.35	0.40
6:D:499:GLN:HA	6:D:500:PRO:HD3	1.95	0.40
4:E:194:SER:HA	4:E:197:HIS:HB3	2.25	0.40
4:E:412:ASN:OD1	4:E:415:ILE:HG13	2.24	0.40
4:E:75:ILE:HD12	5:B:516:ARG:HG3	2.03	0.40
1:F:19:LEU:O	1:F:23:VAL:HG23	2.21	0.40
1:F:384:THR:HB	1:F:385:HIS:H	1.67	0.40
1:F:495:ILE:HG13	1:F:497:ASP:HB2	2.04	0.40
3:G:244:LEU:HD13	3:G:248:LEU:HD11	2.18	0.40
2:H:234:GLY:O	2:H:235:HIS:ND1	2.55	0.40
7:I:456:LEU:HD11	7:I:478:ARG:HH11	1.86	0.40
5:J:14:ARG:O	5:J:15:ALA:C	2.68	0.40
5:J:152:ASP:O	5:J:156:ILE:HG12	2.48	0.40
1:N:326:GLU:HG2	8:K:232:PRO:HG3	2.02	0.40
8:K:35:ILE:CG2	8:K:94:THR:HG23	2.52	0.40
6:L:196:LEU:HD22	6:L:394:LEU:HD13	2.50	0.40
6:L:35:ILE:HD12	6:L:97:VAL:HG11	2.02	0.40
1:N:457:THR:HG22	1:N:460:LYS:HD2	2.10	0.40
3:O:139:LYS:O	3:O:143:LEU:HB2	2.22	0.40
3:O:388:GLU:O	3:O:392:SER:HB2	2.22	0.40
7:A:12:THR:CB	7:A:14:PHE:HE2	2.64	0.40
7:A:390:ALA:HA	8:C:512:THR:HG22	2.32	0.40
5:B:14:ARG:HG2	5:B:15:ALA:N	2.37	0.40
5:B:461:SER:O	5:B:465:ASN:HB2	2.49	0.40
8:C:224:LEU:HD11	8:C:365:PHE:HB3	2.02	0.40
6:D:257:TYR:HB3	7:A:272:GLN:HB3	2.03	0.40
6:D:336:ILE:C	6:D:338:LEU:N	2.75	0.40
6:D:416:ALA:HB3	6:D:417:PRO:HD3	2.03	0.40
6:D:486:ARG:O	6:D:487:SER:HB3	2.21	0.40
4:E:363:VAL:HG21	4:E:369:LEU:HD12	2.41	0.40
1:F:532:GLU:O	1:F:533:LEU:HD23	2.21	0.40
3:G:335:GLN:HG3	3:G:341:ILE:HG12	2.04	0.40
2:H:108:GLY:O	2:H:112:ASN:HB2	2.32	0.40
2:H:236:VAL:HA	2:H:319:LEU:HD13	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:SER:HA	2:H:245:HIS:CE1	2.57	0.40
7:I:109:LEU:HG	7:I:535:CYS:HB2	2.03	0.40
7:I:477:LEU:HD11	7:I:502:LEU:HD13	2.04	0.40
5:J:15:ALA:HB1	5:J:19:ARG:HH12	2.14	0.40
8:K:481:THR:HB	8:K:493:ASP:OD1	2.28	0.40
7:I:52:MET:HE2	8:K:526:ILE:HG12	2.06	0.40
1:N:173:ILE:HG23	1:N:209:PHE:HB2	2.15	0.40
3:O:125:ILE:O	3:O:438:ILE:HG21	2.21	0.40
3:O:292:ILE:HD13	3:O:352:PHE:CD1	2.67	0.40
2:P:180:GLU:O	2:P:184:GLU:HB2	2.43	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	536/546 (98%)	477 (89%)	56 (10%)	3 (1%)	25	62
1	N	536/546 (98%)	483 (90%)	51 (10%)	2 (0%)	34	70
1	f	536/546 (98%)	484 (90%)	49 (9%)	3 (1%)	25	62
1	n	536/546 (98%)	486 (91%)	48 (9%)	2 (0%)	34	70
2	H	513/568 (90%)	445 (87%)	57 (11%)	11 (2%)	7	40
2	P	513/568 (90%)	458 (89%)	47 (9%)	8 (2%)	9	44
2	h	513/568 (90%)	460 (90%)	46 (9%)	7 (1%)	11	46
2	p	513/568 (90%)	450 (88%)	53 (10%)	10 (2%)	8	42
3	G	524/550 (95%)	467 (89%)	48 (9%)	9 (2%)	9	43
3	O	524/550 (95%)	479 (91%)	36 (7%)	9 (2%)	9	43
3	g	524/550 (95%)	477 (91%)	38 (7%)	9 (2%)	9	43
3	o	524/550 (95%)	472 (90%)	41 (8%)	11 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	533/562 (95%)	482 (90%)	45 (8%)	6 (1%)	14	51
4	M	533/562 (95%)	494 (93%)	31 (6%)	8 (2%)	10	46
4	e	533/562 (95%)	500 (94%)	27 (5%)	6 (1%)	14	51
4	m	533/562 (95%)	492 (92%)	33 (6%)	8 (2%)	10	46
5	B	516/527 (98%)	452 (88%)	48 (9%)	16 (3%)	4	33
5	J	516/527 (98%)	460 (89%)	42 (8%)	14 (3%)	5	35
5	b	516/527 (98%)	461 (89%)	41 (8%)	14 (3%)	5	35
5	j	516/527 (98%)	459 (89%)	47 (9%)	10 (2%)	8	42
6	D	521/528 (99%)	457 (88%)	46 (9%)	18 (4%)	3	31
6	L	521/528 (99%)	474 (91%)	33 (6%)	14 (3%)	5	35
6	d	521/528 (99%)	473 (91%)	34 (6%)	14 (3%)	5	35
6	l	521/528 (99%)	469 (90%)	41 (8%)	11 (2%)	7	40
7	A	533/559 (95%)	470 (88%)	50 (9%)	13 (2%)	6	37
7	I	533/559 (95%)	483 (91%)	36 (7%)	14 (3%)	5	36
7	a	533/559 (95%)	482 (90%)	43 (8%)	8 (2%)	10	46
7	i	533/559 (95%)	484 (91%)	37 (7%)	12 (2%)	6	38
8	C	507/590 (86%)	445 (88%)	54 (11%)	8 (2%)	9	44
8	K	507/590 (86%)	454 (90%)	43 (8%)	10 (2%)	7	41
8	c	507/590 (86%)	456 (90%)	44 (9%)	7 (1%)	11	46
8	k	507/590 (86%)	448 (88%)	50 (10%)	9 (2%)	8	42
All	All	16732/17720 (94%)	15033 (90%)	1395 (8%)	304 (2%)	8	42

All (304) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	323	VAL
2	H	442	PRO
2	H	502	ASP
3	G	8	PRO
4	E	389	LYS
5	B	15	ALA
5	B	163	SER
5	B	220	ASN
5	B	255	THR
6	D	159	SER

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Mol	Chain	Res	Type
6	D	160	SER
6	D	368	ASN
7	A	257	ALA
8	C	163	TYR
8	C	239	GLU
2	P	323	VAL
2	P	442	PRO
2	P	502	ASP
3	O	8	PRO
4	M	190	SER
4	M	389	LYS
5	J	15	ALA
5	J	163	SER
5	J	220	ASN
5	J	255	THR
5	J	328	THR
6	L	160	SER
6	L	182	SER
6	L	368	ASN
7	I	257	ALA
8	K	163	TYR
2	h	323	VAL
2	h	442	PRO
2	h	502	ASP
3	g	8	PRO
4	e	389	LYS
5	b	15	ALA
5	b	163	SER
5	b	220	ASN
5	b	255	THR
5	b	328	THR
6	d	368	ASN
8	c	163	TYR
2	p	323	VAL
2	p	442	PRO
2	p	502	ASP
3	o	8	PRO
4	m	190	SER
4	m	389	LYS
5	j	15	ALA
5	j	163	SER
5	j	220	ASN

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Mol	Chain	Res	Type
5	j	255	THR
5	j	328	THR
6	l	282	LYS
6	l	368	ASN
8	k	163	TYR
2	H	26	GLY
3	G	151	LYS
3	G	168	SER
3	G	381	GLY
3	G	432	ALA
4	E	189	GLY
4	E	190	SER
4	E	194	SER
5	B	246	PHE
5	B	328	THR
5	B	451	ASP
6	D	183	ASP
6	D	189	VAL
6	D	282	LYS
6	D	296	ALA
7	A	56	ASP
7	A	65	ASP
7	A	200	VAL
7	A	201	LYS
7	A	256	MET
8	C	60	ASP
8	C	319	ARG
8	C	361	GLY
3	O	151	LYS
3	O	168	SER
3	O	432	ALA
4	M	345	TRP
6	L	186	SER
6	L	296	ALA
7	I	56	ASP
7	I	65	ASP
7	I	256	MET
7	I	367	SER
7	I	369	ASP
8	K	160	GLY
8	K	166	HIS
8	K	319	ARG

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Mol	Chain	Res	Type
8	K	361	GLY
3	g	168	SER
3	g	381	GLY
4	e	189	GLY
4	e	190	SER
5	b	59	ASP
5	b	145	ASP
5	b	246	PHE
6	d	182	SER
6	d	189	VAL
7	a	56	ASP
7	a	65	ASP
7	a	256	MET
7	a	257	ALA
8	c	160	GLY
8	c	239	GLU
3	o	168	SER
3	o	381	GLY
4	m	194	SER
5	j	247	GLY
6	l	160	SER
6	l	182	SER
6	l	189	VAL
6	l	296	ALA
7	i	56	ASP
7	i	201	LYS
7	i	256	MET
7	i	257	ALA
8	k	160	GLY
1	F	437	LYS
2	H	7	GLN
2	H	303	ALA
4	E	268	LYS
5	B	219	GLY
5	B	350	GLU
6	D	182	SER
6	D	186	SER
6	D	187	LYS
6	D	337	GLU
7	A	369	ASP
1	N	202	LEU
1	N	436	ALA

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Mol	Chain	Res	Type
3	O	190	ASP
3	O	381	GLY
4	M	364	PRO
5	J	143	SER
5	J	310	ASP
5	J	451	ASP
6	L	159	SER
6	L	189	VAL
6	L	282	LYS
6	L	293	LEU
6	L	315	ASP
7	I	549	PRO
1	f	437	LYS
2	h	23	ASN
3	g	151	LYS
3	g	227	ALA
5	b	162	SER
5	b	451	ASP
6	d	160	SER
6	d	186	SER
6	d	433	GLU
8	c	319	ARG
8	c	361	GLY
2	p	7	GLN
2	p	23	ASN
3	o	190	ASP
3	o	432	ALA
4	m	189	GLY
4	m	437	SER
5	j	59	ASP
6	l	187	LYS
6	l	249	GLU
7	i	65	ASP
7	i	118	ASN
7	i	367	SER
7	i	390	ALA
7	i	549	PRO
8	k	60	ASP
8	k	221	LYS
8	k	239	GLU
8	k	319	ARG
8	k	361	GLY

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Mol	Chain	Res	Type
1	F	163	ASP
2	H	41	MET
2	H	96	MET
3	G	369	PRO
5	B	59	ASP
5	B	133	ASP
5	B	143	SER
6	D	293	LEU
6	D	329	GLY
7	A	118	ASN
7	A	367	SER
8	C	160	GLY
2	P	23	ASN
3	O	171	ILE
4	M	189	GLY
5	J	59	ASP
5	J	247	GLY
5	J	423	ASP
6	L	183	ASP
7	I	340	SER
7	I	390	ALA
7	I	467	ALA
1	f	202	LEU
2	h	7	GLN
2	h	148	GLY
3	g	190	ASP
3	g	432	ALA
4	e	194	SER
4	e	345	TRP
5	b	143	SER
6	d	159	SER
6	d	162	ILE
6	d	187	LYS
6	d	296	ALA
6	d	479	ASN
7	a	369	ASP
8	c	60	ASP
8	c	511	LYS
1	n	201	HIS
2	p	148	GLY
4	m	202	GLU
4	m	268	LYS

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Mol	Chain	Res	Type
6	l	186	SER
7	i	267	PRO
7	i	369	ASP
8	k	80	GLU
1	F	373	PRO
2	H	418	LYS
3	G	251	LYS
4	E	437	SER
5	B	312	GLU
6	D	162	ILE
6	D	315	ASP
8	C	41	PRO
8	C	80	GLU
2	P	7	GLN
2	P	470	ASP
4	M	194	SER
4	M	268	LYS
4	M	462	ARG
5	J	350	GLU
6	L	249	GLU
7	I	118	ASN
4	e	268	LYS
5	b	241	ASP
5	b	350	GLU
6	d	294	ARG
7	a	267	PRO
2	p	153	LYS
3	o	151	LYS
3	o	249	GLU
5	j	145	ASP
5	j	312	GLU
3	G	171	ILE
3	G	190	ASP
5	B	241	ASP
5	B	470	SER
6	D	243	PRO
7	A	489	PRO
5	J	241	ASP
8	K	41	PRO
8	K	108	ALA
8	K	207	GLU
8	K	435	GLU

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Mol	Chain	Res	Type
3	g	343	PRO
5	b	247	GLY
7	a	118	ASN
7	a	489	PRO
1	n	437	LYS
2	p	418	LYS
3	o	343	PRO
5	j	241	ASP
6	l	159	SER
8	k	435	GLU
7	A	267	PRO
7	A	549	PRO
2	P	26	GLY
5	J	39	PRO
6	L	373	PRO
3	g	369	PRO
7	i	489	PRO
6	D	373	PRO
3	O	369	PRO
6	L	365	GLY
1	f	162	VAL
3	o	431	ILE
2	H	324	PRO
5	B	247	GLY
7	A	22	GLY
7	I	489	PRO
2	h	17	GLY
6	d	329	GLY
3	o	239	PRO
2	H	441	THR
6	D	242	SER
2	P	234	GLY
3	O	343	PRO
7	I	200	VAL
7	I	267	PRO
8	K	384	GLY
2	p	17	GLY
2	p	441	THR
3	o	369	PRO
6	l	353	ILE
6	d	243	PRO
4	m	192	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	380/463 (82%)	342 (90%)	38 (10%)	7	32
1	N	380/463 (82%)	352 (93%)	28 (7%)	13	44
1	f	380/463 (82%)	354 (93%)	26 (7%)	16	47
1	n	380/463 (82%)	353 (93%)	27 (7%)	14	45
2	H	352/473 (74%)	314 (89%)	38 (11%)	6	30
2	P	352/473 (74%)	323 (92%)	29 (8%)	11	40
2	h	352/473 (74%)	320 (91%)	32 (9%)	9	36
2	p	352/473 (74%)	315 (90%)	37 (10%)	7	30
3	G	373/454 (82%)	332 (89%)	41 (11%)	6	29
3	O	373/454 (82%)	340 (91%)	33 (9%)	10	38
3	g	373/454 (82%)	334 (90%)	39 (10%)	7	30
3	o	373/454 (82%)	340 (91%)	33 (9%)	10	38
4	E	382/483 (79%)	340 (89%)	42 (11%)	6	29
4	M	382/483 (79%)	346 (91%)	36 (9%)	8	35
4	e	382/483 (79%)	340 (89%)	42 (11%)	6	29
4	m	382/483 (79%)	346 (91%)	36 (9%)	8	35
5	B	374/441 (85%)	325 (87%)	49 (13%)	4	23
5	J	374/441 (85%)	340 (91%)	34 (9%)	9	36
5	b	374/441 (85%)	330 (88%)	44 (12%)	5	26
5	j	374/441 (85%)	339 (91%)	35 (9%)	8	35
6	D	374/454 (82%)	340 (91%)	34 (9%)	9	36
6	L	374/454 (82%)	344 (92%)	30 (8%)	12	42
6	d	374/454 (82%)	342 (91%)	32 (9%)	10	40
6	l	374/454 (82%)	341 (91%)	33 (9%)	10	38
7	A	375/471 (80%)	335 (89%)	40 (11%)	6	30
7	I	375/471 (80%)	341 (91%)	34 (9%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	a	375/471 (80%)	347 (92%)	28 (8%)	13	44
7	i	375/471 (80%)	348 (93%)	27 (7%)	14	45
8	C	359/497 (72%)	312 (87%)	47 (13%)	4	23
8	K	359/497 (72%)	318 (89%)	41 (11%)	5	28
8	c	359/497 (72%)	325 (90%)	34 (10%)	8	34
8	k	359/497 (72%)	320 (89%)	39 (11%)	6	29
All	All	11876/14944 (80%)	10738 (90%)	1138 (10%)	8	34

All (1138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	16	ASP
1	F	19	LEU
1	F	22	ASN
1	F	30	GLN
1	F	35	THR
1	F	56	THR
1	F	62	LEU
1	F	72	THR
1	F	92	THR
1	F	103	ARG
1	F	107	ARG
1	F	111	GLU
1	F	162	VAL
1	F	165	ASP
1	F	187	ASP
1	F	206	ASP
1	F	217	HIS
1	F	223	ASP
1	F	237	ASN
1	F	239	SER
1	F	251	PHE
1	F	257	ASP
1	F	324	ASN
1	F	340	VAL
1	F	368	THR
1	F	370	ASN
1	F	379	LEU
1	F	390	GLN
1	F	396	ARG

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Mol	Chain	Res	Type
1	F	399	LEU
1	F	408	ASP
1	F	453	VAL
1	F	479	ASP
1	F	497	ASP
1	F	499	CYS
1	F	511	ARG
1	F	514	ARG
1	F	535	ARG
2	H	20	SER
2	H	21	TYR
2	H	25	ASP
2	H	31	SER
2	H	41	MET
2	H	62	ILE
2	H	91	GLN
2	H	92	GLN
2	H	98	ASP
2	H	101	ASN
2	H	102	LEU
2	H	105	ILE
2	H	110	LEU
2	H	145	MET
2	H	206	SER
2	H	221	THR
2	H	223	ILE
2	H	245	HIS
2	H	256	ILE
2	H	260	GLU
2	H	291	ILE
2	H	320	VAL
2	H	327	PHE
2	H	341	LEU
2	H	344	LEU
2	H	348	THR
2	H	354	LEU
2	H	357	THR
2	H	358	VAL
2	H	371	PHE
2	H	392	ASN
2	H	409	LYS
2	H	432	SER

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Mol	Chain	Res	Type
2	H	441	THR
2	H	470	ASP
2	H	502	ASP
2	H	519	ASP
2	H	539	LEU
3	G	10	ILE
3	G	11	VAL
3	G	20	SER
3	G	37	GLN
3	G	43	THR
3	G	61	THR
3	G	88	ARG
3	G	96	ASP
3	G	102	THR
3	G	104	LEU
3	G	108	LEU
3	G	122	SER
3	G	155	ARG
3	G	161	CYS
3	G	187	LEU
3	G	194	LEU
3	G	195	ASP
3	G	196	ASP
3	G	197	LYS
3	G	268	GLN
3	G	272	ASP
3	G	277	LEU
3	G	282	LEU
3	G	284	GLN
3	G	291	ASN
3	G	330	VAL
3	G	338	THR
3	G	365	PHE
3	G	374	CYS
3	G	377	LEU
3	G	398	MET
3	G	399	ILE
3	G	409	ILE
3	G	410	VAL
3	G	435	GLN
3	G	440	ASN
3	G	483	PHE

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Mol	Chain	Res	Type
3	G	485	THR
3	G	488	ILE
3	G	511	THR
3	G	515	ASN
4	E	29	PHE
4	E	30	ILE
4	E	37	ASN
4	E	59	SER
4	E	68	ARG
4	E	74	LEU
4	E	82	THR
4	E	107	LEU
4	E	111	GLN
4	E	120	THR
4	E	125	LEU
4	E	166	ASP
4	E	168	ILE
4	E	206	GLU
4	E	227	GLN
4	E	240	ILE
4	E	283	THR
4	E	294	GLU
4	E	300	THR
4	E	329	ASP
4	E	336	LEU
4	E	344	ARG
4	E	378	SER
4	E	381	TYR
4	E	385	PHE
4	E	387	THR
4	E	388	THR
4	E	404	VAL
4	E	406	CYS
4	E	412	ASN
4	E	414	MET
4	E	427	LEU
4	E	431	ARG
4	E	436	ASP
4	E	455	SER
4	E	459	ASP
4	E	487	SER
4	E	492	ILE

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Mol	Chain	Res	Type
4	E	498	LEU
4	E	519	SER
4	E	544	LEU
4	E	552	ASP
5	B	8	ASP
5	B	11	THR
5	B	48	SER
5	B	52	ASN
5	B	57	THR
5	B	62	THR
5	B	93	THR
5	B	99	SER
5	B	104	ARG
5	B	115	ILE
5	B	119	THR
5	B	124	TYR
5	B	132	LEU
5	B	135	LEU
5	B	141	ASP
5	B	147	THR
5	B	156	ILE
5	B	167	SER
5	B	183	ARG
5	B	199	LEU
5	B	214	LEU
5	B	226	ILE
5	B	237	THR
5	B	240	THR
5	B	241	ASP
5	B	245	ILE
5	B	246	PHE
5	B	308	HIS
5	B	316	ARG
5	B	319	LEU
5	B	321	THR
5	B	341	ASP
5	B	373	THR
5	B	390	VAL
5	B	397	GLU
5	B	402	LEU
5	B	408	GLU
5	B	416	ASP

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Mol	Chain	Res	Type
5	B	423	ASP
5	B	440	LEU
5	B	452	SER
5	B	455	LEU
5	B	457	SER
5	B	459	LEU
5	B	469	THR
5	B	474	LEU
5	B	476	ASN
5	B	509	LEU
5	B	512	ASP
6	D	36	ARG
6	D	38	SER
6	D	85	GLN
6	D	123	SER
6	D	124	PHE
6	D	140	HIS
6	D	169	PHE
6	D	170	LEU
6	D	177	SER
6	D	181	ILE
6	D	198	LYS
6	D	209	MET
6	D	218	THR
6	D	248	THR
6	D	255	ASN
6	D	264	LEU
6	D	266	GLU
6	D	305	LEU
6	D	312	VAL
6	D	340	THR
6	D	349	LEU
6	D	366	ILE
6	D	383	ASN
6	D	385	MET
6	D	399	CYS
6	D	411	ILE
6	D	440	TRP
6	D	467	THR
6	D	475	ASN
6	D	482	ILE
6	D	486	ARG

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Mol	Chain	Res	Type
6	D	502	LEU
6	D	520	ARG
6	D	522	ASP
7	A	26	ARG
7	A	47	VAL
7	A	56	ASP
7	A	61	THR
7	A	68	THR
7	A	75	VAL
7	A	86	LEU
7	A	89	GLN
7	A	90	GLN
7	A	92	ARG
7	A	109	LEU
7	A	118	ASN
7	A	126	ILE
7	A	177	SER
7	A	179	MET
7	A	200	VAL
7	A	212	SER
7	A	224	LEU
7	A	247	LEU
7	A	281	VAL
7	A	299	THR
7	A	319	ARG
7	A	320	ARG
7	A	321	CYS
7	A	328	ARG
7	A	354	TYR
7	A	373	LEU
7	A	396	ASP
7	A	397	GLU
7	A	404	ASP
7	A	419	VAL
7	A	424	CYS
7	A	426	GLU
7	A	439	THR
7	A	442	SER
7	A	457	ILE
7	A	512	GLU
7	A	535	CYS
7	A	542	ASP

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Mol	Chain	Res	Type
7	A	543	THR
8	C	23	SER
8	C	52	MET
8	C	55	LEU
8	C	58	THR
8	C	78	MET
8	C	79	LEU
8	C	81	LEU
8	C	89	VAL
8	C	95	THR
8	C	102	GLU
8	C	107	CYS
8	C	130	THR
8	C	138	GLN
8	C	143	VAL
8	C	148	ASP
8	C	151	MET
8	C	163	TYR
8	C	167	TRP
8	C	177	ASP
8	C	204	VAL
8	C	206	VAL
8	C	215	LEU
8	C	251	GLU
8	C	257	SER
8	C	260	ASN
8	C	290	VAL
8	C	293	THR
8	C	309	LEU
8	C	322	LYS
8	C	325	ASN
8	C	335	THR
8	C	336	ILE
8	C	346	SER
8	C	348	VAL
8	C	350	THR
8	C	354	LEU
8	C	387	ASP
8	C	396	LEU
8	C	398	ASP
8	C	404	ARG
8	C	455	THR

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Mol	Chain	Res	Type
8	C	468	LEU
8	C	481	THR
8	C	484	ILE
8	C	504	VAL
8	C	521	LEU
8	C	528	SER
1	N	16	ASP
1	N	30	GLN
1	N	35	THR
1	N	56	THR
1	N	62	LEU
1	N	72	THR
1	N	74	VAL
1	N	75	LEU
1	N	103	ARG
1	N	107	ARG
1	N	162	VAL
1	N	187	ASP
1	N	190	ASP
1	N	217	HIS
1	N	223	ASP
1	N	237	ASN
1	N	251	PHE
1	N	257	ASP
1	N	324	ASN
1	N	368	THR
1	N	379	LEU
1	N	390	GLN
1	N	399	LEU
1	N	408	ASP
1	N	442	THR
1	N	453	VAL
1	N	497	ASP
1	N	499	CYS
2	P	32	ILE
2	P	42	CYS
2	P	62	ILE
2	P	65	THR
2	P	95	ASP
2	P	105	ILE
2	P	145	MET
2	P	221	THR

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Mol	Chain	Res	Type
2	P	226	MET
2	P	245	HIS
2	P	256	ILE
2	P	260	GLU
2	P	341	LEU
2	P	344	LEU
2	P	348	THR
2	P	354	LEU
2	P	357	THR
2	P	369	THR
2	P	371	PHE
2	P	392	ASN
2	P	403	ASP
2	P	409	LYS
2	P	432	SER
2	P	441	THR
2	P	470	ASP
2	P	502	ASP
2	P	519	ASP
2	P	539	LEU
2	P	544	ILE
3	O	3	PHE
3	O	10	ILE
3	O	11	VAL
3	O	37	GLN
3	O	43	THR
3	O	50	ASP
3	O	96	ASP
3	O	102	THR
3	O	104	LEU
3	O	155	ARG
3	O	194	LEU
3	O	196	ASP
3	O	197	LYS
3	O	267	TYR
3	O	268	GLN
3	O	277	LEU
3	O	282	LEU
3	O	284	GLN
3	O	330	VAL
3	O	374	CYS
3	O	377	LEU

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Mol	Chain	Res	Type
3	O	398	MET
3	O	399	ILE
3	O	409	ILE
3	O	410	VAL
3	O	440	ASN
3	O	468	LEU
3	O	483	PHE
3	O	485	THR
3	O	488	ILE
3	O	508	ASN
3	O	521	ASP
3	O	525	THR
4	M	25	MET
4	M	29	PHE
4	M	30	ILE
4	M	37	ASN
4	M	74	LEU
4	M	82	THR
4	M	92	SER
4	M	107	LEU
4	M	111	GLN
4	M	125	LEU
4	M	129	LEU
4	M	166	ASP
4	M	168	ILE
4	M	206	GLU
4	M	283	THR
4	M	294	GLU
4	M	336	LEU
4	M	344	ARG
4	M	378	SER
4	M	385	PHE
4	M	387	THR
4	M	388	THR
4	M	406	CYS
4	M	408	VAL
4	M	412	ASN
4	M	414	MET
4	M	427	LEU
4	M	431	ARG
4	M	436	ASP
4	M	459	ASP

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Mol	Chain	Res	Type
4	M	464	ILE
4	M	487	SER
4	M	492	ILE
4	M	498	LEU
4	M	513	ASP
4	M	552	ASP
5	J	21	SER
5	J	57	THR
5	J	93	THR
5	J	104	ARG
5	J	119	THR
5	J	124	TYR
5	J	132	LEU
5	J	135	LEU
5	J	141	ASP
5	J	147	THR
5	J	199	LEU
5	J	214	LEU
5	J	226	ILE
5	J	237	THR
5	J	240	THR
5	J	241	ASP
5	J	246	PHE
5	J	283	THR
5	J	308	HIS
5	J	316	ARG
5	J	319	LEU
5	J	321	THR
5	J	341	ASP
5	J	390	VAL
5	J	397	GLU
5	J	408	GLU
5	J	423	ASP
5	J	427	SER
5	J	450	PHE
5	J	452	SER
5	J	455	LEU
5	J	459	LEU
5	J	474	LEU
5	J	509	LEU
6	L	36	ARG
6	L	63	THR

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Mol	Chain	Res	Type
6	L	124	PHE
6	L	140	HIS
6	L	162	ILE
6	L	169	PHE
6	L	170	LEU
6	L	181	ILE
6	L	198	LYS
6	L	206	ASP
6	L	209	MET
6	L	216	THR
6	L	218	THR
6	L	248	THR
6	L	255	ASN
6	L	305	LEU
6	L	312	VAL
6	L	336	ILE
6	L	340	THR
6	L	364	THR
6	L	366	ILE
6	L	385	MET
6	L	411	ILE
6	L	440	TRP
6	L	463	ILE
6	L	482	ILE
6	L	486	ARG
6	L	502	LEU
6	L	513	GLU
6	L	520	ARG
7	I	6	ASN
7	I	26	ARG
7	I	47	VAL
7	I	51	LYS
7	I	56	ASP
7	I	61	THR
7	I	63	THR
7	I	68	THR
7	I	86	LEU
7	I	89	GLN
7	I	90	GLN
7	I	100	SER
7	I	172	ASP
7	I	177	SER

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Mol	Chain	Res	Type
7	I	185	LEU
7	I	200	VAL
7	I	228	VAL
7	I	281	VAL
7	I	328	ARG
7	I	337	LEU
7	I	373	LEU
7	I	377	THR
7	I	396	ASP
7	I	404	ASP
7	I	407	SER
7	I	419	VAL
7	I	426	GLU
7	I	439	THR
7	I	442	SER
7	I	457	ILE
7	I	471	SER
7	I	535	CYS
7	I	542	ASP
7	I	543	THR
8	K	23	SER
8	K	34	VAL
8	K	38	CYS
8	K	52	MET
8	K	58	THR
8	K	78	MET
8	K	79	LEU
8	K	81	LEU
8	K	89	VAL
8	K	95	THR
8	K	107	CYS
8	K	130	THR
8	K	138	GLN
8	K	148	ASP
8	K	154	LEU
8	K	167	TRP
8	K	206	VAL
8	K	215	LEU
8	K	251	GLU
8	K	260	ASN
8	K	290	VAL
8	K	293	THR

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Mol	Chain	Res	Type
8	K	297	THR
8	K	309	LEU
8	K	310	LEU
8	K	322	LYS
8	K	325	ASN
8	K	335	THR
8	K	354	LEU
8	K	369	ASP
8	K	396	LEU
8	K	398	ASP
8	K	404	ARG
8	K	420	GLU
8	K	451	CYS
8	K	468	LEU
8	K	481	THR
8	K	504	VAL
8	K	509	SER
8	K	521	LEU
8	K	528	SER
1	f	19	LEU
1	f	22	ASN
1	f	30	GLN
1	f	35	THR
1	f	56	THR
1	f	72	THR
1	f	75	LEU
1	f	96	CYS
1	f	103	ARG
1	f	107	ARG
1	f	124	ILE
1	f	162	VAL
1	f	187	ASP
1	f	190	ASP
1	f	217	HIS
1	f	237	ASN
1	f	251	PHE
1	f	368	THR
1	f	379	LEU
1	f	390	GLN
1	f	396	ARG
1	f	399	LEU
1	f	453	VAL

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Mol	Chain	Res	Type
1	f	479	ASP
1	f	497	ASP
1	f	499	CYS
2	h	41	MET
2	h	42	CYS
2	h	65	THR
2	h	91	GLN
2	h	95	ASP
2	h	98	ASP
2	h	101	ASN
2	h	102	LEU
2	h	105	ILE
2	h	145	MET
2	h	221	THR
2	h	223	ILE
2	h	245	HIS
2	h	256	ILE
2	h	258	ASN
2	h	264	THR
2	h	277	SER
2	h	333	CYS
2	h	341	LEU
2	h	344	LEU
2	h	348	THR
2	h	354	LEU
2	h	357	THR
2	h	371	PHE
2	h	392	ASN
2	h	403	ASP
2	h	409	LYS
2	h	432	SER
2	h	441	THR
2	h	502	ASP
2	h	519	ASP
2	h	539	LEU
3	g	3	PHE
3	g	10	ILE
3	g	11	VAL
3	g	30	ILE
3	g	37	GLN
3	g	43	THR
3	g	50	ASP

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Mol	Chain	Res	Type
3	g	55	THR
3	g	61	THR
3	g	88	ARG
3	g	96	ASP
3	g	104	LEU
3	g	155	ARG
3	g	158	LEU
3	g	194	LEU
3	g	195	ASP
3	g	196	ASP
3	g	197	LYS
3	g	272	ASP
3	g	277	LEU
3	g	282	LEU
3	g	284	GLN
3	g	291	ASN
3	g	330	VAL
3	g	374	CYS
3	g	377	LEU
3	g	398	MET
3	g	399	ILE
3	g	409	ILE
3	g	410	VAL
3	g	423	CYS
3	g	430	THR
3	g	468	LEU
3	g	485	THR
3	g	488	ILE
3	g	508	ASN
3	g	511	THR
3	g	515	ASN
3	g	521	ASP
4	e	25	MET
4	e	29	PHE
4	e	30	ILE
4	e	37	ASN
4	e	59	SER
4	e	61	ILE
4	e	74	LEU
4	e	82	THR
4	e	92	SER
4	e	107	LEU

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Mol	Chain	Res	Type
4	e	109	LYS
4	e	111	GLN
4	e	125	LEU
4	e	129	LEU
4	e	159	SER
4	e	166	ASP
4	e	168	ILE
4	e	206	GLU
4	e	283	THR
4	e	291	SER
4	e	294	GLU
4	e	329	ASP
4	e	336	LEU
4	e	344	ARG
4	e	381	TYR
4	e	385	PHE
4	e	387	THR
4	e	388	THR
4	e	404	VAL
4	e	406	CYS
4	e	412	ASN
4	e	414	MET
4	e	427	LEU
4	e	429	VAL
4	e	431	ARG
4	e	436	ASP
4	e	455	SER
4	e	464	ILE
4	e	487	SER
4	e	492	ILE
4	e	498	LEU
4	e	552	ASP
5	b	11	THR
5	b	21	SER
5	b	52	ASN
5	b	57	THR
5	b	62	THR
5	b	94	SER
5	b	99	SER
5	b	104	ARG
5	b	115	ILE
5	b	119	THR

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Mol	Chain	Res	Type
5	b	132	LEU
5	b	135	LEU
5	b	141	ASP
5	b	145	ASP
5	b	147	THR
5	b	150	ARG
5	b	195	ILE
5	b	199	LEU
5	b	214	LEU
5	b	237	THR
5	b	240	THR
5	b	241	ASP
5	b	246	PHE
5	b	308	HIS
5	b	316	ARG
5	b	319	LEU
5	b	321	THR
5	b	341	ASP
5	b	365	CYS
5	b	390	VAL
5	b	397	GLU
5	b	400	THR
5	b	402	LEU
5	b	406	CYS
5	b	408	GLU
5	b	416	ASP
5	b	423	ASP
5	b	440	LEU
5	b	452	SER
5	b	459	LEU
5	b	474	LEU
5	b	476	ASN
5	b	509	LEU
5	b	512	ASP
6	d	33	ASP
6	d	36	ARG
6	d	63	THR
6	d	85	GLN
6	d	103	LEU
6	d	123	SER
6	d	124	PHE
6	d	136	LEU

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Mol	Chain	Res	Type
6	d	140	HIS
6	d	150	LEU
6	d	162	ILE
6	d	169	PHE
6	d	181	ILE
6	d	198	LYS
6	d	218	THR
6	d	248	THR
6	d	255	ASN
6	d	266	GLU
6	d	299	ASP
6	d	305	LEU
6	d	312	VAL
6	d	340	THR
6	d	366	ILE
6	d	385	MET
6	d	411	ILE
6	d	440	TRP
6	d	482	ILE
6	d	486	ARG
6	d	502	LEU
6	d	513	GLU
6	d	520	ARG
6	d	522	ASP
7	a	6	ASN
7	a	26	ARG
7	a	47	VAL
7	a	51	LYS
7	a	56	ASP
7	a	61	THR
7	a	68	THR
7	a	86	LEU
7	a	89	GLN
7	a	90	GLN
7	a	92	ARG
7	a	109	LEU
7	a	177	SER
7	a	179	MET
7	a	228	VAL
7	a	320	ARG
7	a	328	ARG
7	a	371	CYS

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Mol	Chain	Res	Type
7	a	377	THR
7	a	392	ASP
7	a	419	VAL
7	a	424	CYS
7	a	426	GLU
7	a	439	THR
7	a	457	ILE
7	a	522	ILE
7	a	535	CYS
7	a	542	ASP
8	c	34	VAL
8	c	52	MET
8	c	58	THR
8	c	78	MET
8	c	79	LEU
8	c	81	LEU
8	c	107	CYS
8	c	130	THR
8	c	138	GLN
8	c	143	VAL
8	c	148	ASP
8	c	154	LEU
8	c	165	ILE
8	c	167	TRP
8	c	199	ASP
8	c	206	VAL
8	c	215	LEU
8	c	245	LEU
8	c	290	VAL
8	c	293	THR
8	c	309	LEU
8	c	310	LEU
8	c	322	LYS
8	c	325	ASN
8	c	354	LEU
8	c	369	ASP
8	c	396	LEU
8	c	398	ASP
8	c	404	ARG
8	c	437	ILE
8	c	468	LEU
8	c	481	THR

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Mol	Chain	Res	Type
8	c	521	LEU
8	c	528	SER
1	n	19	LEU
1	n	24	THR
1	n	30	GLN
1	n	35	THR
1	n	55	LEU
1	n	56	THR
1	n	62	LEU
1	n	72	THR
1	n	96	CYS
1	n	103	ARG
1	n	107	ARG
1	n	124	ILE
1	n	162	VAL
1	n	187	ASP
1	n	217	HIS
1	n	237	ASN
1	n	251	PHE
1	n	368	THR
1	n	371	THR
1	n	379	LEU
1	n	390	GLN
1	n	399	LEU
1	n	453	VAL
1	n	479	ASP
1	n	497	ASP
1	n	499	CYS
1	n	511	ARG
2	p	21	TYR
2	p	25	ASP
2	p	31	SER
2	p	32	ILE
2	p	41	MET
2	p	42	CYS
2	p	45	SER
2	p	62	ILE
2	p	65	THR
2	p	98	ASP
2	p	101	ASN
2	p	102	LEU
2	p	105	ILE

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Mol	Chain	Res	Type
2	p	113	VAL
2	p	145	MET
2	p	221	THR
2	p	223	ILE
2	p	245	HIS
2	p	256	ILE
2	p	258	ASN
2	p	308	LEU
2	p	333	CYS
2	p	341	LEU
2	p	344	LEU
2	p	348	THR
2	p	354	LEU
2	p	357	THR
2	p	358	VAL
2	p	371	PHE
2	p	392	ASN
2	p	409	LYS
2	p	432	SER
2	p	441	THR
2	p	470	ASP
2	p	502	ASP
2	p	519	ASP
2	p	539	LEU
3	o	3	PHE
3	o	10	ILE
3	o	11	VAL
3	o	37	GLN
3	o	43	THR
3	o	50	ASP
3	o	55	THR
3	o	61	THR
3	o	96	ASP
3	o	102	THR
3	o	104	LEU
3	o	155	ARG
3	o	161	CYS
3	o	173	ASN
3	o	194	LEU
3	o	195	ASP
3	o	196	ASP
3	o	268	GLN

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Mol	Chain	Res	Type
3	o	277	LEU
3	o	282	LEU
3	o	284	GLN
3	o	302	LEU
3	o	330	VAL
3	o	374	CYS
3	o	377	LEU
3	o	398	MET
3	o	399	ILE
3	o	409	ILE
3	o	410	VAL
3	o	440	ASN
3	o	485	THR
3	o	488	ILE
3	o	511	THR
4	m	29	PHE
4	m	30	ILE
4	m	37	ASN
4	m	59	SER
4	m	68	ARG
4	m	74	LEU
4	m	82	THR
4	m	89	THR
4	m	92	SER
4	m	107	LEU
4	m	111	GLN
4	m	125	LEU
4	m	166	ASP
4	m	168	ILE
4	m	240	ILE
4	m	283	THR
4	m	294	GLU
4	m	300	THR
4	m	312	ASP
4	m	336	LEU
4	m	344	ARG
4	m	385	PHE
4	m	387	THR
4	m	388	THR
4	m	406	CYS
4	m	412	ASN
4	m	414	MET

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Mol	Chain	Res	Type
4	m	427	LEU
4	m	431	ARG
4	m	436	ASP
4	m	464	ILE
4	m	487	SER
4	m	492	ILE
4	m	498	LEU
4	m	519	SER
4	m	552	ASP
5	j	8	ASP
5	j	21	SER
5	j	31	ASP
5	j	52	ASN
5	j	57	THR
5	j	80	ILE
5	j	104	ARG
5	j	119	THR
5	j	124	TYR
5	j	135	LEU
5	j	141	ASP
5	j	147	THR
5	j	199	LEU
5	j	214	LEU
5	j	226	ILE
5	j	237	THR
5	j	240	THR
5	j	246	PHE
5	j	308	HIS
5	j	319	LEU
5	j	321	THR
5	j	341	ASP
5	j	397	GLU
5	j	402	LEU
5	j	408	GLU
5	j	416	ASP
5	j	423	ASP
5	j	440	LEU
5	j	443	ILE
5	j	455	LEU
5	j	459	LEU
5	j	474	LEU
5	j	476	ASN

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Mol	Chain	Res	Type
5	j	509	LEU
5	j	512	ASP
6	l	36	ARG
6	l	38	SER
6	l	103	LEU
6	l	123	SER
6	l	124	PHE
6	l	140	HIS
6	l	162	ILE
6	l	169	PHE
6	l	170	LEU
6	l	181	ILE
6	l	198	LYS
6	l	209	MET
6	l	218	THR
6	l	248	THR
6	l	251	ASN
6	l	255	ASN
6	l	283	CYS
6	l	312	VAL
6	l	340	THR
6	l	349	LEU
6	l	364	THR
6	l	366	ILE
6	l	375	VAL
6	l	385	MET
6	l	411	ILE
6	l	440	TRP
6	l	467	THR
6	l	482	ILE
6	l	486	ARG
6	l	502	LEU
6	l	513	GLU
6	l	520	ARG
6	l	522	ASP
7	i	26	ARG
7	i	47	VAL
7	i	56	ASP
7	i	61	THR
7	i	68	THR
7	i	86	LEU
7	i	89	GLN

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Mol	Chain	Res	Type
7	i	90	GLN
7	i	92	ARG
7	i	281	VAL
7	i	319	ARG
7	i	320	ARG
7	i	328	ARG
7	i	337	LEU
7	i	373	LEU
7	i	377	THR
7	i	392	ASP
7	i	407	SER
7	i	419	VAL
7	i	424	CYS
7	i	426	GLU
7	i	438	THR
7	i	442	SER
7	i	457	ILE
7	i	542	ASP
7	i	543	THR
7	i	546	THR
8	k	23	SER
8	k	34	VAL
8	k	52	MET
8	k	58	THR
8	k	78	MET
8	k	79	LEU
8	k	81	LEU
8	k	102	GLU
8	k	107	CYS
8	k	130	THR
8	k	138	GLN
8	k	143	VAL
8	k	148	ASP
8	k	154	LEU
8	k	167	TRP
8	k	206	VAL
8	k	215	LEU
8	k	251	GLU
8	k	257	SER
8	k	260	ASN
8	k	290	VAL
8	k	293	THR

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Mol	Chain	Res	Type
8	k	309	LEU
8	k	310	LEU
8	k	322	LYS
8	k	325	ASN
8	k	335	THR
8	k	336	ILE
8	k	348	VAL
8	k	354	LEU
8	k	396	LEU
8	k	398	ASP
8	k	404	ARG
8	k	438	GLN
8	k	468	LEU
8	k	481	THR
8	k	504	VAL
8	k	516	SER
8	k	521	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (228) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	22	ASN
1	F	83	GLN
1	F	104	GLN
1	F	142	ASN
1	F	145	ASN
1	F	221	HIS
1	F	248	ASN
1	F	324	ASN
1	F	338	ASN
2	H	27	GLN
2	H	311	HIS
2	H	392	ASN
3	G	21	GLN
3	G	37	GLN
3	G	123	HIS
3	G	172	HIS
3	G	173	ASN
3	G	245	ASN
3	G	268	GLN
3	G	384	GLN
3	G	472	HIS

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Mol	Chain	Res	Type
3	G	491	ASN
3	G	508	ASN
3	G	515	ASN
4	E	93	GLN
4	E	98	ASN
4	E	111	GLN
4	E	148	ASN
4	E	296	GLN
4	E	333	HIS
4	E	337	GLN
4	E	502	GLN
5	B	52	ASN
5	B	79	ASN
5	B	192	HIS
5	B	385	HIS
6	D	24	ASN
6	D	72	HIS
6	D	85	GLN
6	D	125	GLN
6	D	255	ASN
6	D	273	ASN
6	D	473	HIS
7	A	6	ASN
7	A	29	ASN
7	A	77	HIS
7	A	90	GLN
7	A	158	ASN
7	A	209	HIS
7	A	231	GLN
7	A	269	GLN
8	C	24	ASN
8	C	72	HIS
8	C	85	GLN
8	C	231	HIS
8	C	237	HIS
8	C	270	ASN
8	C	370	ASN
8	C	405	ASN
1	N	22	ASN
1	N	83	GLN
1	N	104	GLN
1	N	142	ASN

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Mol	Chain	Res	Type
1	N	145	ASN
1	N	221	HIS
1	N	248	ASN
1	N	324	ASN
1	N	338	ASN
1	N	430	ASN
2	P	27	GLN
2	P	203	ASN
2	P	311	HIS
2	P	392	ASN
3	O	37	GLN
3	O	174	ASN
3	O	384	GLN
3	O	491	ASN
3	O	505	ASN
3	O	508	ASN
3	O	515	ASN
4	M	93	GLN
4	M	98	ASN
4	M	253	GLN
4	M	432	ASN
4	M	502	GLN
4	M	520	ASN
5	J	52	ASN
5	J	79	ASN
5	J	142	ASN
5	J	192	HIS
5	J	286	ASN
5	J	375	GLN
5	J	385	HIS
6	L	24	ASN
6	L	59	ASN
6	L	72	HIS
6	L	85	GLN
6	L	125	GLN
6	L	149	GLN
6	L	251	ASN
6	L	255	ASN
6	L	303	HIS
6	L	473	HIS
7	I	6	ASN
7	I	29	ASN

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Mol	Chain	Res	Type
7	I	64	ASN
7	I	77	HIS
7	I	90	GLN
7	I	231	GLN
7	I	269	GLN
8	K	24	ASN
8	K	85	GLN
8	K	115	ASN
8	K	138	GLN
8	K	231	HIS
8	K	237	HIS
8	K	270	ASN
8	K	370	ASN
8	K	405	ASN
1	f	22	ASN
1	f	83	GLN
1	f	142	ASN
1	f	145	ASN
1	f	221	HIS
1	f	248	ASN
1	f	324	ASN
1	f	338	ASN
1	f	430	ASN
2	h	27	GLN
2	h	79	HIS
2	h	311	HIS
2	h	392	ASN
3	g	21	GLN
3	g	37	GLN
3	g	141	ASN
3	g	245	ASN
3	g	384	GLN
3	g	472	HIS
3	g	491	ASN
3	g	505	ASN
3	g	508	ASN
4	e	98	ASN
4	e	148	ASN
4	e	296	GLN
4	e	432	ASN
4	e	502	GLN
4	e	520	ASN

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Mol	Chain	Res	Type
5	b	52	ASN
5	b	79	ASN
5	b	84	GLN
5	b	308	HIS
5	b	375	GLN
5	b	385	HIS
5	b	513	ASN
6	d	24	ASN
6	d	59	ASN
6	d	125	GLN
6	d	255	ASN
6	d	473	HIS
7	a	6	ASN
7	a	29	ASN
7	a	77	HIS
7	a	90	GLN
7	a	158	ASN
7	a	231	GLN
7	a	269	GLN
7	a	485	GLN
8	c	12	GLN
8	c	24	ASN
8	c	72	HIS
8	c	85	GLN
8	c	138	GLN
8	c	231	HIS
8	c	237	HIS
8	c	351	ASN
8	c	370	ASN
1	n	22	ASN
1	n	83	GLN
1	n	104	GLN
1	n	142	ASN
1	n	145	ASN
1	n	221	HIS
1	n	324	ASN
1	n	338	ASN
1	n	430	ASN
2	p	27	GLN
2	p	79	HIS
3	o	21	GLN
3	o	37	GLN

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Mol	Chain	Res	Type
3	o	172	HIS
3	o	174	ASN
3	o	472	HIS
3	o	491	ASN
3	o	505	ASN
3	o	515	ASN
4	m	93	GLN
4	m	98	ASN
4	m	111	GLN
4	m	296	GLN
4	m	432	ASN
4	m	502	GLN
4	m	520	ASN
5	j	52	ASN
5	j	79	ASN
5	j	286	ASN
5	j	288	GLN
5	j	385	HIS
6	l	24	ASN
6	l	72	HIS
6	l	85	GLN
6	l	125	GLN
6	l	255	ASN
6	l	303	HIS
6	l	473	HIS
7	i	6	ASN
7	i	28	GLN
7	i	29	ASN
7	i	77	HIS
7	i	90	GLN
7	i	158	ASN
7	i	269	GLN
7	i	485	GLN
8	k	24	ASN
8	k	72	HIS
8	k	85	GLN
8	k	270	ASN
8	k	370	ASN
8	k	405	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 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	BEF	k	1103	10	0,3,3	0.00	-	-		
10	ADP	L	602	11,9	24,29,29	1.01	2 (8%)	29,45,45	1.42	4 (13%)
11	BEF	f	603	10	0,3,3	0.00	-	-		
10	ADP	E	602	9,11	24,29,29	0.99	1 (4%)	29,45,45	1.44	5 (17%)
10	ADP	d	602	11,9	24,29,29	0.94	1 (4%)	29,45,45	1.34	4 (13%)
10	ADP	F	602	11,9	24,29,29	0.98	1 (4%)	29,45,45	1.19	2 (6%)
10	ADP	H	602	9	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
11	BEF	j	603	10	0,3,3	0.00	-	-		
10	ADP	O	602	9	24,29,29	0.98	1 (4%)	29,45,45	1.39	4 (13%)
10	ADP	l	602	11,9	24,29,29	1.01	1 (4%)	29,45,45	1.44	4 (13%)
11	BEF	N	603	10	0,3,3	0.00	-	-		
10	ADP	n	602	11,9	24,29,29	1.03	2 (8%)	29,45,45	1.34	4 (13%)
11	BEF	d	603	10	0,3,3	0.00	-	-		
10	ADP	p	602	9	24,29,29	0.99	2 (8%)	29,45,45	1.39	4 (13%)
10	ADP	k	1102	11,9	24,29,29	1.02	2 (8%)	29,45,45	1.48	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	BEF	P	603	-	0,3,3	0.00	-	-		
11	BEF	G	603	-	0,3,3	0.00	-	-		
11	BEF	I	603	10	0,3,3	0.00	-	-		
10	ADP	e	602	11,9	24,29,29	0.99	2 (8%)	29,45,45	1.41	4 (13%)
10	ADP	B	602	11,9	24,29,29	0.96	1 (4%)	29,45,45	1.24	4 (13%)
11	BEF	c	1103	10	0,3,3	0.00	-	-		
10	ADP	f	602	11,9	24,29,29	1.08	3 (12%)	29,45,45	1.33	4 (13%)
10	ADP	h	602	9	24,29,29	0.97	2 (8%)	29,45,45	1.30	4 (13%)
10	ADP	m	602	9,11	24,29,29	1.05	2 (8%)	29,45,45	1.32	3 (10%)
10	ADP	J	602	11,9	24,29,29	1.00	1 (4%)	29,45,45	1.37	3 (10%)
10	ADP	o	602	9	24,29,29	1.04	2 (8%)	29,45,45	1.44	5 (17%)
11	BEF	o	603	-	0,3,3	0.00	-	-		
11	BEF	n	603	10	0,3,3	0.00	-	-		
10	ADP	A	602	9,11	24,29,29	1.02	2 (8%)	29,45,45	1.47	4 (13%)
11	BEF	F	603	10	0,3,3	0.00	-	-		
11	BEF	C	1103	10	0,3,3	0.00	-	-		
11	BEF	M	603	10	0,3,3	0.00	-	-		
11	BEF	p	603	-	0,3,3	0.00	-	-		
10	ADP	b	602	11,9	24,29,29	1.02	2 (8%)	29,45,45	1.29	4 (13%)
10	ADP	g	602	9	24,29,29	0.99	1 (4%)	29,45,45	1.40	4 (13%)
10	ADP	P	602	9	24,29,29	0.97	2 (8%)	29,45,45	1.36	4 (13%)
11	BEF	K	1103	10	0,3,3	0.00	-	-		
11	BEF	L	603	10	0,3,3	0.00	-	-		
11	BEF	H	603	-	0,3,3	0.00	-	-		
10	ADP	j	602	11,9	24,29,29	1.02	2 (8%)	29,45,45	1.29	4 (13%)
10	ADP	a	602	9,11	24,29,29	1.00	1 (4%)	29,45,45	1.39	4 (13%)
11	BEF	A	603	10	0,3,3	0.00	-	-		
11	BEF	B	603	10	0,3,3	0.00	-	-		
11	BEF	a	603	10	0,3,3	0.00	-	-		
10	ADP	C	1102	11,9	24,29,29	1.01	2 (8%)	29,45,45	1.45	4 (13%)
10	ADP	I	602	9,11	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
11	BEF	E	603	10	0,3,3	0.00	-	-		
10	ADP	M	602	11,9	24,29,29	0.98	1 (4%)	29,45,45	1.38	4 (13%)
11	BEF	i	603	10	0,3,3	0.00	-	-		
11	BEF	h	603	-	0,3,3	0.00	-	-		
10	ADP	D	602	11,9	24,29,29	0.97	1 (4%)	29,45,45	1.32	4 (13%)
11	BEF	l	603	10	0,3,3	0.00	-	-		
10	ADP	c	1102	11,9	24,29,29	0.97	1 (4%)	29,45,45	1.36	4 (13%)
11	BEF	J	603	10	0,3,3	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	BEF	e	603	10	0,3,3	0.00	-	-		
11	BEF	O	603	-	0,3,3	0.00	-	-		
10	ADP	N	602	9,11	24,29,29	1.00	1 (4%)	29,45,45	1.36	4 (13%)
11	BEF	D	603	10	0,3,3	0.00	-	-		
10	ADP	K	1102	11,9	24,29,29	0.99	1 (4%)	29,45,45	1.41	5 (17%)
11	BEF	b	603	10	0,3,3	0.00	-	-		
11	BEF	g	603	-	0,3,3	0.00	-	-		
10	ADP	i	602	11,9	24,29,29	1.01	2 (8%)	29,45,45	1.42	4 (13%)
10	ADP	G	602	9	24,29,29	0.98	2 (8%)	29,45,45	1.46	4 (13%)
11	BEF	m	603	10	0,3,3	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	E	602	9,11	-	7/12/32/32	0/3/3/3
10	ADP	d	602	11,9	-	6/12/32/32	0/3/3/3
10	ADP	F	602	11,9	-	8/12/32/32	0/3/3/3
10	ADP	H	602	9	-	1/12/32/32	0/3/3/3
10	ADP	M	602	11,9	-	8/12/32/32	0/3/3/3
10	ADP	O	602	9	-	4/12/32/32	0/3/3/3
10	ADP	l	602	11,9	-	6/12/32/32	0/3/3/3
10	ADP	n	602	11,9	-	8/12/32/32	0/3/3/3
10	ADP	p	602	9	-	1/12/32/32	0/3/3/3
10	ADP	e	602	11,9	-	8/12/32/32	0/3/3/3
10	ADP	B	602	11,9	-	3/12/32/32	0/3/3/3
10	ADP	G	602	9	-	5/12/32/32	0/3/3/3
10	ADP	f	602	11,9	-	7/12/32/32	0/3/3/3
10	ADP	h	602	9	-	1/12/32/32	0/3/3/3
10	ADP	m	602	9,11	-	7/12/32/32	0/3/3/3
10	ADP	J	602	11,9	-	2/12/32/32	0/3/3/3
10	ADP	o	602	9	-	5/12/32/32	0/3/3/3
10	ADP	A	602	9,11	-	5/12/32/32	0/3/3/3
10	ADP	b	602	11,9	-	2/12/32/32	0/3/3/3
10	ADP	g	602	9	-	5/12/32/32	0/3/3/3
10	ADP	P	602	9	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	j	602	11,9	-	2/12/32/32	0/3/3/3
10	ADP	a	602	9,11	-	5/12/32/32	0/3/3/3
10	ADP	k	1102	11,9	-	2/12/32/32	0/3/3/3
10	ADP	C	1102	11,9	-	2/12/32/32	0/3/3/3
10	ADP	I	602	9,11	-	5/12/32/32	0/3/3/3
10	ADP	D	602	11,9	-	6/12/32/32	0/3/3/3
10	ADP	c	1102	11,9	-	2/12/32/32	0/3/3/3
10	ADP	L	602	11,9	-	7/12/32/32	0/3/3/3
10	ADP	N	602	9,11	-	8/12/32/32	0/3/3/3
10	ADP	K	1102	11,9	-	1/12/32/32	0/3/3/3
10	ADP	i	602	11,9	-	6/12/32/32	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	f	602	ADP	C5-C4	2.75	1.48	1.40
10	m	602	ADP	C5-C4	2.72	1.48	1.40
10	n	602	ADP	C5-C4	2.71	1.48	1.40
10	b	602	ADP	C5-C4	2.68	1.48	1.40
10	k	1102	ADP	C5-C4	2.65	1.47	1.40
10	A	602	ADP	C5-C4	2.64	1.47	1.40
10	j	602	ADP	C5-C4	2.63	1.47	1.40
10	l	602	ADP	C5-C4	2.61	1.47	1.40
10	C	1102	ADP	C5-C4	2.61	1.47	1.40
10	c	1102	ADP	C5-C4	2.59	1.47	1.40
10	N	602	ADP	C5-C4	2.59	1.47	1.40
10	G	602	ADP	C5-C4	2.59	1.47	1.40
10	g	602	ADP	C5-C4	2.58	1.47	1.40
10	L	602	ADP	C5-C4	2.54	1.47	1.40
10	i	602	ADP	C5-C4	2.54	1.47	1.40
10	P	602	ADP	C5-C4	2.53	1.47	1.40
10	H	602	ADP	C5-C4	2.53	1.47	1.40
10	o	602	ADP	C5-C4	2.53	1.47	1.40
10	O	602	ADP	C5-C4	2.53	1.47	1.40
10	F	602	ADP	C5-C4	2.52	1.47	1.40
10	e	602	ADP	C5-C4	2.52	1.47	1.40
10	J	602	ADP	C5-C4	2.52	1.47	1.40
10	E	602	ADP	C5-C4	2.50	1.47	1.40
10	a	602	ADP	C5-C4	2.50	1.47	1.40
10	M	602	ADP	C5-C4	2.48	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	p	602	ADP	C5-C4	2.47	1.47	1.40
10	K	1102	ADP	C5-C4	2.47	1.47	1.40
10	I	602	ADP	C5-C4	2.45	1.47	1.40
10	d	602	ADP	C5-C4	2.44	1.47	1.40
10	h	602	ADP	C5-C4	2.44	1.47	1.40
10	D	602	ADP	C5-C4	2.41	1.47	1.40
10	B	602	ADP	C5-C4	2.39	1.47	1.40
10	m	602	ADP	C2-N3	2.28	1.35	1.32
10	f	602	ADP	C2-N3	2.17	1.35	1.32
10	o	602	ADP	O4'-C1'	2.17	1.44	1.41
10	i	602	ADP	O4'-C1'	2.11	1.44	1.41
10	f	602	ADP	O4'-C1'	2.11	1.44	1.41
10	b	602	ADP	C2-N3	2.08	1.35	1.32
10	P	602	ADP	C2-N3	2.07	1.35	1.32
10	p	602	ADP	C2-N3	2.06	1.35	1.32
10	C	1102	ADP	C2-N3	2.04	1.35	1.32
10	n	602	ADP	C2-N3	2.02	1.35	1.32
10	j	602	ADP	C2-N3	2.02	1.35	1.32
10	e	602	ADP	C2-N3	2.01	1.35	1.32
10	A	602	ADP	C2-N3	2.01	1.35	1.32
10	k	1102	ADP	C2-N3	2.01	1.35	1.32
10	h	602	ADP	C2-N3	2.01	1.35	1.32
10	L	602	ADP	C2-N3	2.00	1.35	1.32
10	G	602	ADP	C2-N3	2.00	1.35	1.32

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	g	602	ADP	C3'-C2'-C1'	3.63	106.45	100.98
10	C	1102	ADP	PA-O3A-PB	-3.63	120.37	132.83
10	M	602	ADP	N3-C2-N1	-3.60	123.06	128.68
10	k	1102	ADP	PA-O3A-PB	-3.57	120.58	132.83
10	J	602	ADP	C3'-C2'-C1'	3.56	106.33	100.98
10	G	602	ADP	C3'-C2'-C1'	3.55	106.33	100.98
10	i	602	ADP	C3'-C2'-C1'	3.55	106.32	100.98
10	E	602	ADP	N3-C2-N1	-3.54	123.14	128.68
10	h	602	ADP	N3-C2-N1	-3.53	123.15	128.68
10	p	602	ADP	N3-C2-N1	-3.53	123.17	128.68
10	o	602	ADP	C3'-C2'-C1'	3.51	106.26	100.98
10	I	602	ADP	N3-C2-N1	-3.50	123.21	128.68
10	O	602	ADP	C3'-C2'-C1'	3.48	106.21	100.98
10	o	602	ADP	N3-C2-N1	-3.47	123.25	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	602	ADP	N3-C2-N1	-3.46	123.27	128.68
10	l	602	ADP	N3-C2-N1	-3.45	123.28	128.68
10	O	602	ADP	N3-C2-N1	-3.44	123.31	128.68
10	H	602	ADP	N3-C2-N1	-3.44	123.31	128.68
10	l	602	ADP	C3'-C2'-C1'	3.43	106.14	100.98
10	P	602	ADP	N3-C2-N1	-3.42	123.33	128.68
10	i	602	ADP	N3-C2-N1	-3.41	123.34	128.68
10	g	602	ADP	N3-C2-N1	-3.39	123.38	128.68
10	G	602	ADP	N3-C2-N1	-3.38	123.39	128.68
10	N	602	ADP	N3-C2-N1	-3.37	123.42	128.68
10	n	602	ADP	N3-C2-N1	-3.36	123.43	128.68
10	m	602	ADP	N3-C2-N1	-3.34	123.46	128.68
10	F	602	ADP	N3-C2-N1	-3.33	123.47	128.68
10	d	602	ADP	N3-C2-N1	-3.33	123.47	128.68
10	K	1102	ADP	N3-C2-N1	-3.30	123.53	128.68
10	f	602	ADP	N3-C2-N1	-3.30	123.53	128.68
10	D	602	ADP	N3-C2-N1	-3.28	123.55	128.68
10	I	602	ADP	PA-O3A-PB	-3.28	121.56	132.83
10	L	602	ADP	N3-C2-N1	-3.28	123.56	128.68
10	L	602	ADP	C3'-C2'-C1'	3.27	105.91	100.98
10	k	1102	ADP	N3-C2-N1	-3.25	123.60	128.68
10	A	602	ADP	N3-C2-N1	-3.25	123.60	128.68
10	j	602	ADP	N3-C2-N1	-3.25	123.60	128.68
10	B	602	ADP	N3-C2-N1	-3.24	123.61	128.68
10	A	602	ADP	C3'-C2'-C1'	3.23	105.85	100.98
10	J	602	ADP	N3-C2-N1	-3.23	123.62	128.68
10	m	602	ADP	C3'-C2'-C1'	3.21	105.82	100.98
10	e	602	ADP	N3-C2-N1	-3.21	123.66	128.68
10	A	602	ADP	C4-C5-N7	-3.20	106.06	109.40
10	K	1102	ADP	PA-O3A-PB	-3.18	121.90	132.83
10	e	602	ADP	C3'-C2'-C1'	3.18	105.77	100.98
10	H	602	ADP	C3'-C2'-C1'	3.17	105.75	100.98
10	C	1102	ADP	N3-C2-N1	-3.17	123.72	128.68
10	k	1102	ADP	C3'-C2'-C1'	3.13	105.69	100.98
10	P	602	ADP	C3'-C2'-C1'	3.10	105.65	100.98
10	b	602	ADP	N3-C2-N1	-3.09	123.85	128.68
10	p	602	ADP	C3'-C2'-C1'	3.08	105.62	100.98
10	E	602	ADP	C3'-C2'-C1'	3.07	105.60	100.98
10	f	602	ADP	C3'-C2'-C1'	3.05	105.57	100.98
10	c	1102	ADP	PA-O3A-PB	-3.04	122.39	132.83
10	G	602	ADP	PA-O3A-PB	-3.03	122.43	132.83
10	M	602	ADP	C3'-C2'-C1'	3.03	105.53	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	c	1102	ADP	N3-C2-N1	-3.02	123.96	128.68
10	J	602	ADP	C4-C5-N7	-3.01	106.26	109.40
10	O	602	ADP	C4-C5-N7	-2.96	106.31	109.40
10	A	602	ADP	PA-O3A-PB	-2.94	122.72	132.83
10	L	602	ADP	C4-C5-N7	-2.93	106.34	109.40
10	C	1102	ADP	C3'-C2'-C1'	2.93	105.39	100.98
10	P	602	ADP	C4-C5-N7	-2.92	106.36	109.40
10	D	602	ADP	C4-C5-N7	-2.91	106.37	109.40
10	N	602	ADP	C4-C5-N7	-2.91	106.37	109.40
10	e	602	ADP	C4-C5-N7	-2.90	106.38	109.40
10	a	602	ADP	C4-C5-N7	-2.90	106.38	109.40
10	n	602	ADP	C4-C5-N7	-2.87	106.41	109.40
10	p	602	ADP	C4-C5-N7	-2.87	106.41	109.40
10	b	602	ADP	C3'-C2'-C1'	2.83	105.25	100.98
10	N	602	ADP	C3'-C2'-C1'	2.81	105.21	100.98
10	f	602	ADP	C4-C5-N7	-2.81	106.47	109.40
10	e	602	ADP	PA-O3A-PB	-2.81	123.19	132.83
10	G	602	ADP	C4-C5-N7	-2.80	106.48	109.40
10	b	602	ADP	C4-C5-N7	-2.79	106.49	109.40
10	i	602	ADP	C4-C5-N7	-2.78	106.50	109.40
10	o	602	ADP	C4-C5-N7	-2.78	106.50	109.40
10	E	602	ADP	PA-O3A-PB	-2.77	123.31	132.83
10	h	602	ADP	C3'-C2'-C1'	2.77	105.15	100.98
10	c	1102	ADP	C4-C5-N7	-2.75	106.53	109.40
10	I	602	ADP	C4-C5-N7	-2.74	106.54	109.40
10	M	602	ADP	C4-C5-N7	-2.74	106.55	109.40
10	m	602	ADP	C4-C5-N7	-2.72	106.57	109.40
10	h	602	ADP	C4-C5-N7	-2.71	106.57	109.40
10	i	602	ADP	PA-O3A-PB	-2.71	123.54	132.83
10	o	602	ADP	PA-O3A-PB	-2.70	123.56	132.83
10	a	602	ADP	PA-O3A-PB	-2.70	123.57	132.83
10	k	1102	ADP	C4-C5-N7	-2.67	106.61	109.40
10	j	602	ADP	C3'-C2'-C1'	2.66	104.98	100.98
10	H	602	ADP	C4-C5-N7	-2.64	106.65	109.40
10	I	602	ADP	C3'-C2'-C1'	2.63	104.94	100.98
10	D	602	ADP	C3'-C2'-C1'	2.63	104.94	100.98
10	c	1102	ADP	C3'-C2'-C1'	2.63	104.93	100.98
10	d	602	ADP	C4-C5-N7	-2.62	106.67	109.40
10	l	602	ADP	C4-C5-N7	-2.62	106.67	109.40
10	d	602	ADP	C3'-C2'-C1'	2.62	104.92	100.98
10	K	1102	ADP	C4-C5-N7	-2.59	106.70	109.40
10	l	602	ADP	PA-O3A-PB	-2.57	124.00	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	602	ADP	C4-C5-N7	-2.56	106.73	109.40
10	B	602	ADP	C4-C5-N7	-2.54	106.75	109.40
10	a	602	ADP	C3'-C2'-C1'	2.54	104.81	100.98
10	n	602	ADP	C3'-C2'-C1'	2.54	104.80	100.98
10	L	602	ADP	PA-O3A-PB	-2.54	124.12	132.83
10	g	602	ADP	PA-O3A-PB	-2.52	124.18	132.83
10	p	602	ADP	PA-O3A-PB	-2.52	124.19	132.83
10	C	1102	ADP	C4-C5-N7	-2.49	106.80	109.40
10	D	602	ADP	PA-O3A-PB	-2.49	124.29	132.83
10	d	602	ADP	PA-O3A-PB	-2.48	124.32	132.83
10	E	602	ADP	C4-C5-N7	-2.44	106.86	109.40
10	N	602	ADP	PA-O3A-PB	-2.41	124.54	132.83
10	g	602	ADP	C4-C5-N7	-2.40	106.89	109.40
10	K	1102	ADP	C3'-C2'-C1'	2.34	104.50	100.98
10	P	602	ADP	PA-O3A-PB	-2.33	124.82	132.83
10	f	602	ADP	PA-O3A-PB	-2.29	124.98	132.83
10	n	602	ADP	PA-O3A-PB	-2.26	125.08	132.83
10	E	602	ADP	C2'-C3'-C4'	2.20	106.93	102.64
10	B	602	ADP	PA-O3A-PB	-2.20	125.29	132.83
10	O	602	ADP	PA-O3A-PB	-2.17	125.37	132.83
10	H	602	ADP	PA-O3A-PB	-2.16	125.40	132.83
10	b	602	ADP	PA-O3A-PB	-2.16	125.43	132.83
10	K	1102	ADP	C2'-C3'-C4'	2.10	106.73	102.64
10	j	602	ADP	C4-C5-N7	-2.09	107.23	109.40
10	j	602	ADP	PA-O3A-PB	-2.08	125.67	132.83
10	h	602	ADP	PA-O3A-PB	-2.07	125.72	132.83
10	B	602	ADP	C3'-C2'-C1'	2.07	104.09	100.98
10	M	602	ADP	PA-O3A-PB	-2.06	125.77	132.83
10	o	602	ADP	C2'-C3'-C4'	2.02	106.56	102.64

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	602	ADP	C5'-O5'-PA-O3A
10	E	602	ADP	C3'-C4'-C5'-O5'
10	d	602	ADP	PB-O3A-PA-O5'
10	d	602	ADP	C5'-O5'-PA-O1A
10	d	602	ADP	C5'-O5'-PA-O2A
10	d	602	ADP	C3'-C4'-C5'-O5'
10	M	602	ADP	C5'-O5'-PA-O1A
10	M	602	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
10	M	602	ADP	C3'-C4'-C5'-O5'
10	l	602	ADP	PA-O3A-PB-O3B
10	l	602	ADP	C5'-O5'-PA-O2A
10	l	602	ADP	C3'-C4'-C5'-O5'
10	n	602	ADP	C5'-O5'-PA-O1A
10	n	602	ADP	C5'-O5'-PA-O2A
10	n	602	ADP	C5'-O5'-PA-O3A
10	n	602	ADP	C3'-C4'-C5'-O5'
10	m	602	ADP	C5'-O5'-PA-O1A
10	m	602	ADP	C5'-O5'-PA-O2A
10	m	602	ADP	O4'-C4'-C5'-O5'
10	m	602	ADP	C3'-C4'-C5'-O5'
10	A	602	ADP	C5'-O5'-PA-O3A
10	A	602	ADP	C3'-C4'-C5'-O5'
10	a	602	ADP	C5'-O5'-PA-O3A
10	a	602	ADP	O4'-C4'-C5'-O5'
10	a	602	ADP	C3'-C4'-C5'-O5'
10	L	602	ADP	C5'-O5'-PA-O1A
10	L	602	ADP	C5'-O5'-PA-O2A
10	L	602	ADP	C3'-C4'-C5'-O5'
10	g	602	ADP	PB-O3A-PA-O5'
10	g	602	ADP	C5'-O5'-PA-O3A
10	g	602	ADP	O4'-C4'-C5'-O5'
10	g	602	ADP	C3'-C4'-C5'-O5'
10	F	602	ADP	C5'-O5'-PA-O1A
10	F	602	ADP	C5'-O5'-PA-O2A
10	O	602	ADP	C5'-O5'-PA-O1A
10	G	602	ADP	C5'-O5'-PA-O1A
10	i	602	ADP	C5'-O5'-PA-O1A
10	i	602	ADP	C5'-O5'-PA-O2A
10	i	602	ADP	C3'-C4'-C5'-O5'
10	p	602	ADP	PA-O3A-PB-O3B
10	e	602	ADP	C5'-O5'-PA-O1A
10	e	602	ADP	C5'-O5'-PA-O3A
10	e	602	ADP	O4'-C4'-C5'-O5'
10	e	602	ADP	C3'-C4'-C5'-O5'
10	f	602	ADP	C5'-O5'-PA-O3A
10	f	602	ADP	C3'-C4'-C5'-O5'
10	o	602	ADP	PB-O3A-PA-O5'
10	o	602	ADP	C5'-O5'-PA-O1A
10	I	602	ADP	PB-O3A-PA-O5'
10	I	602	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
10	I	602	ADP	O4'-C4'-C5'-O5'
10	I	602	ADP	C3'-C4'-C5'-O5'
10	D	602	ADP	C5'-O5'-PA-O2A
10	D	602	ADP	C3'-C4'-C5'-O5'
10	N	602	ADP	C5'-O5'-PA-O1A
10	N	602	ADP	C5'-O5'-PA-O2A
10	N	602	ADP	C3'-C4'-C5'-O5'
10	E	602	ADP	O4'-C4'-C5'-O5'
10	F	602	ADP	C3'-C4'-C5'-O5'
10	O	602	ADP	O4'-C4'-C5'-O5'
10	O	602	ADP	C3'-C4'-C5'-O5'
10	G	602	ADP	O4'-C4'-C5'-O5'
10	G	602	ADP	C3'-C4'-C5'-O5'
10	o	602	ADP	O4'-C4'-C5'-O5'
10	o	602	ADP	C3'-C4'-C5'-O5'
10	d	602	ADP	O4'-C4'-C5'-O5'
10	M	602	ADP	O4'-C4'-C5'-O5'
10	n	602	ADP	O4'-C4'-C5'-O5'
10	A	602	ADP	O4'-C4'-C5'-O5'
10	L	602	ADP	O4'-C4'-C5'-O5'
10	i	602	ADP	O4'-C4'-C5'-O5'
10	f	602	ADP	O4'-C4'-C5'-O5'
10	N	602	ADP	O4'-C4'-C5'-O5'
10	l	602	ADP	O4'-C4'-C5'-O5'
10	F	602	ADP	O4'-C4'-C5'-O5'
10	D	602	ADP	O4'-C4'-C5'-O5'
10	A	602	ADP	PB-O3A-PA-O5'
10	a	602	ADP	PB-O3A-PA-O5'
10	O	602	ADP	PB-O3A-PA-O5'
10	G	602	ADP	PB-O3A-PA-O5'
10	i	602	ADP	PB-O3A-PA-O5'
10	D	602	ADP	PB-O3A-PA-O5'
10	M	602	ADP	PA-O3A-PB-O1B
10	n	602	ADP	PA-O3A-PB-O1B
10	e	602	ADP	PA-O3A-PB-O1B
10	f	602	ADP	PA-O3A-PB-O1B
10	l	602	ADP	C5'-O5'-PA-O3A
10	D	602	ADP	C5'-O5'-PA-O3A
10	N	602	ADP	C5'-O5'-PA-O3A
10	j	602	ADP	PB-O3A-PA-O2A
10	c	1102	ADP	PB-O3A-PA-O2A
10	E	602	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	l	602	ADP	C5'-O5'-PA-O1A
10	A	602	ADP	C5'-O5'-PA-O1A
10	a	602	ADP	C5'-O5'-PA-O1A
10	g	602	ADP	C5'-O5'-PA-O1A
10	e	602	ADP	C5'-O5'-PA-O2A
10	f	602	ADP	C5'-O5'-PA-O1A
10	I	602	ADP	C5'-O5'-PA-O1A
10	D	602	ADP	C5'-O5'-PA-O1A
10	J	602	ADP	C3'-C4'-C5'-O5'
10	N	602	ADP	PA-O3A-PB-O1B
10	b	602	ADP	PB-O3A-PA-O2A
10	B	602	ADP	PB-O3A-PA-O2A
10	G	602	ADP	PB-O3A-PA-O1A
10	k	1102	ADP	PB-O3A-PA-O2A
10	C	1102	ADP	PB-O3A-PA-O2A
10	K	1102	ADP	PB-O3A-PA-O2A
10	b	602	ADP	C3'-C4'-C5'-O5'
10	E	602	ADP	PA-O3A-PB-O1B
10	m	602	ADP	PA-O3A-PB-O1B
10	F	602	ADP	PA-O3A-PB-O1B
10	J	602	ADP	PB-O3A-PA-O2A
10	L	602	ADP	PB-O3A-PA-O5'
10	B	602	ADP	C3'-C4'-C5'-O5'
10	E	602	ADP	PA-O3A-PB-O2B
10	E	602	ADP	PA-O3A-PB-O3B
10	M	602	ADP	PA-O3A-PB-O2B
10	M	602	ADP	PA-O3A-PB-O3B
10	n	602	ADP	PA-O3A-PB-O2B
10	n	602	ADP	PA-O3A-PB-O3B
10	m	602	ADP	PA-O3A-PB-O2B
10	L	602	ADP	PA-O3A-PB-O3B
10	H	602	ADP	PA-O3A-PB-O3B
10	F	602	ADP	PA-O3A-PB-O2B
10	F	602	ADP	PA-O3A-PB-O3B
10	h	602	ADP	PA-O3A-PB-O3B
10	P	602	ADP	PA-O3A-PB-O3B
10	e	602	ADP	PA-O3A-PB-O2B
10	e	602	ADP	PA-O3A-PB-O3B
10	f	602	ADP	PA-O3A-PB-O2B
10	f	602	ADP	PA-O3A-PB-O3B
10	o	602	ADP	PA-O3A-PB-O3B
10	N	602	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
10	N	602	ADP	PA-O3A-PB-O3B
10	d	602	ADP	C5'-O5'-PA-O3A
10	M	602	ADP	C5'-O5'-PA-O3A
10	m	602	ADP	C5'-O5'-PA-O3A
10	L	602	ADP	C5'-O5'-PA-O3A
10	F	602	ADP	C5'-O5'-PA-O3A
10	i	602	ADP	C5'-O5'-PA-O3A
10	B	602	ADP	PB-O3A-PA-O1A
10	j	602	ADP	PB-O3A-PA-O1A
10	k	1102	ADP	PB-O3A-PA-O1A
10	C	1102	ADP	PB-O3A-PA-O1A
10	c	1102	ADP	PB-O3A-PA-O1A

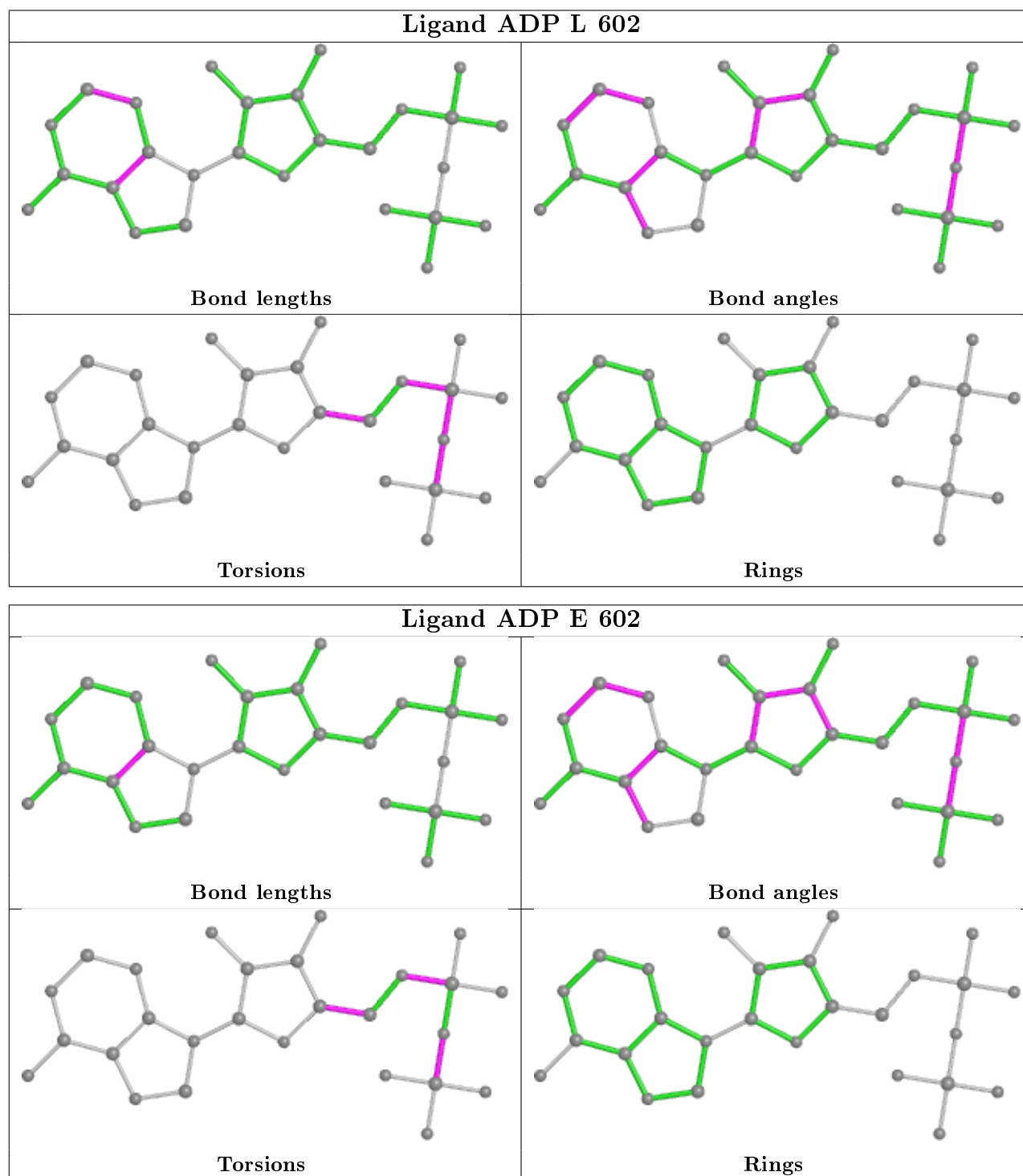
There are no ring outliers.

18 monomers are involved in 19 short contacts:

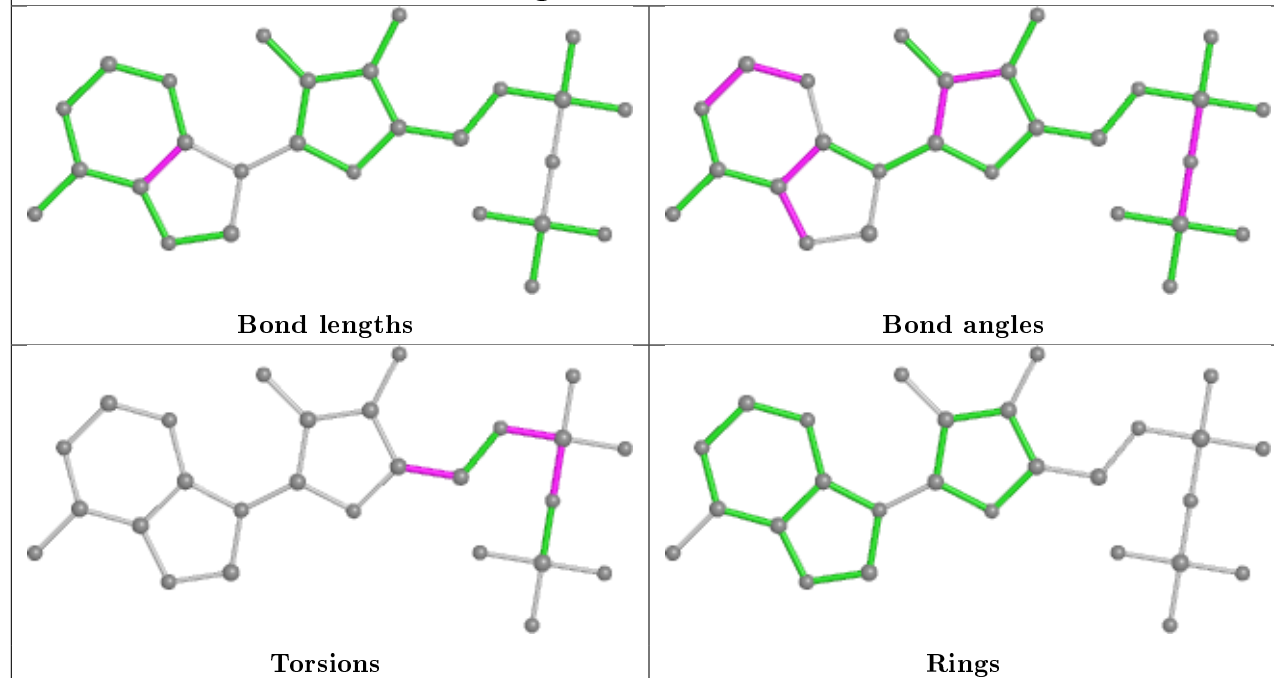
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	602	ADP	1	0
11	G	603	BEF	1	0
10	B	602	ADP	3	0
10	J	602	ADP	2	0
10	A	602	ADP	1	0
11	C	1103	BEF	2	0
11	M	603	BEF	1	0
11	K	1103	BEF	1	0
11	B	603	BEF	2	0
10	C	1102	ADP	5	0
10	I	602	ADP	1	0
11	E	603	BEF	1	0
10	M	602	ADP	1	0
10	D	602	ADP	1	0
11	J	603	BEF	1	0
11	O	603	BEF	1	0
11	D	603	BEF	1	0
10	K	1102	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

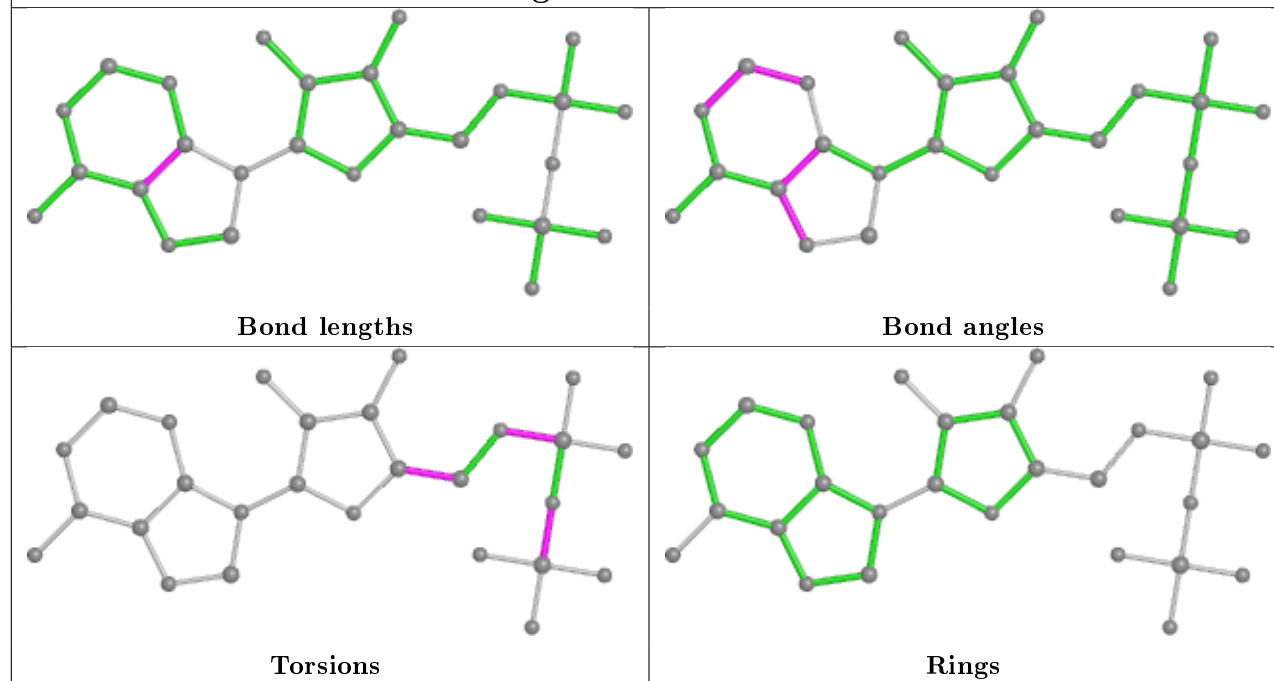
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

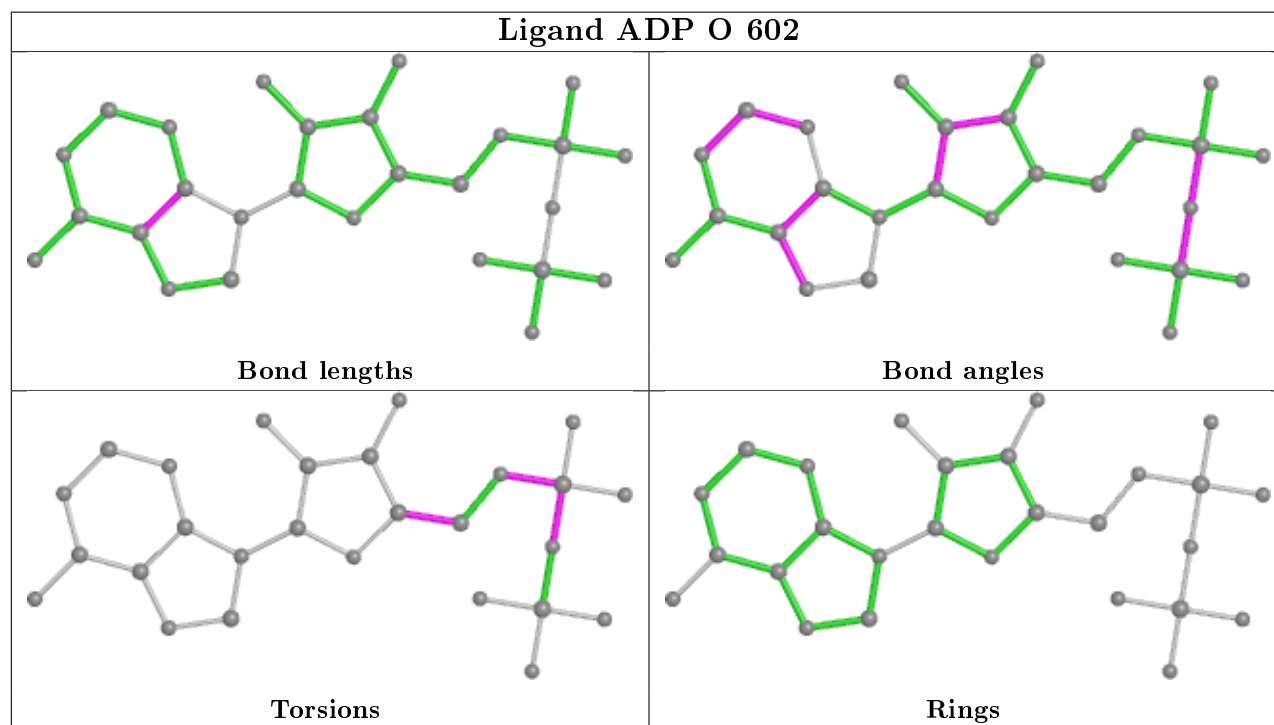
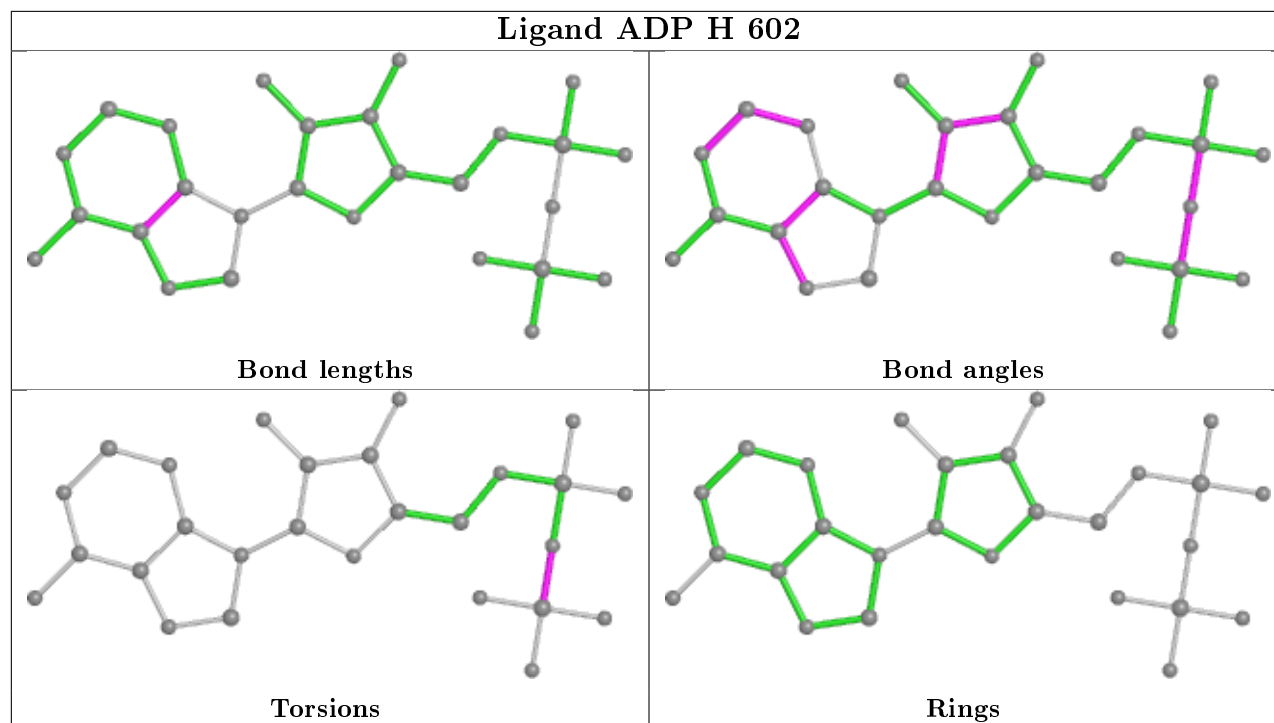


## Ligand ADP d 602

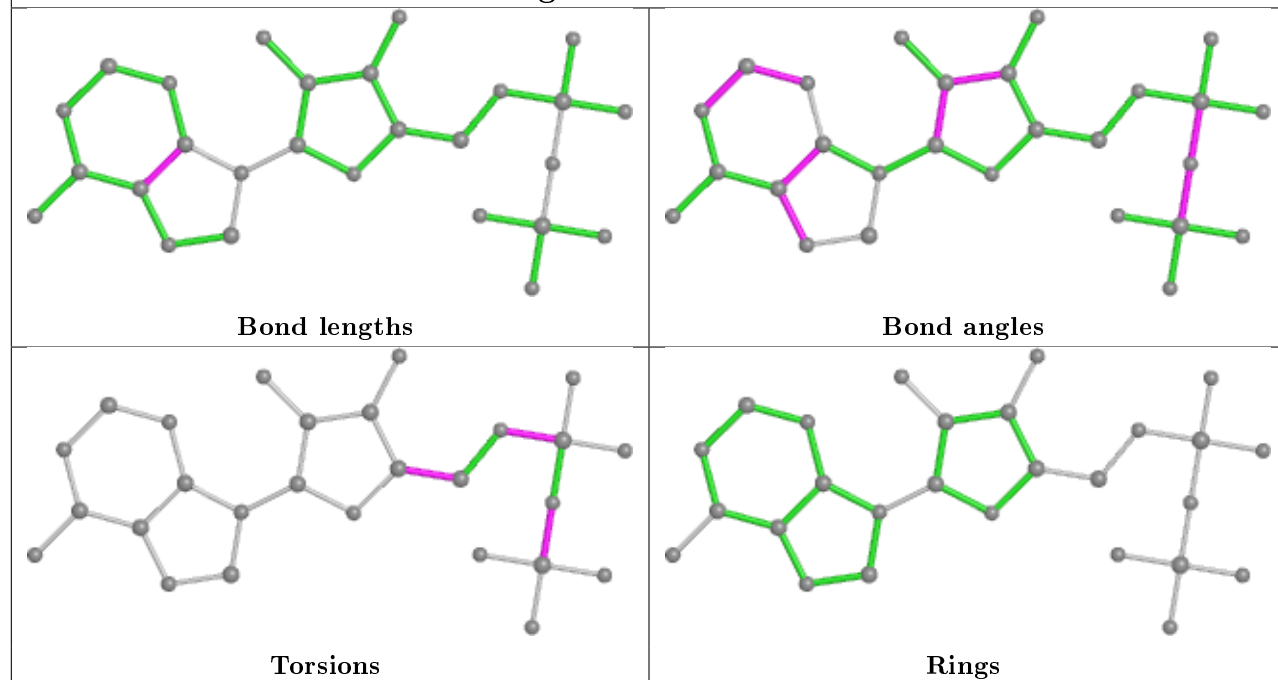


## Ligand ADP F 602

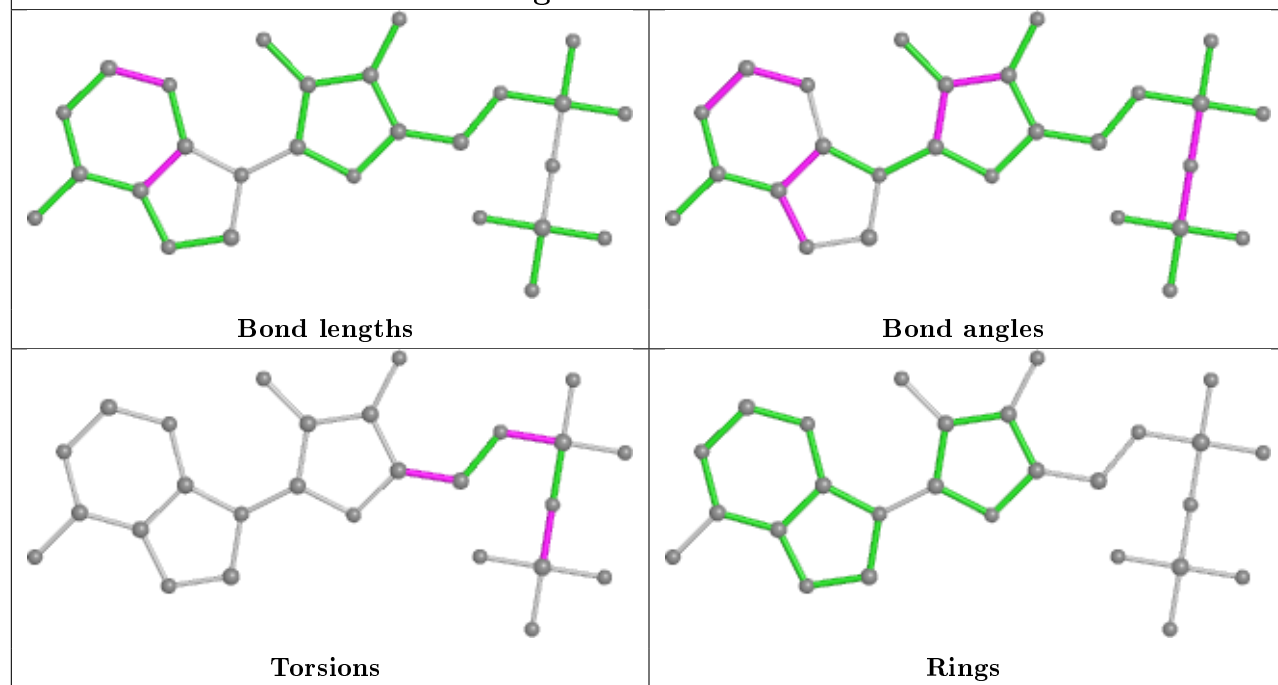




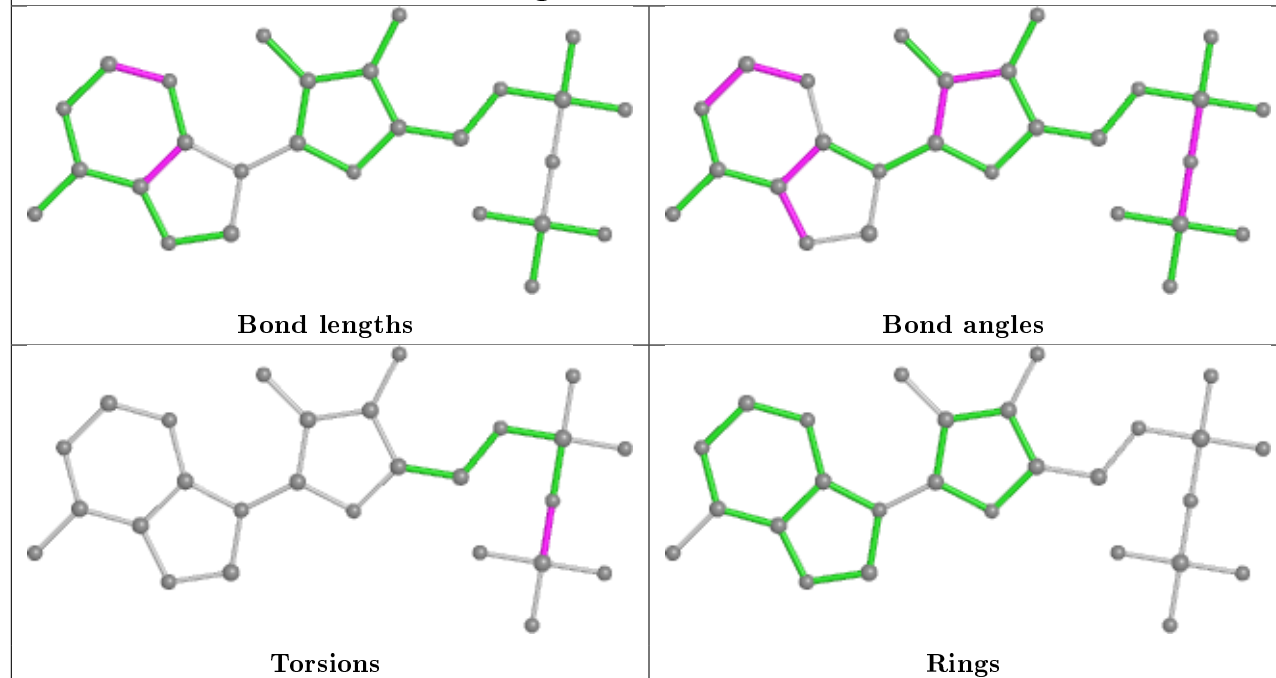
## Ligand ADP 1 602



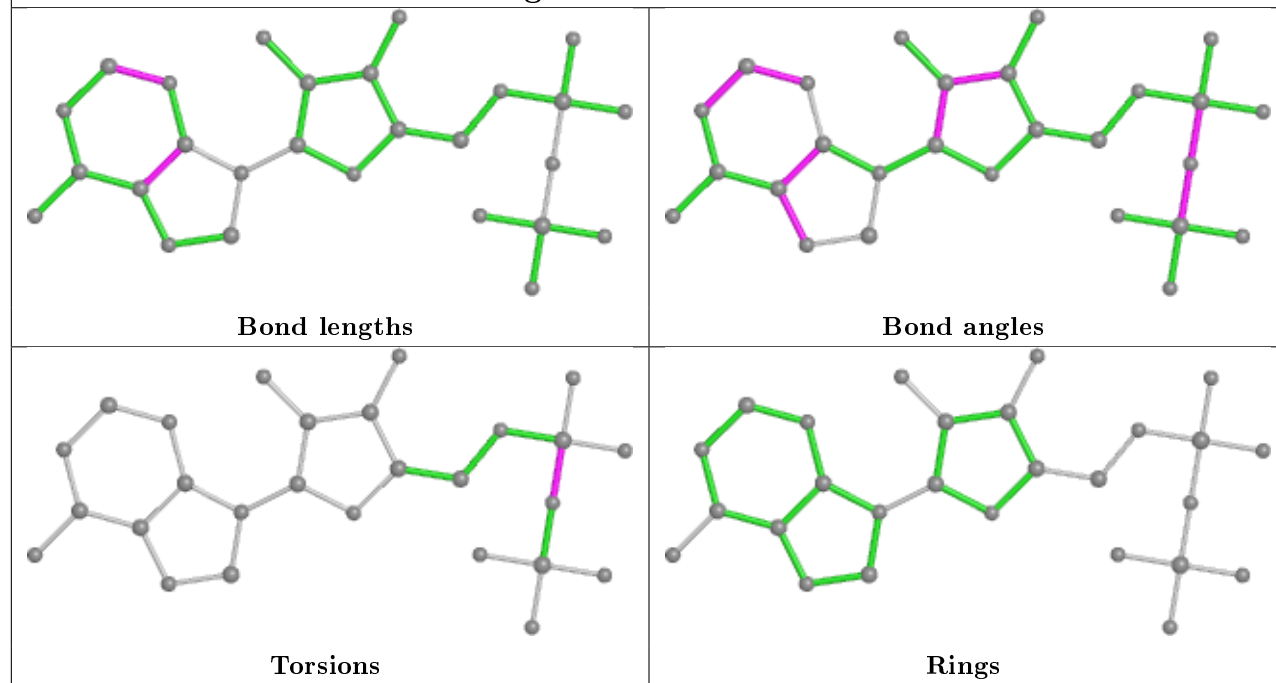
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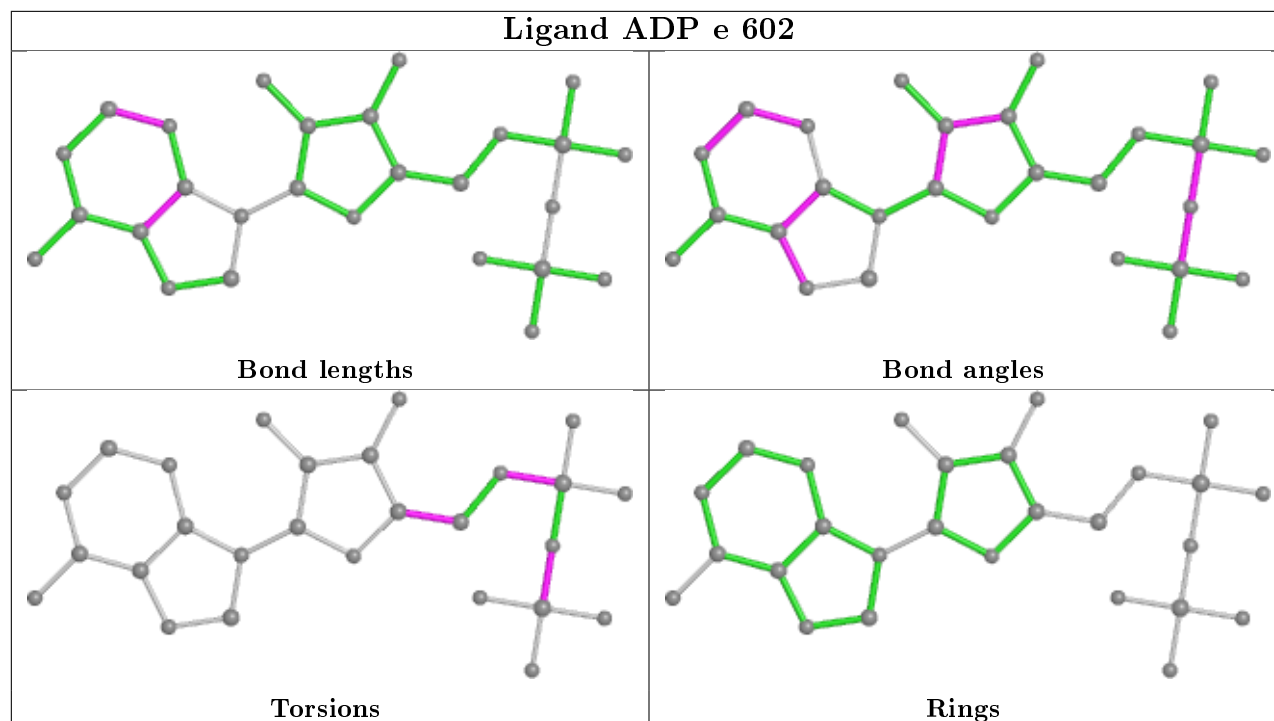
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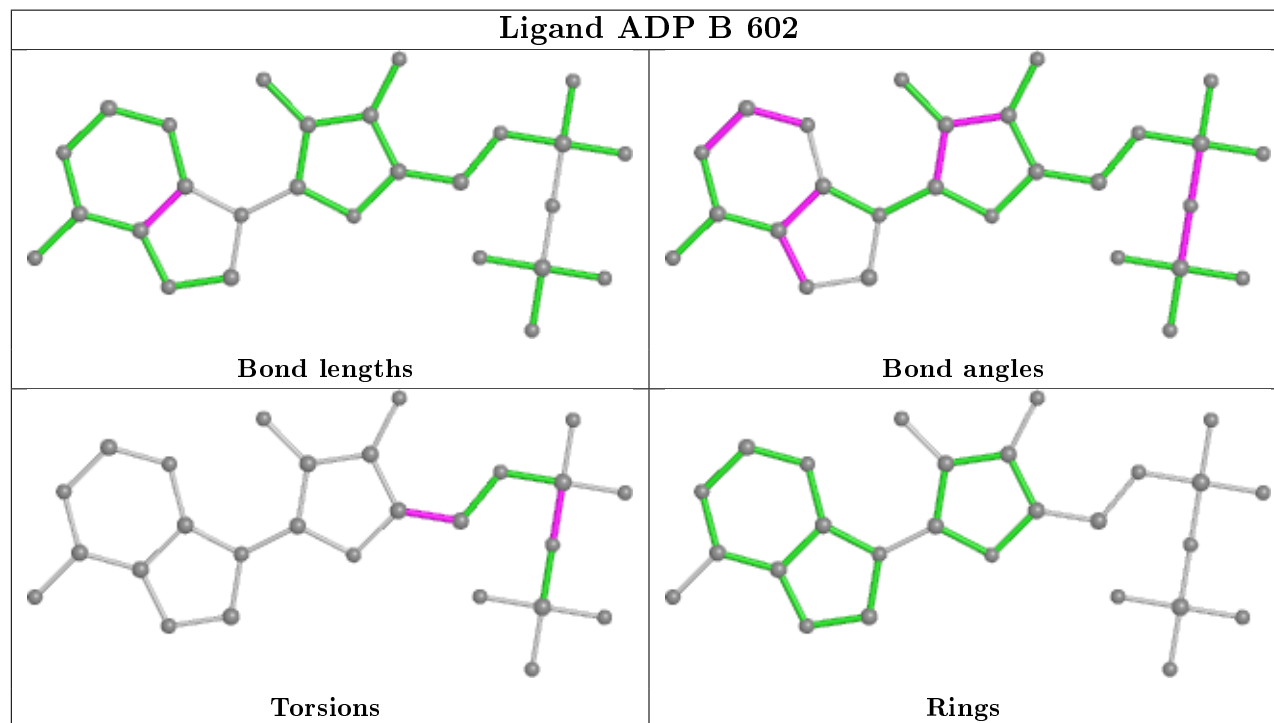
## Ligand ADP k 1102



## Ligand ADP e 602

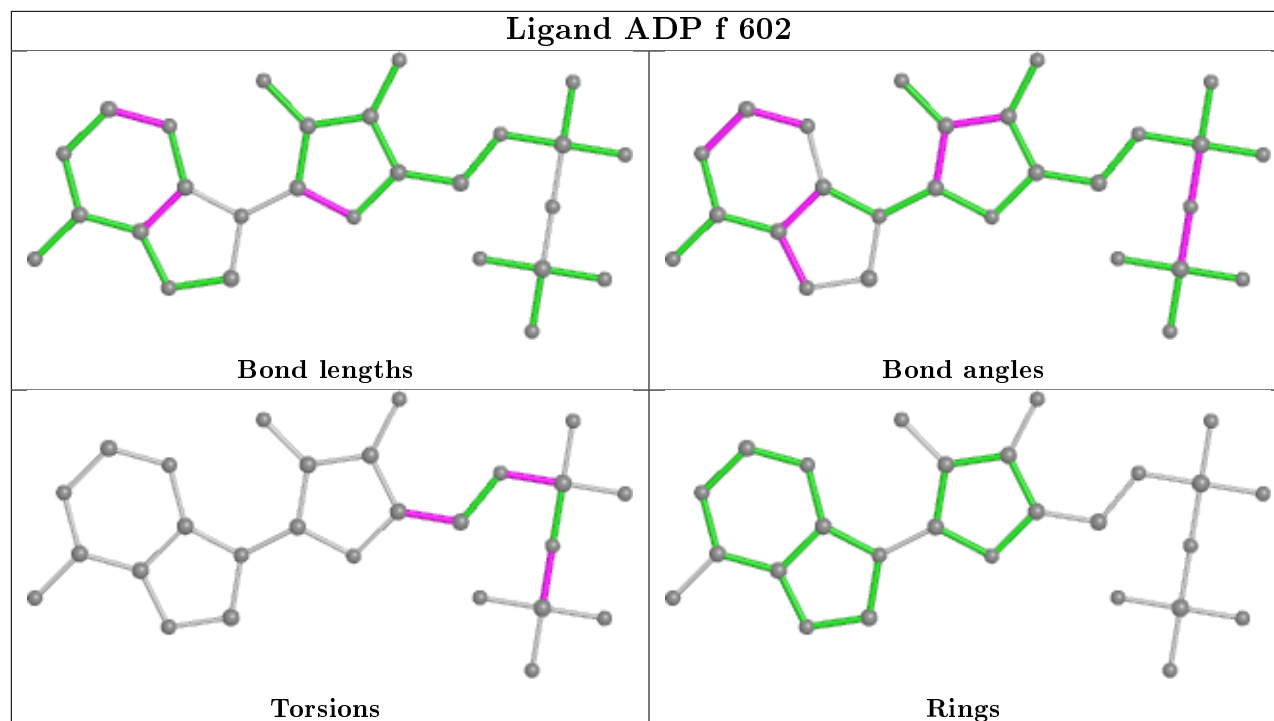


## Ligand ADP B 602

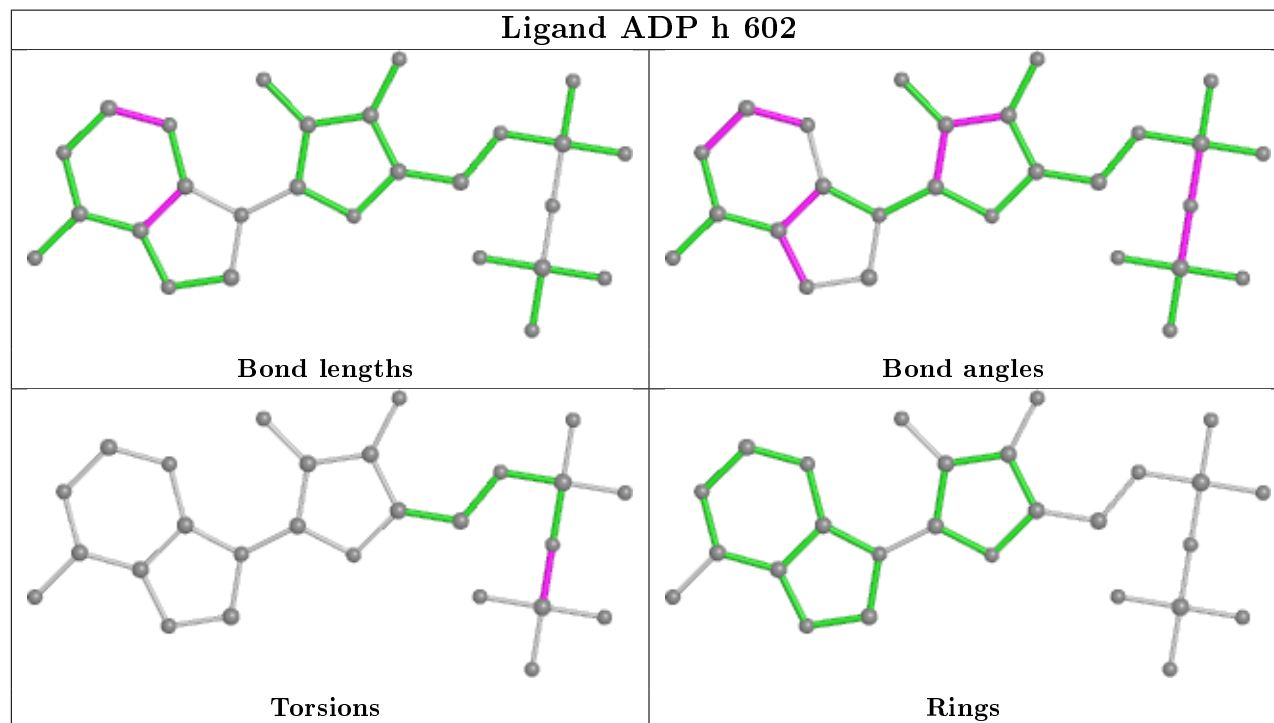


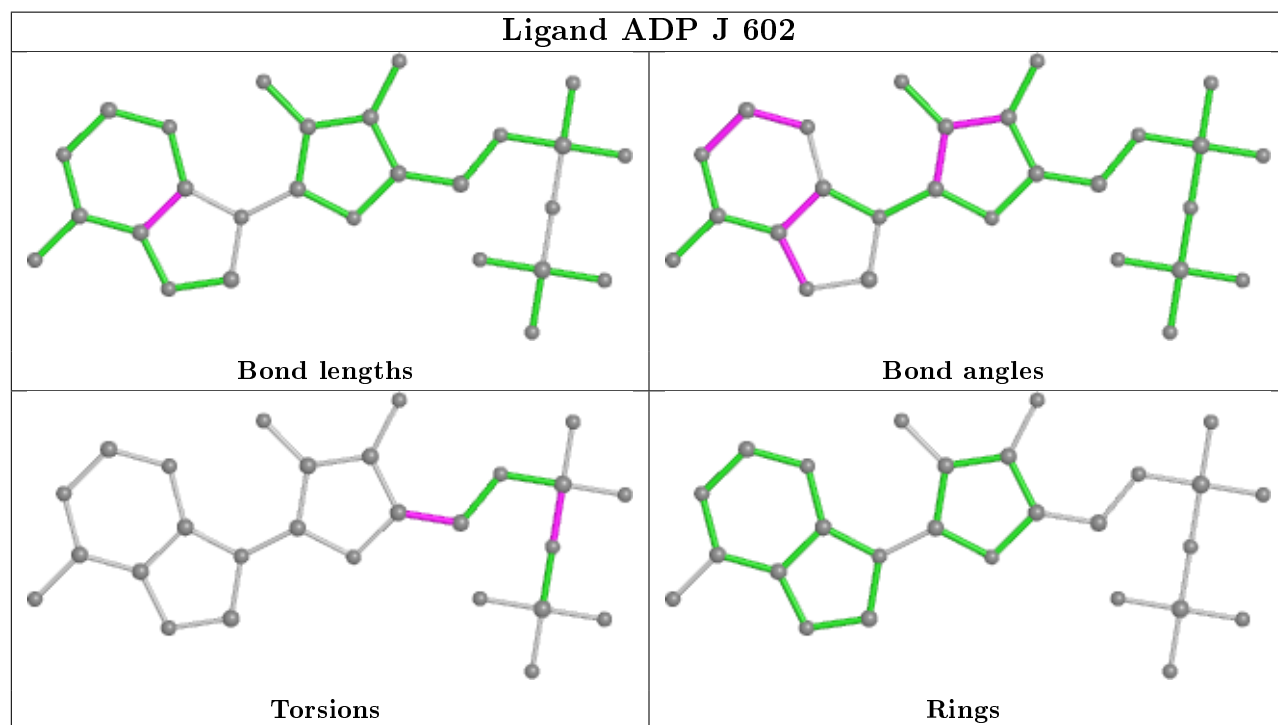
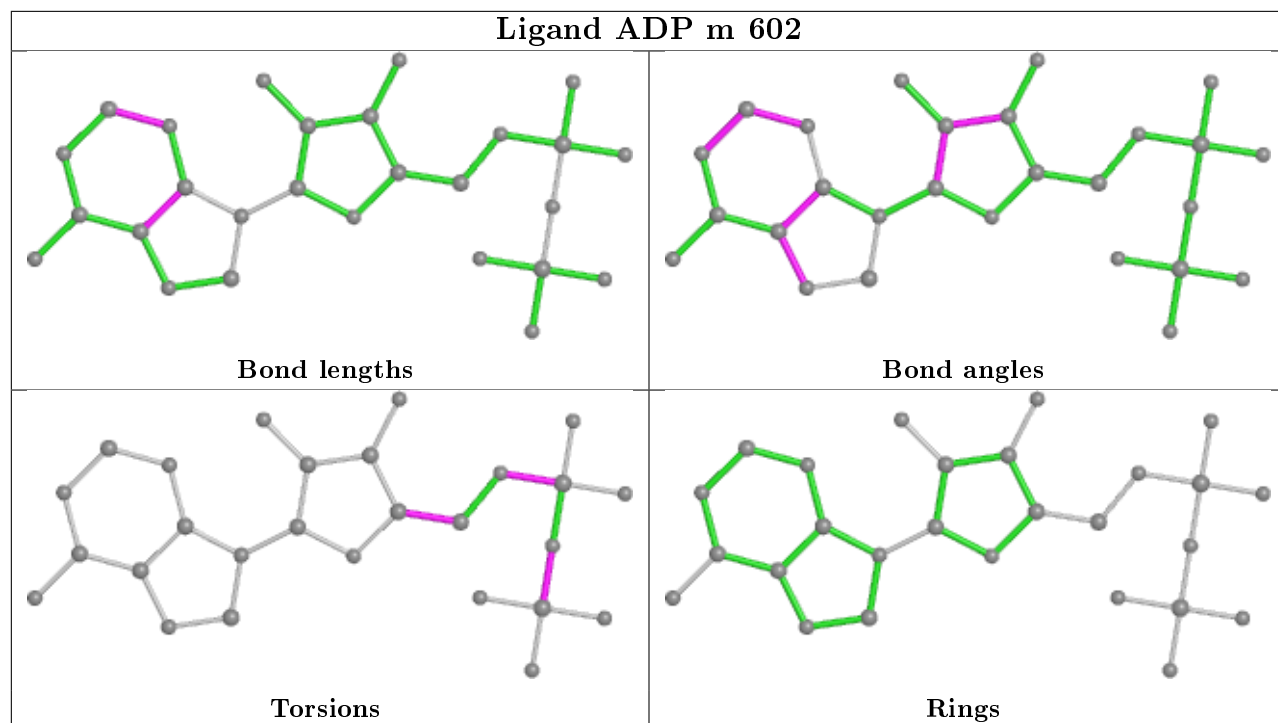


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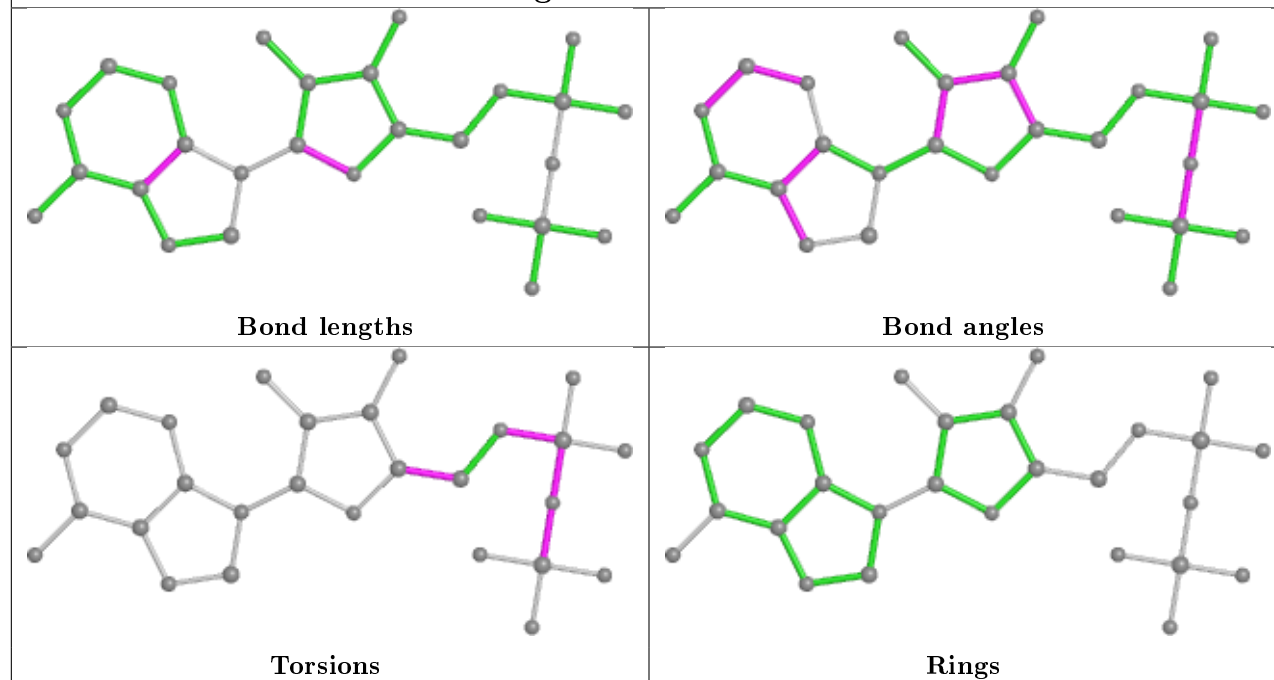


## Ligand ADP h 602

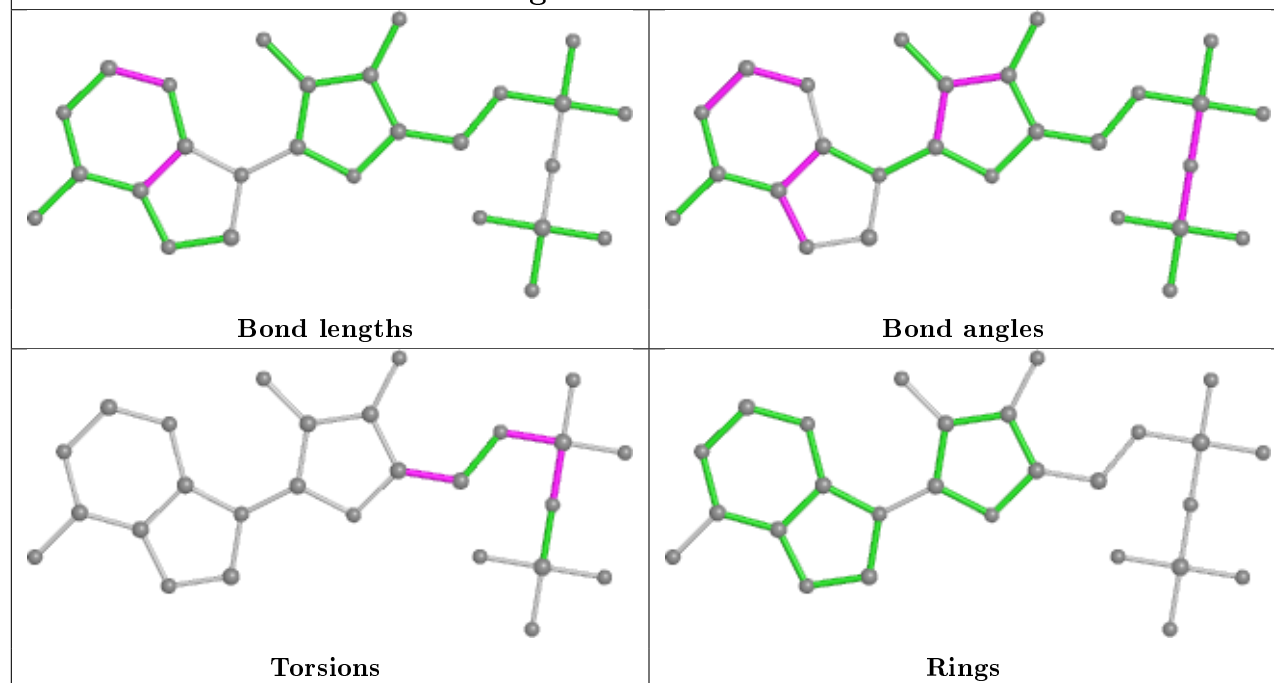




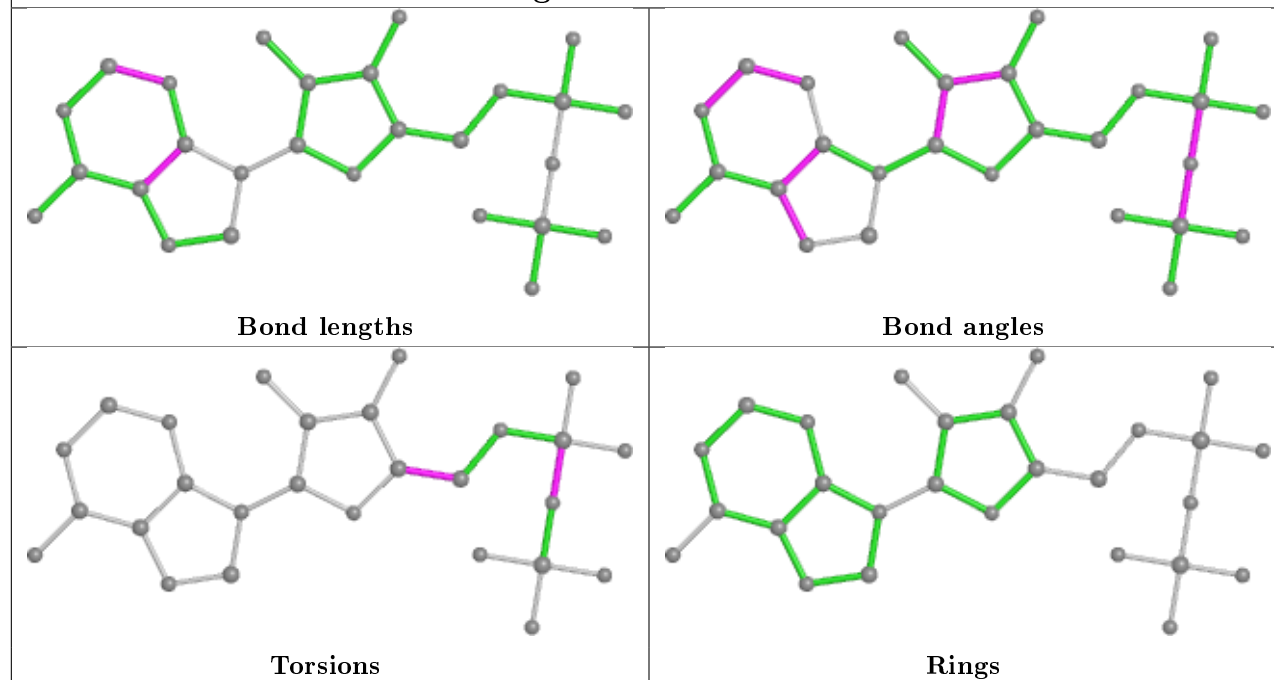
## Ligand ADP o 602



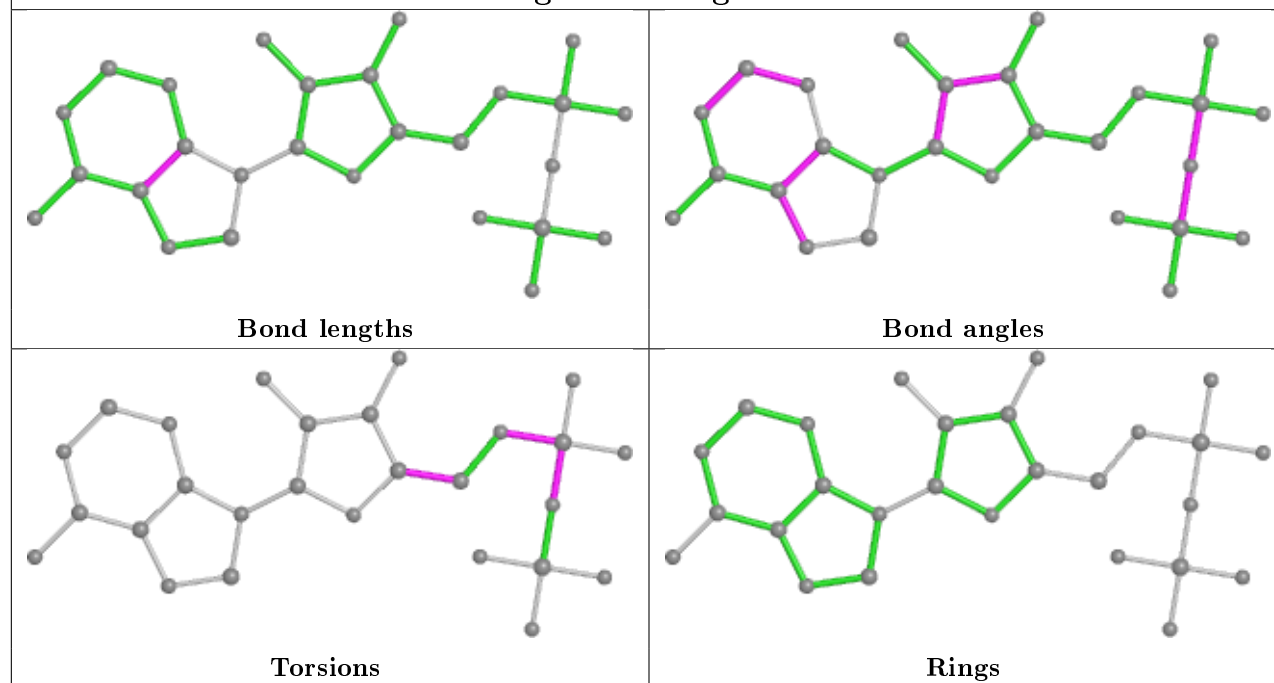
## Ligand ADP A 602

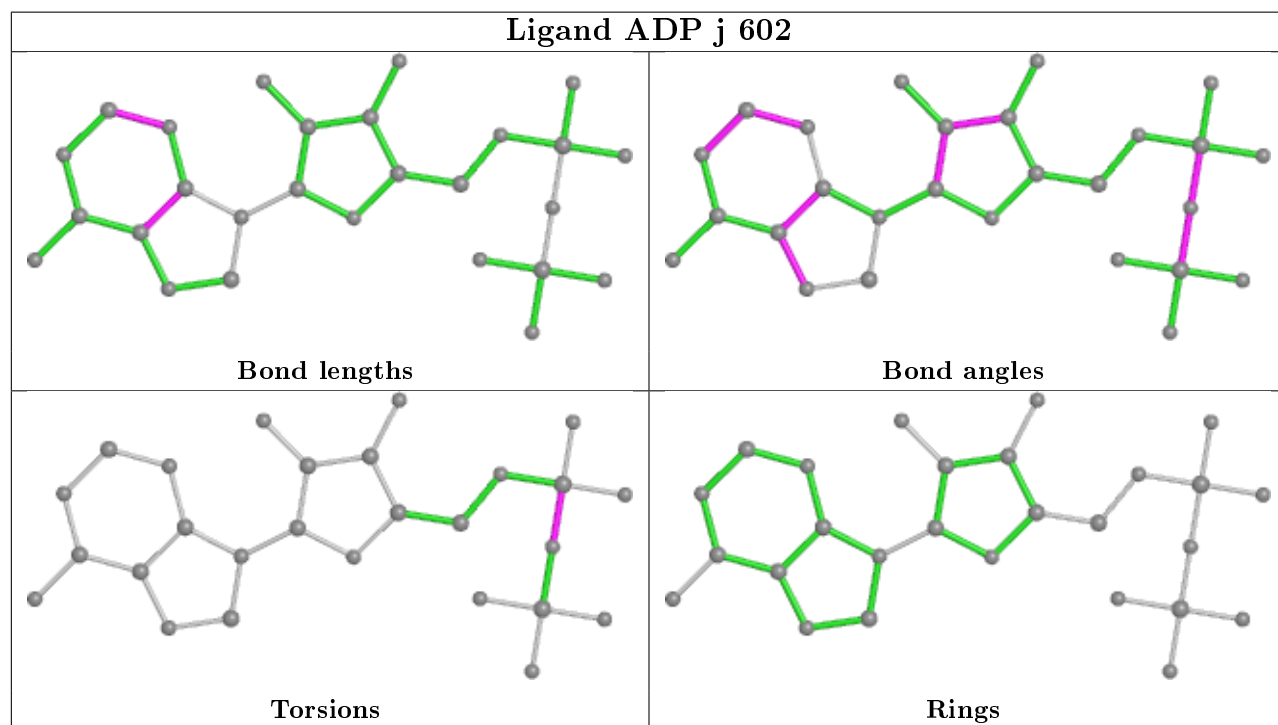
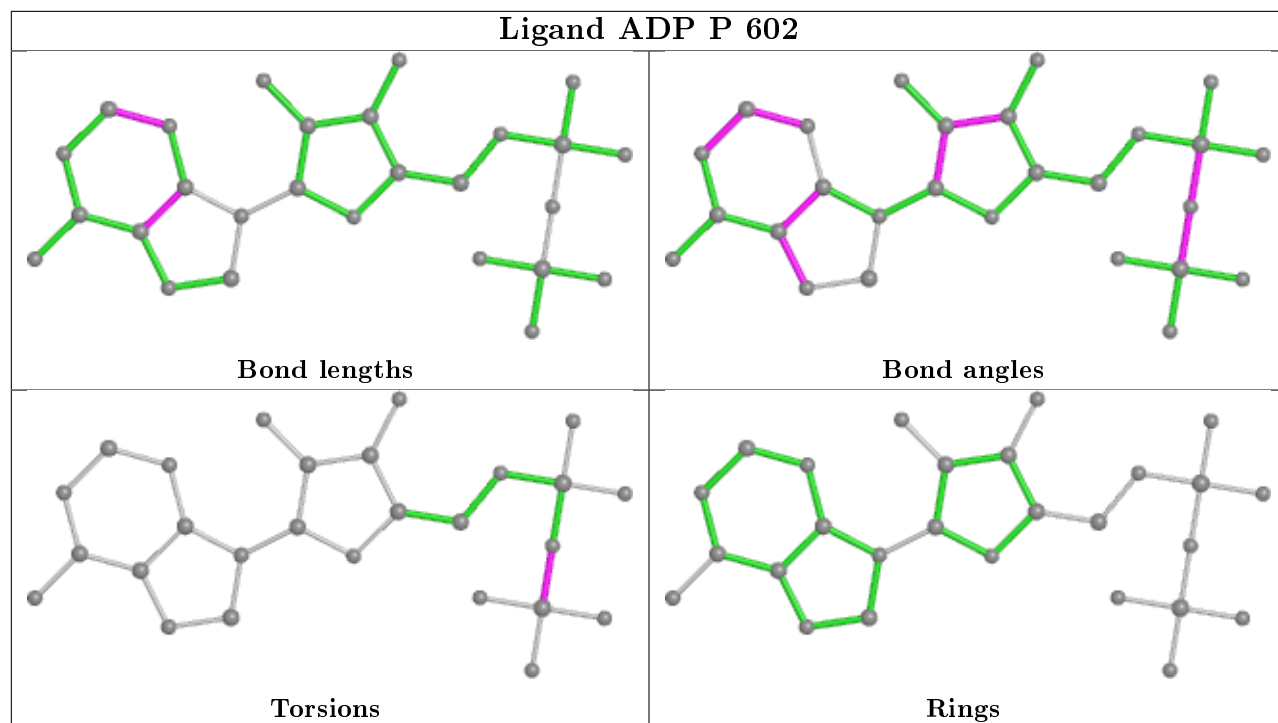


## Ligand ADP b 602

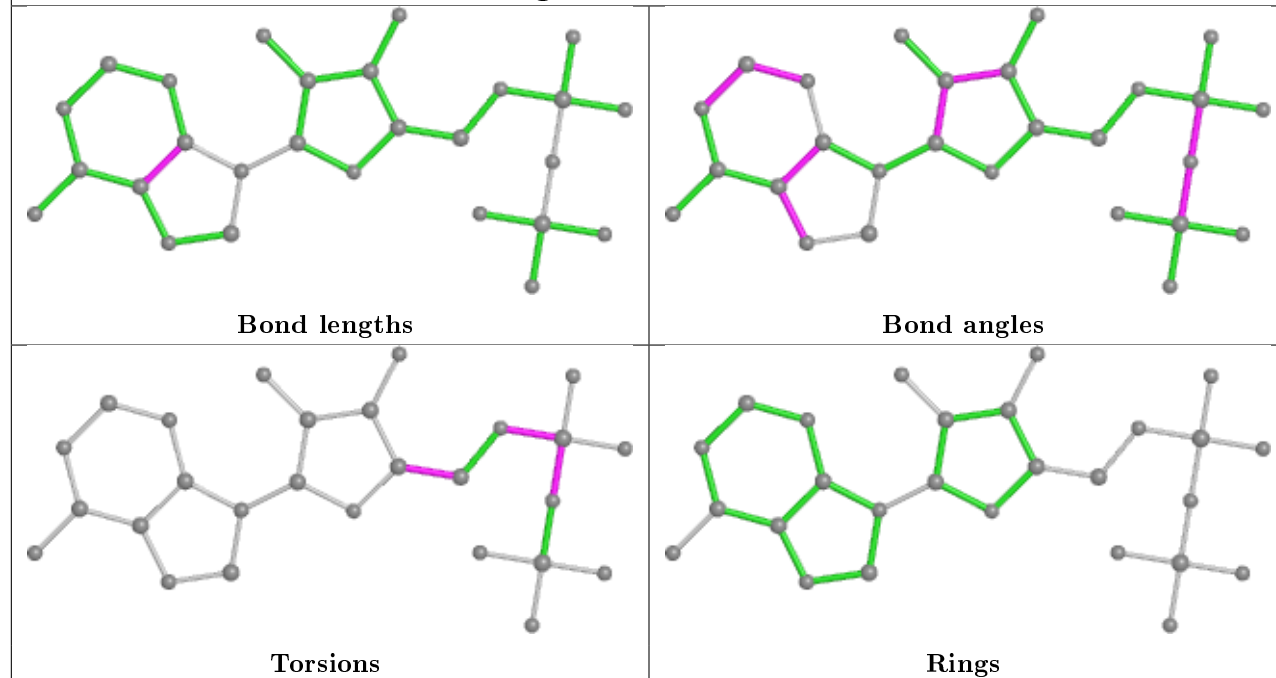


## Ligand ADP g 602

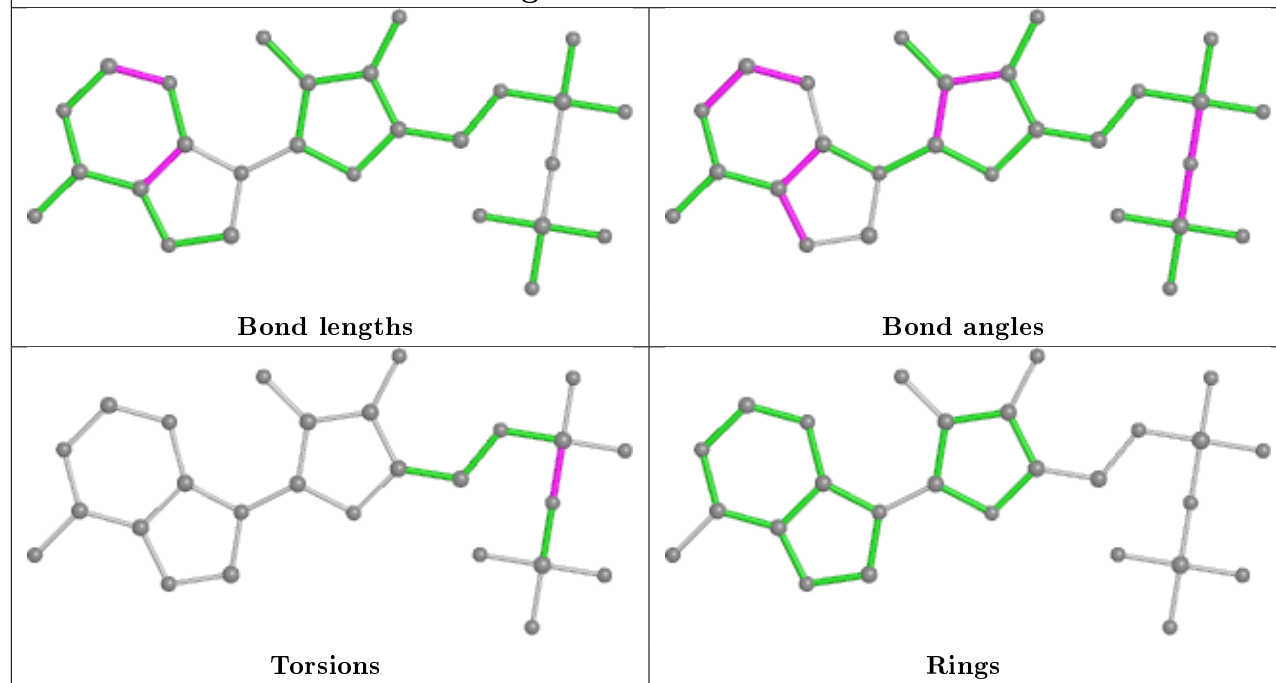




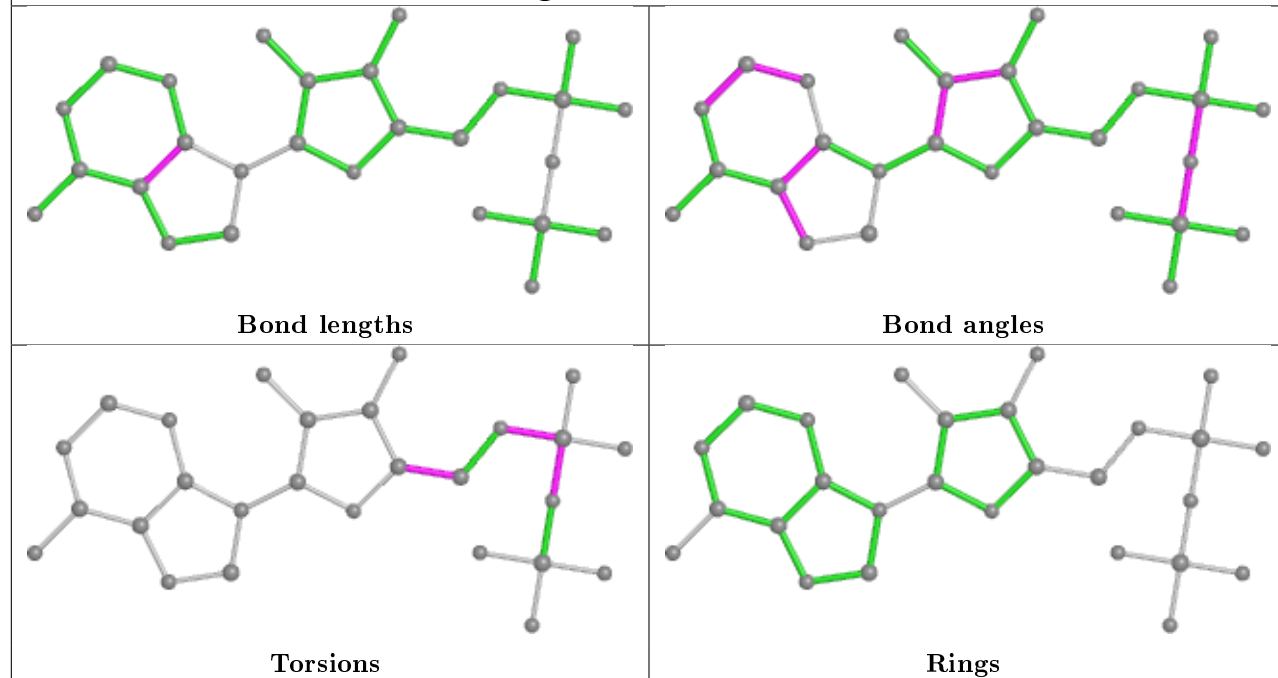
## Ligand ADP a 602



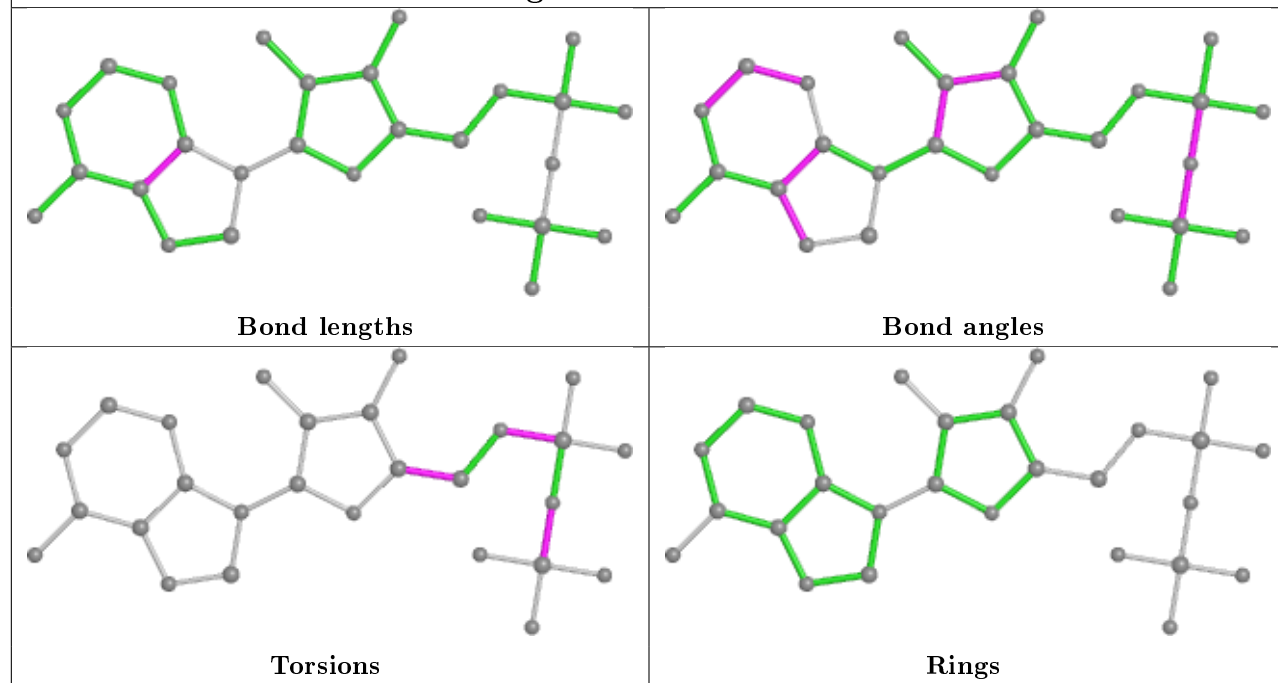
## Ligand ADP C 1102

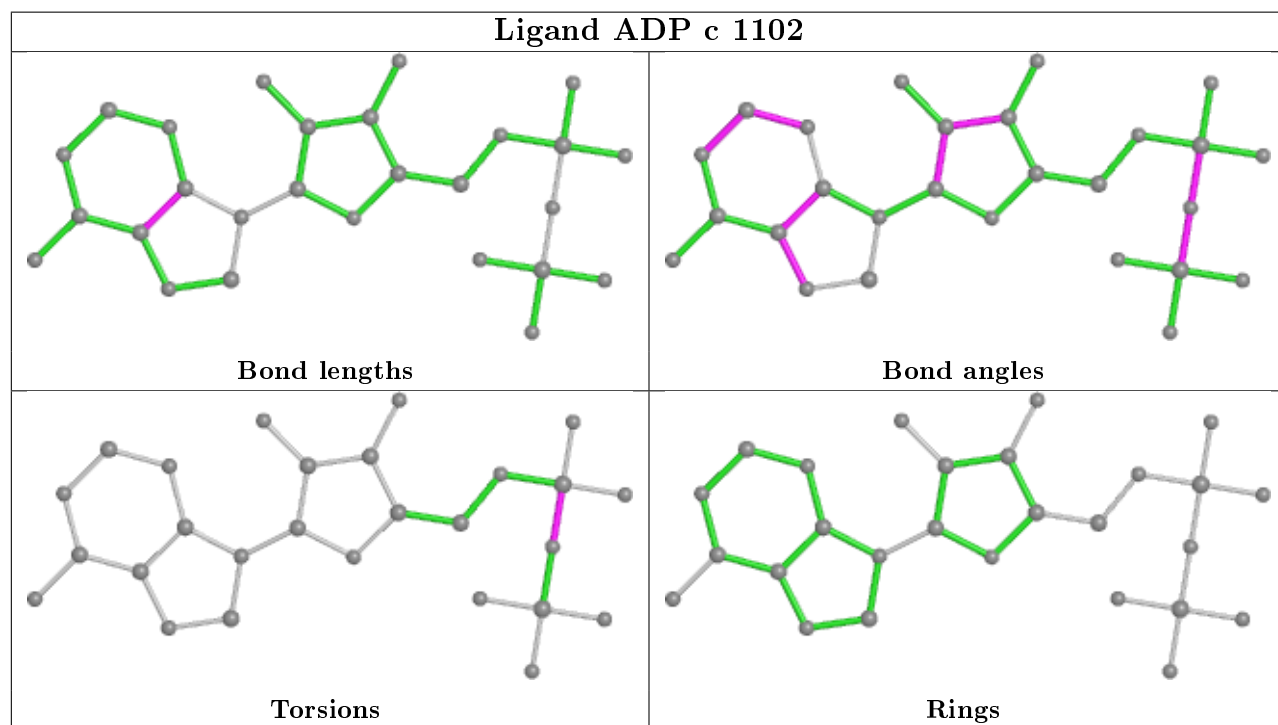
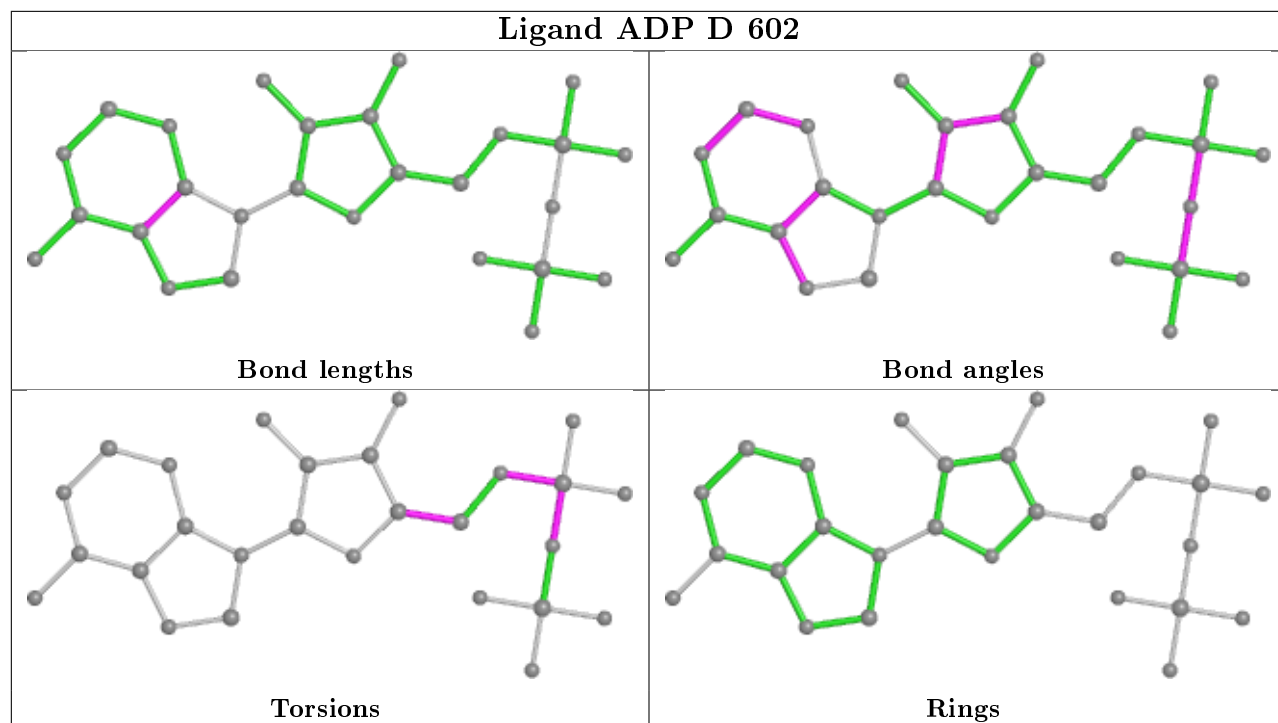


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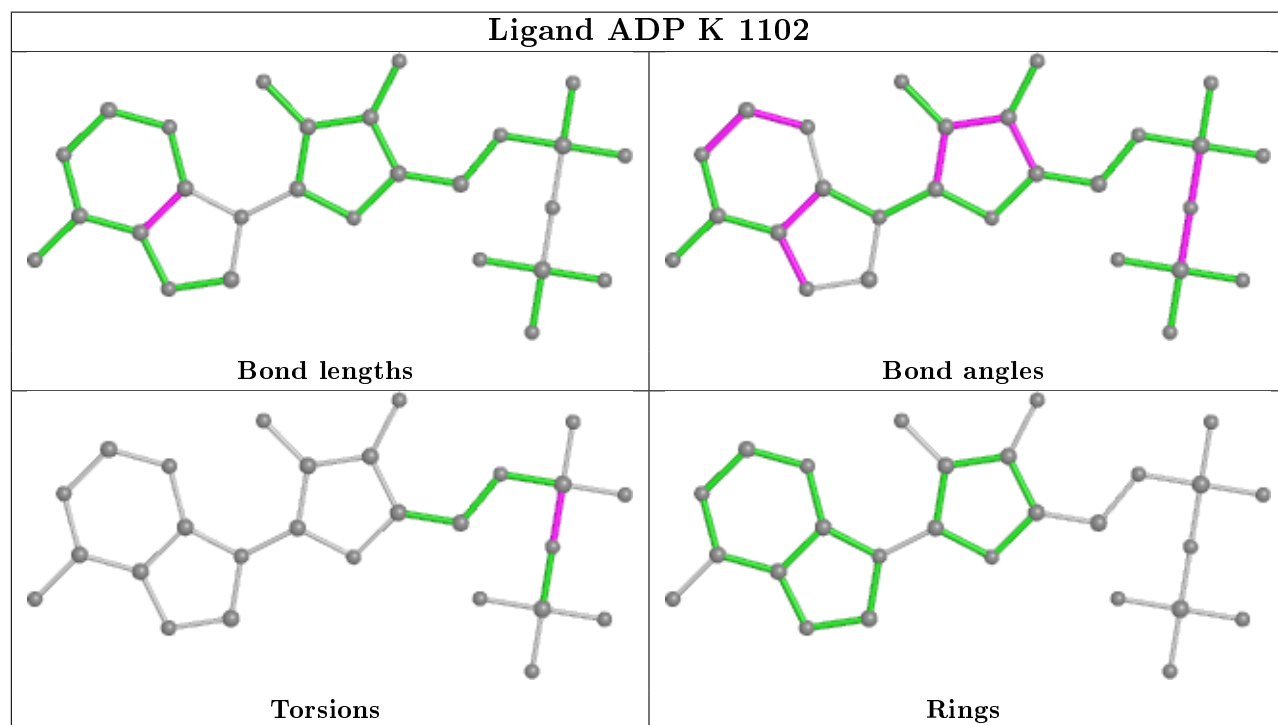
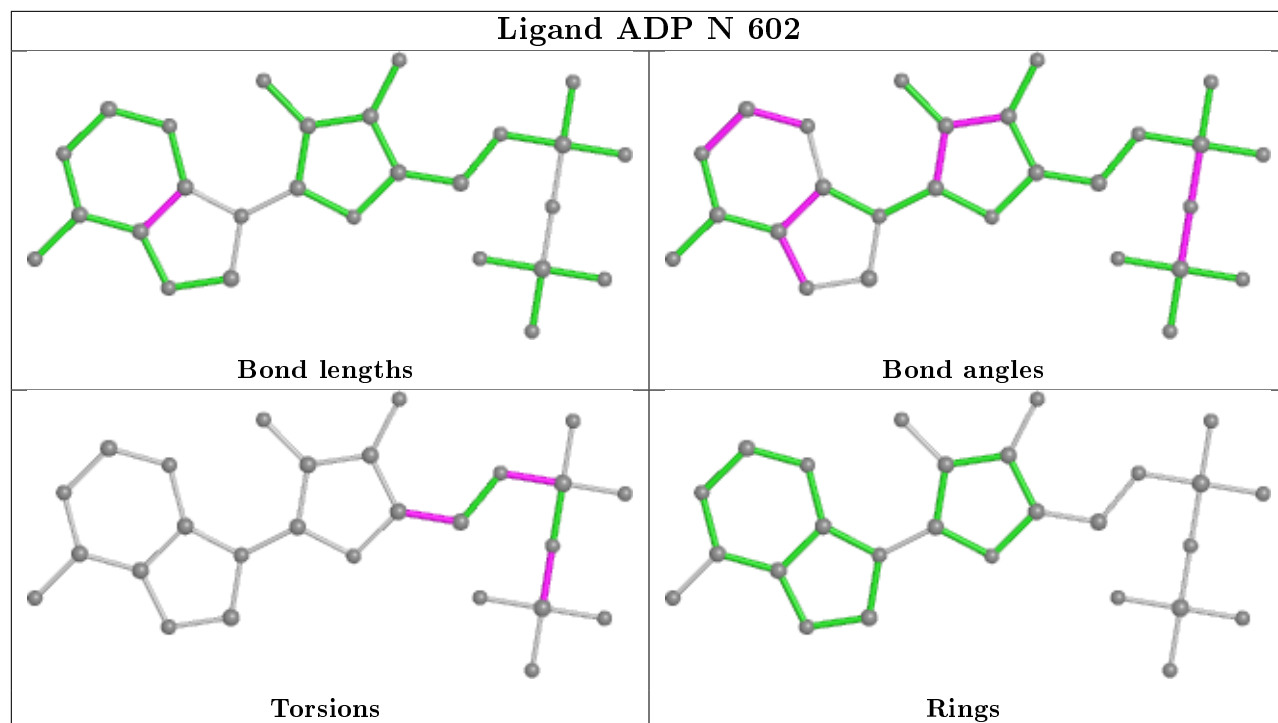


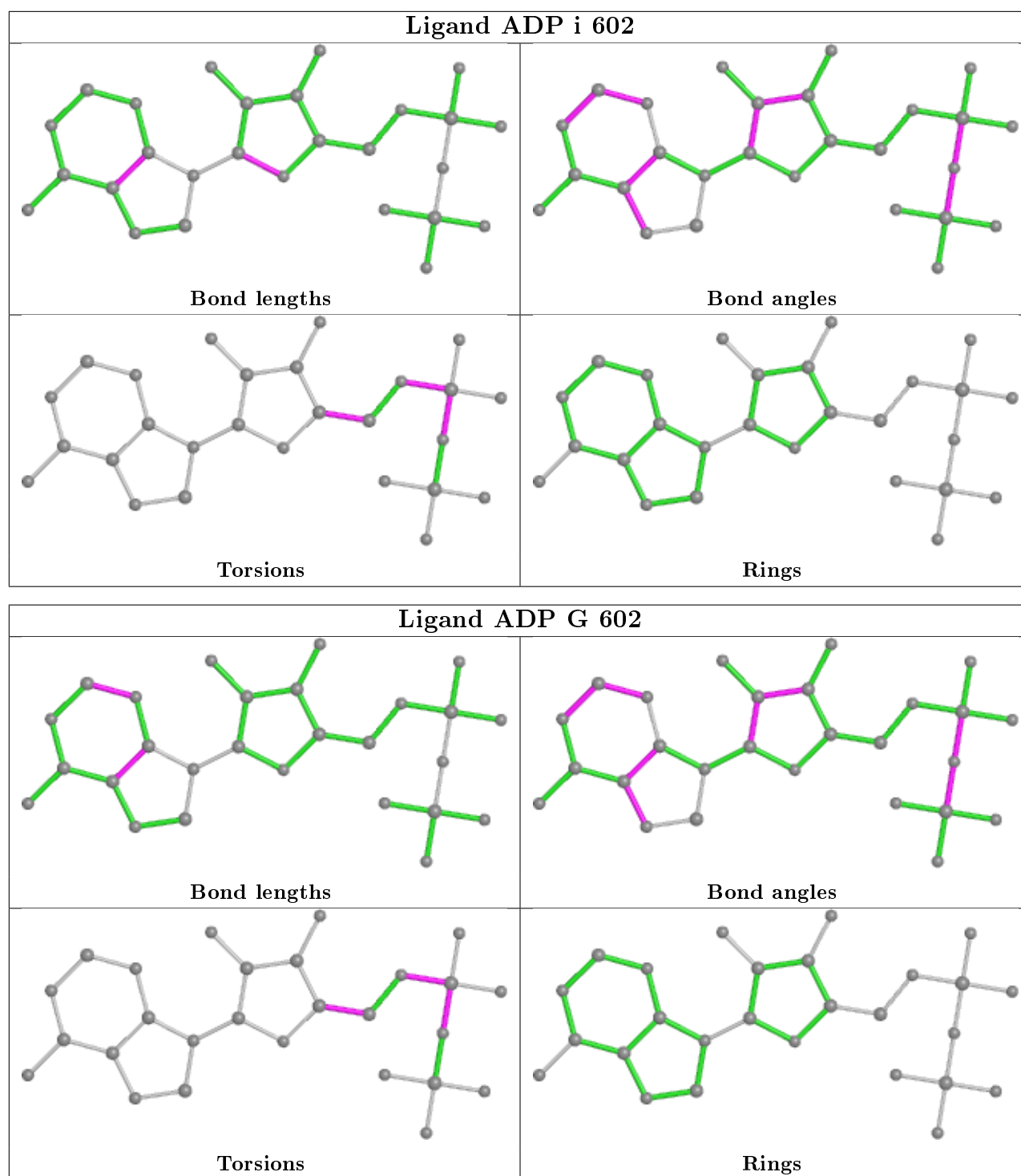
## Ligand ADP M 602











## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	F	538/546 (98%)	-0.40	3 (0%) 89 85	94, 122, 163, 189	0
1	N	538/546 (98%)	0.05	14 (2%) 56 47	111, 164, 220, 255	0
1	f	538/546 (98%)	0.06	14 (2%) 56 47	132, 160, 198, 229	0
1	n	538/546 (98%)	-0.15	9 (1%) 70 62	112, 129, 161, 201	0
2	H	521/568 (91%)	-0.34	0 100 100	94, 131, 172, 189	0
2	P	521/568 (91%)	-0.02	12 (2%) 60 52	119, 171, 234, 265	0
2	h	521/568 (91%)	-0.03	8 (1%) 73 66	133, 160, 194, 273	0
2	p	521/568 (91%)	-0.19	5 (0%) 82 76	101, 140, 177, 203	0
3	G	526/550 (95%)	-0.33	5 (0%) 82 76	95, 137, 174, 196	0
3	O	526/550 (95%)	-0.02	13 (2%) 57 49	106, 157, 253, 338	0
3	g	526/550 (95%)	-0.11	6 (1%) 80 74	115, 141, 181, 238	0
3	o	526/550 (95%)	-0.24	6 (1%) 80 74	99, 128, 174, 247	0
4	E	535/562 (95%)	-0.36	1 (0%) 95 94	88, 130, 172, 189	0
4	M	535/562 (95%)	-0.08	9 (1%) 70 62	106, 140, 233, 319	0
4	e	535/562 (95%)	-0.23	2 (0%) 92 89	100, 124, 173, 249	0
4	m	535/562 (95%)	-0.33	3 (0%) 89 85	94, 113, 161, 235	0
5	B	518/527 (98%)	-0.48	0 100 100	75, 100, 146, 172	0
5	J	518/527 (98%)	-0.16	2 (0%) 92 89	101, 127, 198, 249	0
5	b	518/527 (98%)	-0.27	2 (0%) 92 89	100, 116, 141, 176	0
5	j	518/527 (98%)	-0.28	0 100 100	90, 110, 131, 155	0
6	D	523/528 (99%)	-0.43	4 (0%) 86 81	78, 119, 153, 183	0
6	L	523/528 (99%)	0.06	10 (1%) 66 59	118, 160, 239, 313	0
6	d	523/528 (99%)	-0.13	8 (1%) 73 66	112, 136, 166, 182	0
6	l	523/528 (99%)	-0.26	4 (0%) 86 81	103, 129, 170, 196	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	A	539/559 (96%)	-0.37	5 (0%) 84 79	88, 120, 160, 203	0
7	I	539/559 (96%)	-0.02	12 (2%) 62 54	107, 144, 223, 317	0
7	a	539/559 (96%)	-0.12	8 (1%) 73 66	112, 135, 177, 208	0
7	i	539/559 (96%)	-0.21	8 (1%) 73 66	101, 132, 185, 212	0
8	C	513/590 (86%)	-0.34	5 (0%) 82 76	91, 121, 154, 181	0
8	K	513/590 (86%)	-0.10	12 (2%) 60 52	103, 150, 238, 312	0
8	c	513/590 (86%)	-0.02	14 (2%) 54 45	121, 143, 186, 223	0
8	k	513/590 (86%)	-0.16	10 (1%) 66 59	114, 131, 176, 246	0
All	All	16852/17720 (95%)	-0.19	214 (1%) 77 70	75, 134, 194, 338	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	292	GLY	6.2
8	K	1055	SER	6.0
1	f	142	ASN	5.7
4	M	289	ILE	5.6
8	K	264	GLU	5.6
8	K	1054	GLY	5.1
1	N	142	ASN	5.1
1	f	430	ASN	5.0
6	d	356	ASP	4.9
6	l	356	ASP	4.3
8	c	10	ALA	4.1
1	f	49	GLY	4.0
1	n	482	ASP	3.9
8	c	6	VAL	3.8
8	K	351	ASN	3.8
3	O	149	SER	3.7
4	M	461	GLN	3.7
8	K	199	ASP	3.7
2	h	19	ASN	3.7
7	I	293	ALA	3.5
8	c	9	ASN	3.5
2	P	151	THR	3.5
8	K	197	GLU	3.5
6	L	488	GLY	3.4
8	c	276	GLU	3.4
1	N	508	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
3	O	2	ASN	3.4
3	o	148	THR	3.3
3	o	2	ASN	3.3
8	K	261	ILE	3.2
2	h	53	LYS	3.2
7	I	194	GLY	3.2
1	n	432	ASN	3.2
3	g	16	GLY	3.2
1	N	291	LYS	3.2
1	f	435	GLY	3.2
7	a	485	GLN	3.2
3	O	148	THR	3.2
3	G	430	THR	3.2
6	L	185	ASN	3.2
8	k	434	LEU	3.1
4	e	461	GLN	3.1
3	g	258	GLU	3.1
2	h	154	ASN	3.1
8	c	434	LEU	3.0
7	A	198	TYR	3.0
8	C	434	LEU	3.0
6	d	182	SER	3.0
2	h	492	THR	2.9
6	L	208	GLU	2.9
7	a	439	THR	2.9
8	c	410	PRO	2.9
1	N	290	ASP	2.9
4	M	290	SER	2.9
8	c	1055	SER	2.9
1	N	435	GLY	2.9
6	L	369	ASN	2.9
3	O	261	VAL	2.9
1	f	436	ALA	2.9
7	i	7	ASN	2.9
1	n	496	GLY	2.8
6	L	356	ASP	2.8
1	N	232	TYR	2.8
7	a	294	GLN	2.8
7	I	264	ILE	2.8
2	p	204	VAL	2.8
6	l	371	ALA	2.8
8	k	9	ASN	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	n	142	ASN	2.8
2	p	154	ASN	2.8
1	N	250	GLY	2.8
8	c	183	ARG	2.8
2	P	354	LEU	2.7
6	L	355	SER	2.7
7	I	309	GLU	2.7
8	c	407	MET	2.7
3	o	252	ALA	2.7
1	f	248	ASN	2.7
7	a	166	SER	2.7
8	C	263	ILE	2.7
3	G	149	SER	2.7
2	h	191	PRO	2.7
8	k	11	SER	2.7
1	f	429	ALA	2.7
3	g	100	SER	2.7
1	n	250	GLY	2.7
1	f	345	PRO	2.7
1	N	359	ILE	2.6
8	K	462	GLY	2.6
5	b	260	GLN	2.6
1	F	142	ASN	2.6
1	n	483	SER	2.6
5	J	250	PHE	2.6
2	P	412	MET	2.6
7	A	264	ILE	2.6
7	I	292	GLY	2.6
1	n	484	ASP	2.6
1	F	188	ASN	2.6
7	a	491	ASP	2.6
8	c	254	LYS	2.6
7	I	490	GLU	2.6
6	d	371	ALA	2.6
4	m	461	GLN	2.6
2	h	229	ASN	2.6
6	L	526	PHE	2.6
1	N	464	PHE	2.6
6	L	95	SER	2.6
6	d	370	ASN	2.6
8	c	531	ARG	2.6
4	e	28	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
7	a	264	ILE	2.5
3	O	289	GLY	2.5
2	h	153	LYS	2.5
8	K	11	SER	2.5
6	D	371	ALA	2.5
4	E	190	SER	2.5
1	f	358	THR	2.5
3	O	147	ILE	2.5
7	a	489	PRO	2.5
2	P	345	GLY	2.5
3	g	430	THR	2.5
4	m	37	ASN	2.5
8	k	307	HIS	2.5
3	o	4	GLY	2.5
2	P	242	ASP	2.5
8	C	199	ASP	2.5
8	K	260	ASN	2.5
7	I	340	SER	2.5
2	h	151	THR	2.5
3	G	157	LEU	2.4
8	k	433	GLN	2.4
7	I	489	PRO	2.4
8	k	1055	SER	2.4
3	g	192	ASN	2.4
4	M	460	LYS	2.4
2	p	506	ASP	2.4
1	N	498	SER	2.4
7	I	389	GLY	2.4
1	f	522	GLY	2.4
3	O	267	TYR	2.4
4	M	390	ASP	2.4
7	i	3	GLN	2.4
1	n	430	ASN	2.4
6	d	369	ASN	2.4
7	a	495	ARG	2.4
1	N	249	SER	2.4
2	P	366	ASP	2.4
3	G	460	ASP	2.4
1	N	143	LEU	2.4
3	O	430	THR	2.4
4	m	507	ILE	2.3
4	M	266	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	p	440	ARG	2.3
7	i	490	GLU	2.3
8	c	58	THR	2.3
4	M	26	GLY	2.3
6	l	369	ASN	2.3
7	i	346	GLY	2.3
2	P	506	ASP	2.3
8	C	489	GLY	2.3
3	o	147	ILE	2.3
8	c	496	SER	2.3
7	i	440	VAL	2.3
7	i	489	PRO	2.3
2	P	357	THR	2.3
6	d	255	ASN	2.3
1	f	216	ASP	2.3
2	p	441	THR	2.3
3	O	306	PHE	2.3
7	i	491	ASP	2.2
7	i	15	LEU	2.2
1	f	432	ASN	2.2
6	l	185	ASN	2.2
6	D	292	ILE	2.2
6	D	186	SER	2.2
6	L	218	THR	2.2
4	M	39	LYS	2.2
6	L	188	ASN	2.2
6	D	369	ASN	2.2
2	P	267	LEU	2.2
8	K	1056	GLY	2.2
8	c	7	PHE	2.2
3	G	487	ASN	2.2
3	O	158	LEU	2.2
6	d	189	VAL	2.2
8	k	8	MET	2.1
5	J	344	GLU	2.1
7	I	260	VAL	2.1
7	A	256	MET	2.1
1	f	525	SER	2.1
2	P	498	GLY	2.1
3	o	149	SER	2.1
8	k	477	GLN	2.1
2	P	444	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	M	218	ASP	2.1
7	I	487	ALA	2.1
3	O	432	ALA	2.1
3	O	431	ILE	2.1
8	K	198	ILE	2.1
8	k	49	LEU	2.1
3	g	497	TRP	2.0
1	F	152	GLN	2.0
1	n	360	GLY	2.0
7	A	194	GLY	2.0
7	A	265	ASP	2.0
2	P	343	ARG	2.0
1	N	486	THR	2.0
3	O	290	ALA	2.0
5	b	278	LYS	2.0
7	I	248	ASP	2.0
8	k	435	GLU	2.0
8	C	198	ILE	2.0
6	d	185	ASN	2.0
1	f	312	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MG	h	601	1/1	0.83	0.22	151,151,151,151	0
10	ADP	c	1102	27/27	0.85	0.35	134,138,142,143	0
10	ADP	k	1102	27/27	0.89	0.33	115,117,120,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	ADP	C	1102	27/27	0.90	0.31	100,111,118,119	0
10	ADP	L	602	27/27	0.90	0.28	135,138,144,147	0
10	ADP	N	602	27/27	0.90	0.39	133,145,153,154	0
11	BEF	h	603	4/4	0.91	0.17	55,55,55,55	0
10	ADP	J	602	27/27	0.91	0.29	104,108,113,113	0
9	MG	N	601	1/1	0.92	0.70	132,132,132,132	0
10	ADP	M	602	27/27	0.93	0.30	104,111,114,115	0
10	ADP	m	602	27/27	0.93	0.26	102,106,108,109	0
11	BEF	L	603	4/4	0.93	0.31	135,138,138,141	0
10	ADP	g	602	27/27	0.93	0.36	132,141,149,150	0
9	MG	c	1101	1/1	0.93	0.38	129,129,129,129	0
10	ADP	b	602	27/27	0.93	0.36	104,109,115,115	0
9	MG	o	601	1/1	0.93	0.35	115,115,115,115	0
10	ADP	P	602	27/27	0.93	0.28	136,143,148,149	0
10	ADP	f	602	27/27	0.93	0.27	149,154,159,160	0
10	ADP	F	602	27/27	0.93	0.24	97,105,112,113	0
9	MG	L	601	1/1	0.94	0.40	124,124,124,124	0
10	ADP	d	602	27/27	0.94	0.36	125,135,149,151	0
10	ADP	j	602	27/27	0.94	0.36	94,100,106,107	0
10	ADP	A	602	27/27	0.94	0.30	98,113,126,127	0
10	ADP	a	602	27/27	0.94	0.33	126,139,146,148	0
10	ADP	l	602	27/27	0.94	0.37	117,129,144,145	0
10	ADP	O	602	27/27	0.94	0.34	109,115,120,121	0
10	ADP	n	602	27/27	0.94	0.20	112,116,123,124	0
11	BEF	N	603	4/4	0.94	0.30	132,135,135,137	0
10	ADP	i	602	27/27	0.94	0.29	113,121,126,127	0
10	ADP	p	602	27/27	0.94	0.34	133,145,154,156	0
10	ADP	e	602	27/27	0.94	0.35	117,124,127,128	0
10	ADP	B	602	27/27	0.94	0.29	78,83,86,87	0
10	ADP	I	602	27/27	0.94	0.28	121,126,133,135	0
10	ADP	h	602	27/27	0.94	0.32	152,159,166,167	0
10	ADP	K	1102	27/27	0.94	0.28	122,131,144,147	0
10	ADP	G	602	27/27	0.95	0.33	111,127,140,142	0
11	BEF	e	603	4/4	0.95	0.40	114,114,116,118	0
10	ADP	E	602	27/27	0.95	0.27	102,115,123,124	0
10	ADP	o	602	27/27	0.95	0.33	119,128,133,134	0
11	BEF	c	1103	4/4	0.95	0.42	126,127,127,129	0
10	ADP	D	602	27/27	0.95	0.24	95,106,120,123	0
11	BEF	K	1103	4/4	0.95	0.36	118,120,120,123	0
10	ADP	H	602	27/27	0.95	0.26	106,117,128,130	0
9	MG	O	601	1/1	0.96	0.32	113,113,113,113	0
11	BEF	p	603	4/4	0.96	0.26	130,132,133,133	0

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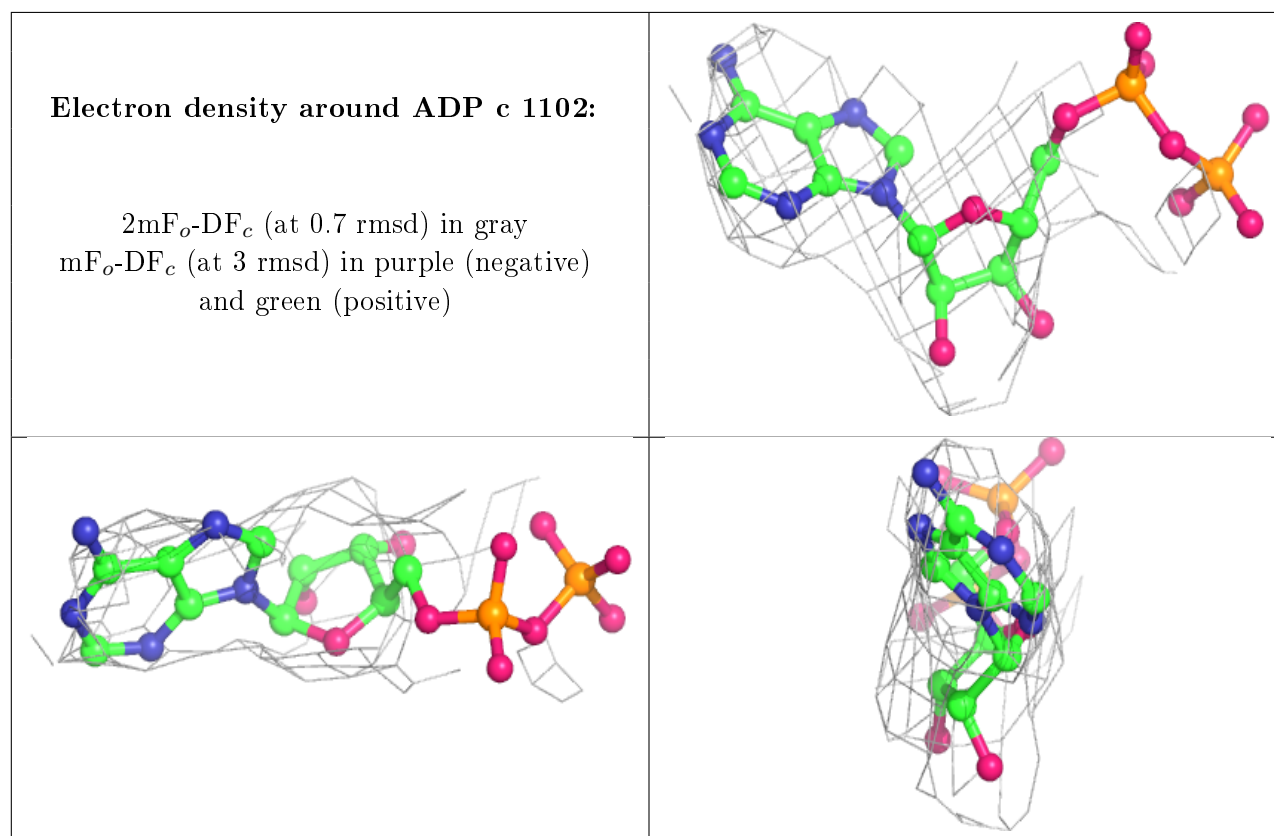
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	BEF	O	603	4/4	0.96	0.46	117,118,119,120	0
9	MG	K	1101	1/1	0.96	0.39	126,126,126,126	0
9	MG	d	601	1/1	0.96	0.59	115,115,115,115	0
11	BEF	f	603	4/4	0.96	0.23	152,152,154,156	0
11	BEF	g	603	4/4	0.96	0.45	128,132,132,134	0
11	BEF	k	1103	4/4	0.96	0.50	110,111,111,112	0
11	BEF	o	603	4/4	0.96	0.31	116,118,119,119	0
11	BEF	E	603	4/4	0.97	0.41	98,98,100,102	0
11	BEF	i	603	4/4	0.97	0.30	104,105,105,106	0
9	MG	g	601	1/1	0.97	0.46	129,129,129,129	0
11	BEF	m	603	4/4	0.97	0.33	99,100,101,103	0
11	BEF	J	603	4/4	0.97	0.41	110,112,113,114	0
11	BEF	n	603	4/4	0.97	0.21	115,115,116,118	0
11	BEF	I	603	4/4	0.97	0.34	119,119,120,122	0
11	BEF	M	603	4/4	0.98	0.26	111,113,114,116	0
11	BEF	D	603	4/4	0.98	0.29	89,89,91,94	0
11	BEF	j	603	4/4	0.98	0.37	93,94,94,96	0
9	MG	l	601	1/1	0.98	0.49	107,107,107,107	0
11	BEF	l	603	4/4	0.98	0.46	107,110,111,111	0
11	BEF	C	1103	4/4	0.98	0.42	91,92,93,94	0
11	BEF	d	603	4/4	0.98	0.43	116,120,121,121	0
11	BEF	P	603	4/4	0.98	0.24	140,141,142,145	0
9	MG	m	601	1/1	0.98	0.32	84,84,84,84	0
9	MG	a	601	1/1	0.98	0.45	126,126,126,126	0
9	MG	F	601	1/1	0.98	0.25	94,94,94,94	0
11	BEF	A	603	4/4	0.98	0.37	91,91,92,95	0
9	MG	n	601	1/1	0.98	0.15	108,108,108,108	0
11	BEF	H	603	4/4	0.98	0.28	105,106,106,108	0
9	MG	i	601	1/1	0.98	0.29	111,111,111,111	0
11	BEF	b	603	4/4	0.98	0.37	103,105,105,107	0
11	BEF	a	603	4/4	0.98	0.40	118,120,121,121	0
11	BEF	G	603	4/4	0.98	0.45	110,110,112,116	0
11	BEF	F	603	4/4	0.98	0.22	99,101,101,102	0
9	MG	p	601	1/1	0.98	0.26	131,131,131,131	0
9	MG	I	601	1/1	0.99	0.38	121,121,121,121	0
9	MG	P	601	1/1	0.99	0.20	140,140,140,140	0
9	MG	b	601	1/1	0.99	0.56	97,97,97,97	0
11	BEF	B	603	4/4	0.99	0.40	76,77,77,78	0
9	MG	f	601	1/1	0.99	0.34	143,143,143,143	0
9	MG	k	1101	1/1	0.99	0.38	111,111,111,111	0
9	MG	C	1101	1/1	0.99	0.28	99,99,99,99	0
9	MG	M	601	1/1	0.99	0.25	96,96,96,96	0

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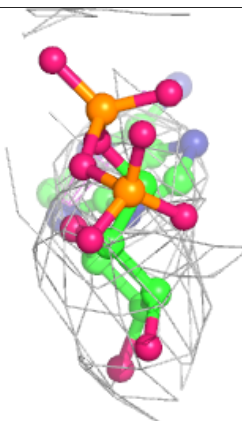
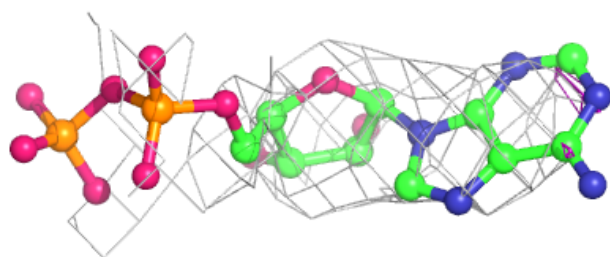
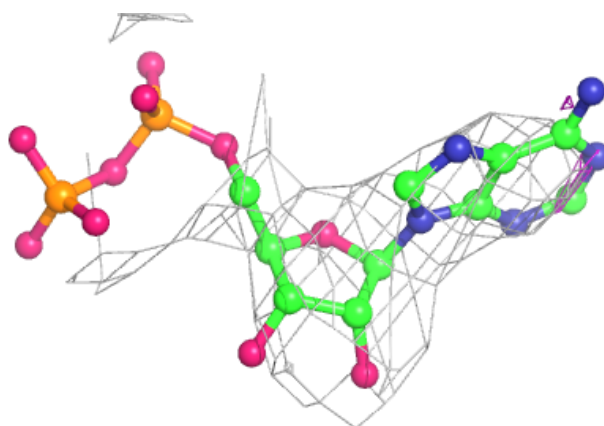
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MG	J	601	1/1	0.99	0.31	101,101,101,101	0
9	MG	j	601	1/1	0.99	0.40	88,88,88,88	0
9	MG	E	601	1/1	0.99	0.33	91,91,91,91	0
9	MG	B	601	1/1	0.99	0.21	70,70,70,70	0
9	MG	e	601	1/1	0.99	0.41	102,102,102,102	0
9	MG	A	601	1/1	0.99	0.37	102,102,102,102	0
9	MG	G	601	1/1	0.99	0.30	113,113,113,113	0
9	MG	D	601	1/1	1.00	0.26	89,89,89,89	0
9	MG	H	601	1/1	1.00	0.20	109,109,109,109	0

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

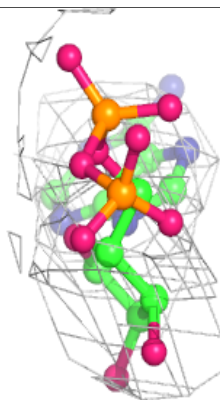
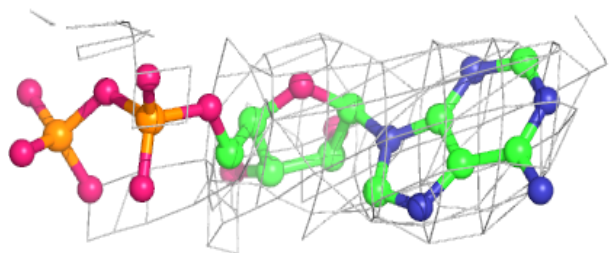


**Electron density around ADP k 1102:**

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

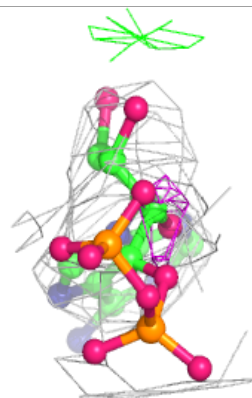
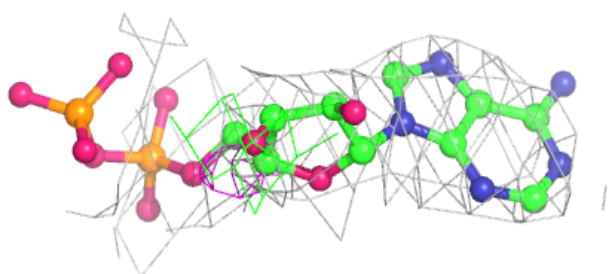
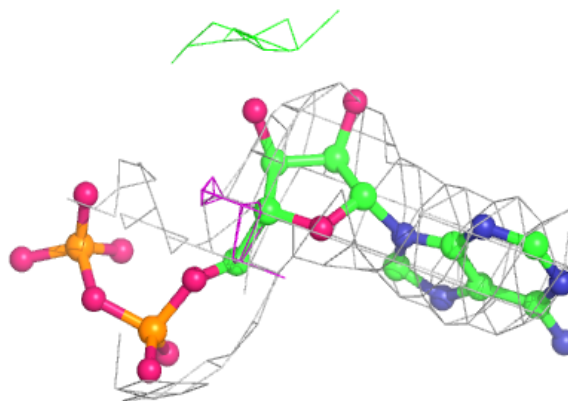
**Electron density around ADP C 1102:**

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

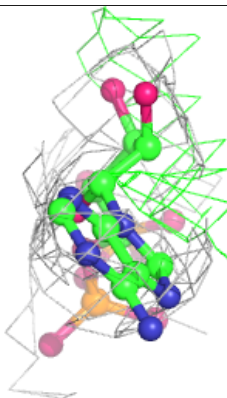
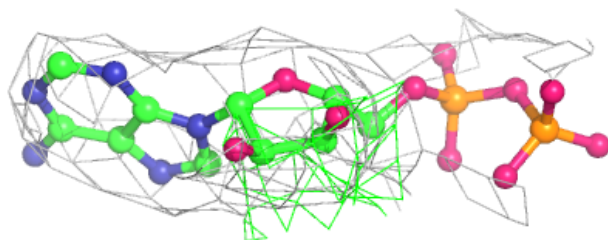
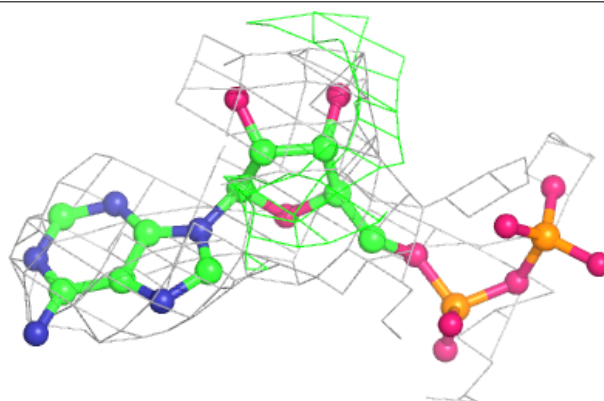


**Electron density around ADP L 602:**

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

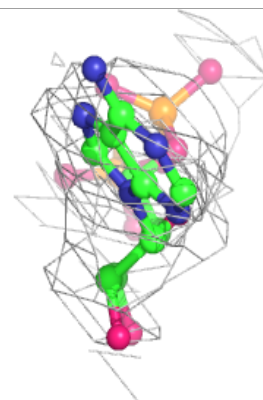
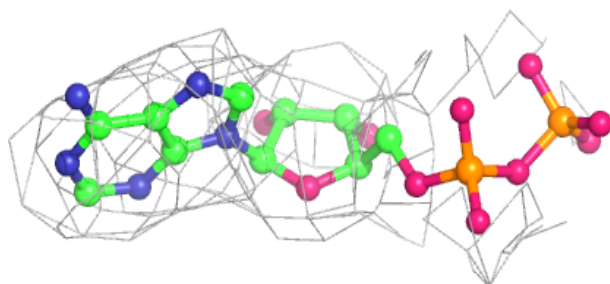
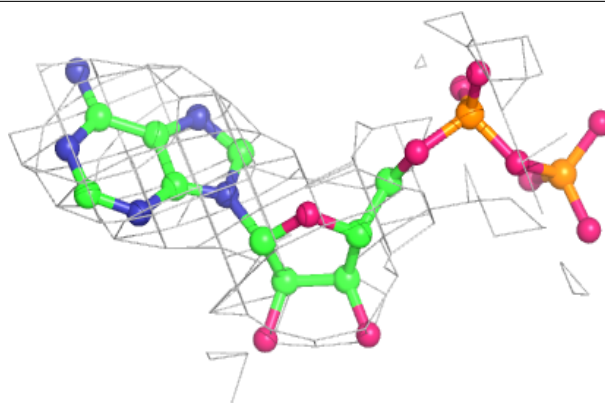
**Electron density around ADP N 602:**

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

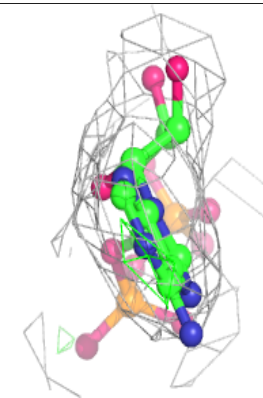
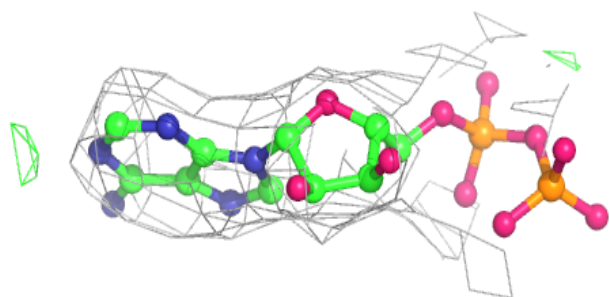
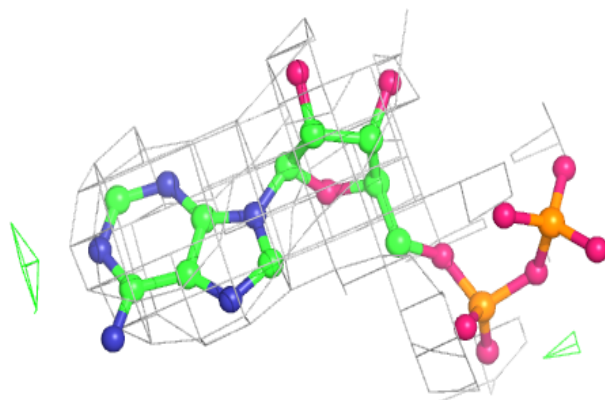


**Electron density around ADP J 602:**

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

**Electron density around ADP M 602:**

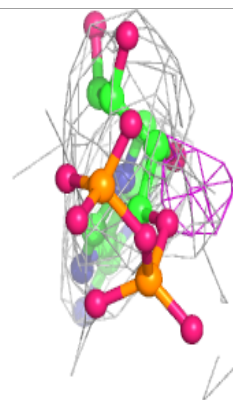
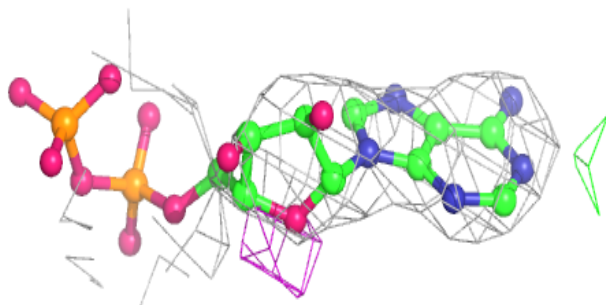
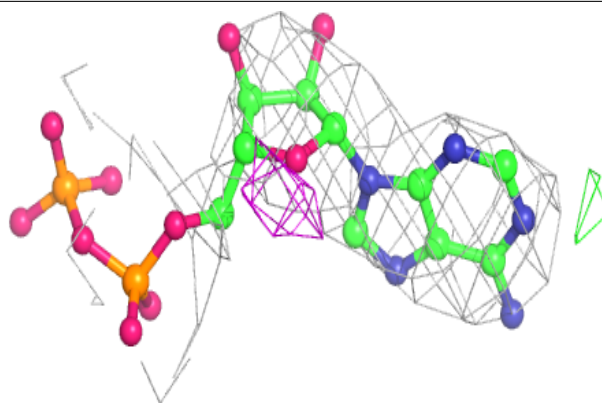
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



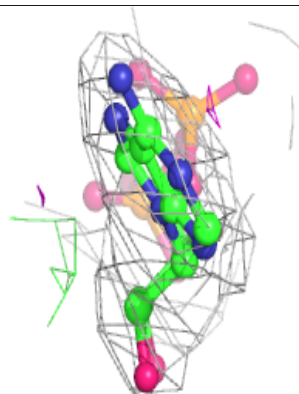
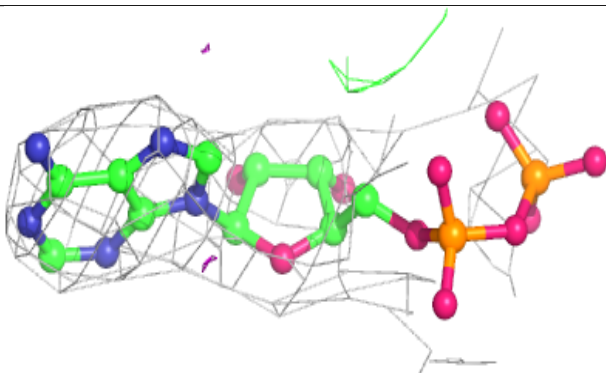
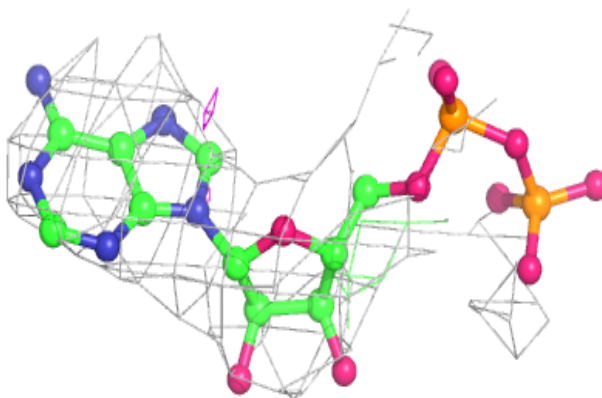


**Electron density around ADP m 602:**

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

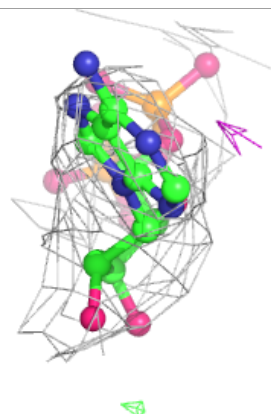
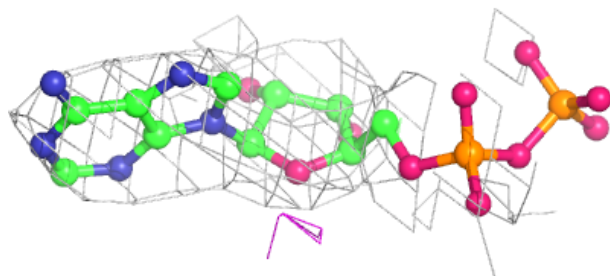
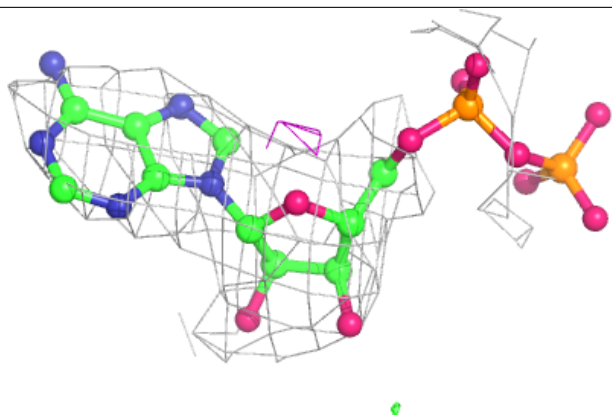
**Electron density around ADP g 602:**

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

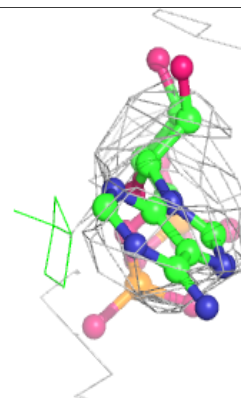
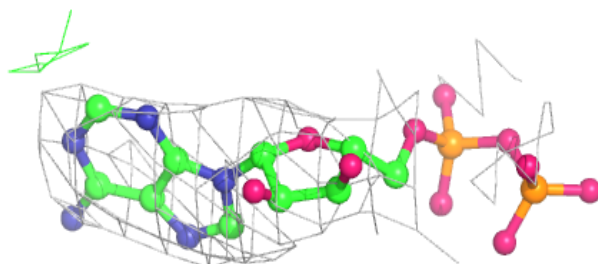
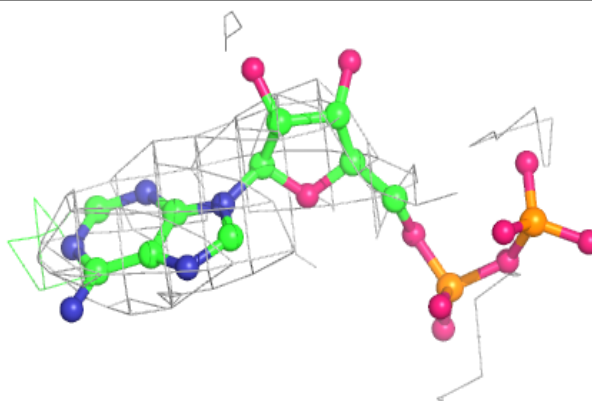


**Electron density around ADP b 602:**

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

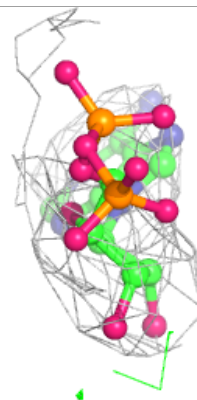
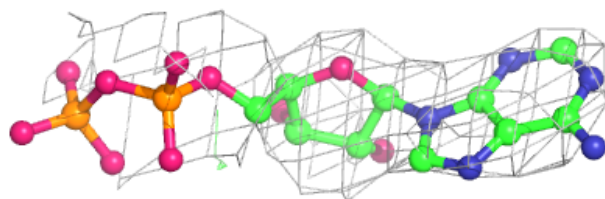
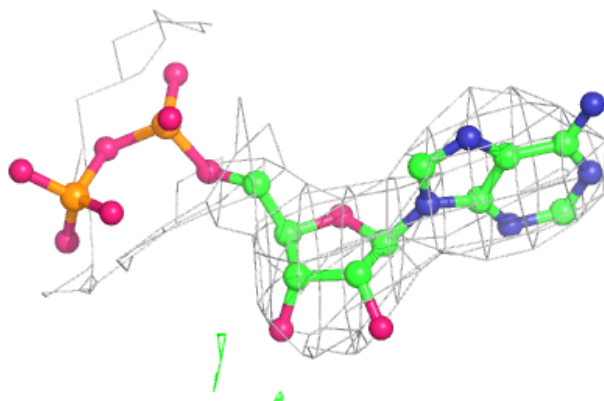
**Electron density around ADP P 602:**

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

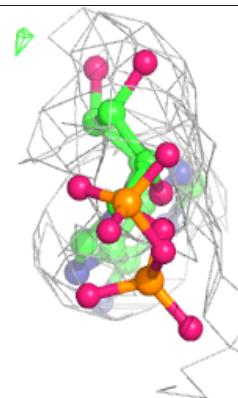
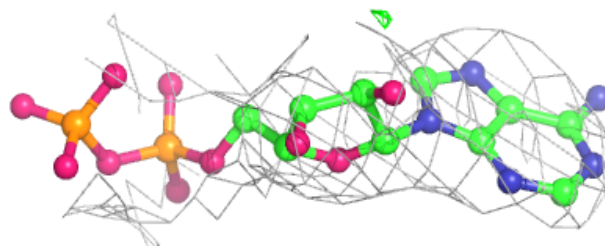
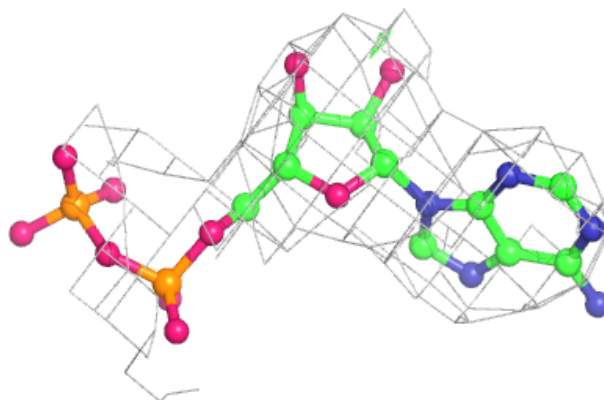


**Electron density around ADP f 602:**

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

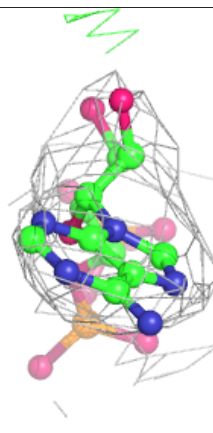
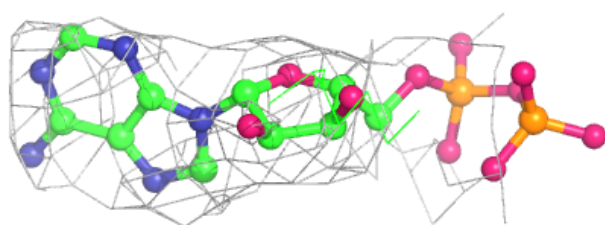
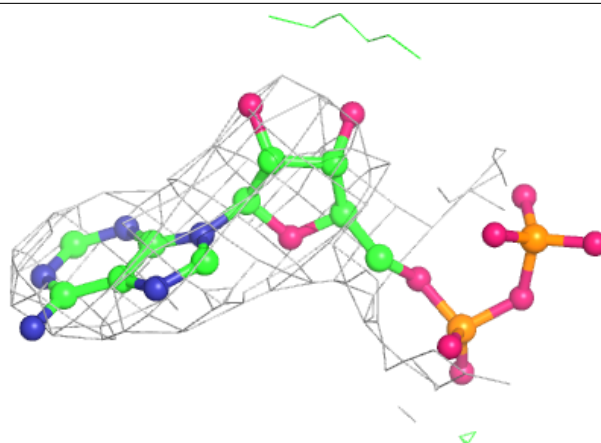
**Electron density around ADP F 602:**

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

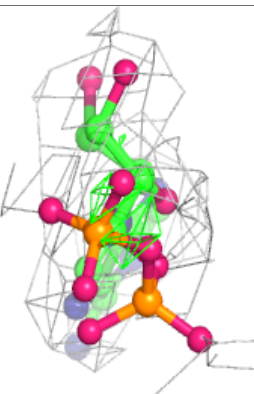
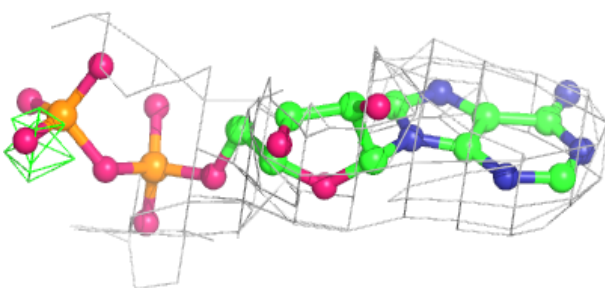
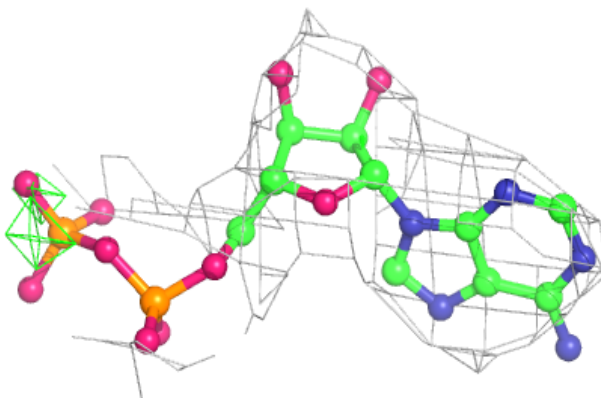


**Electron density around ADP d 602:**

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

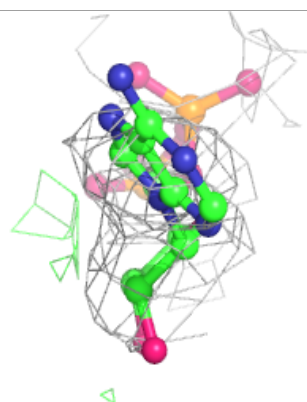
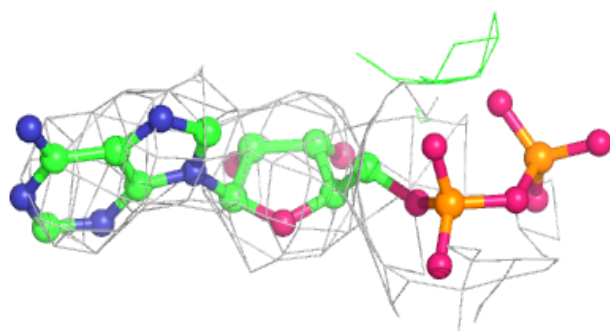
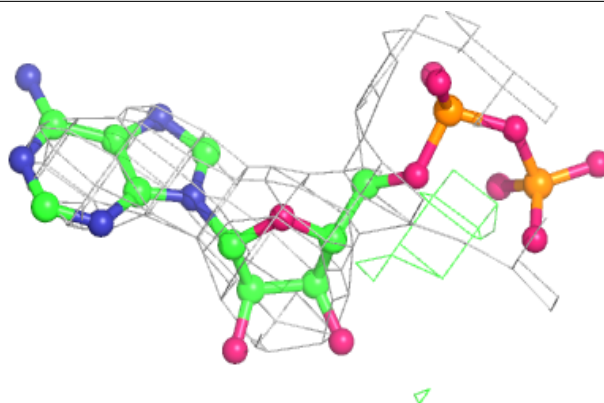
**Electron density around ADP j 602:**

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

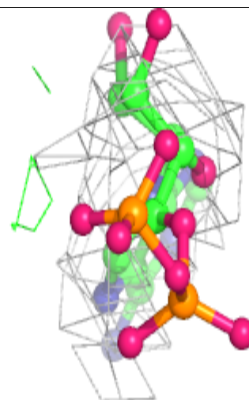
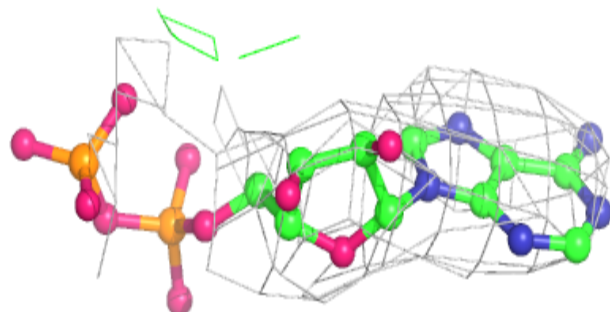
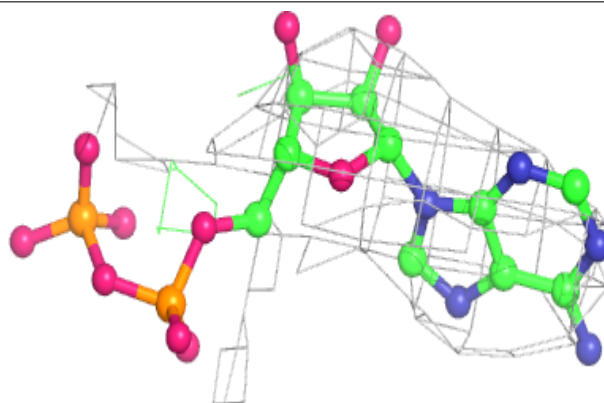


**Electron density around ADP A 602:**

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

**Electron density around ADP a 602:**

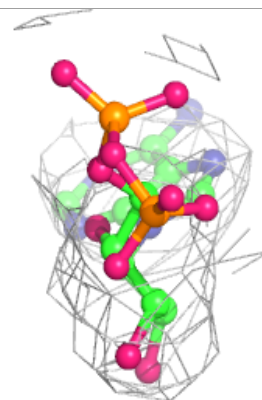
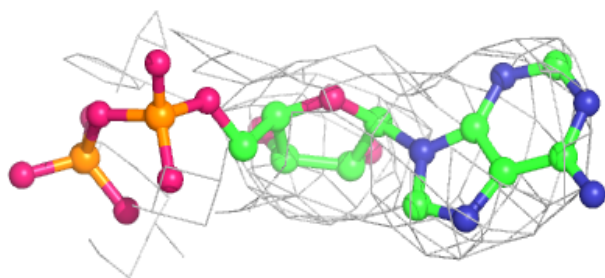
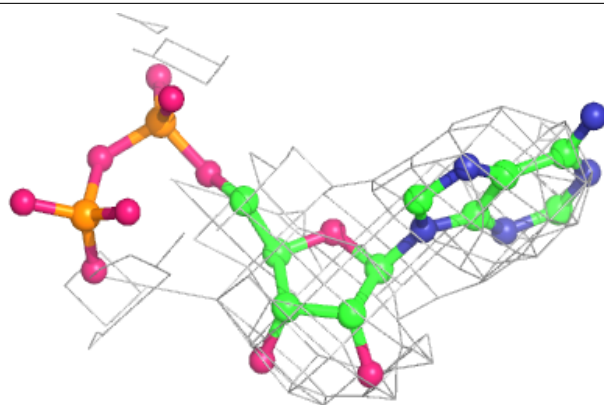
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



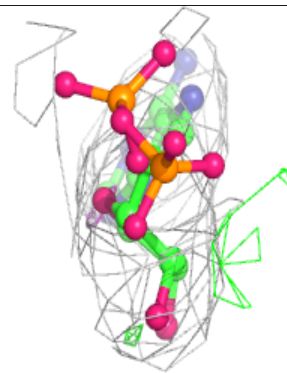
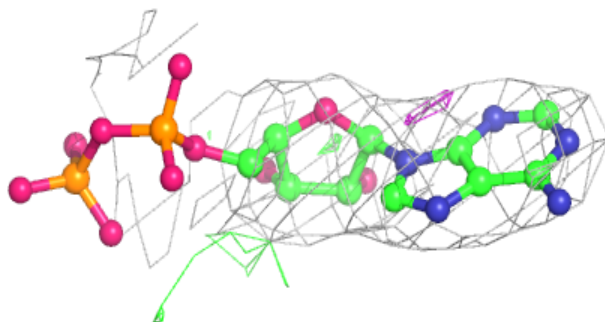
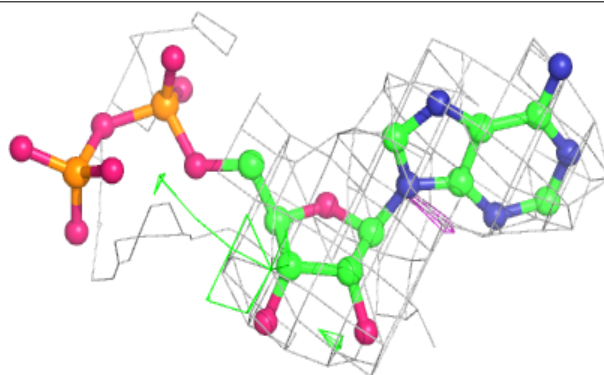


**Electron density around ADP 1 602:**

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

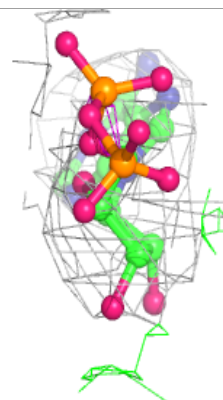
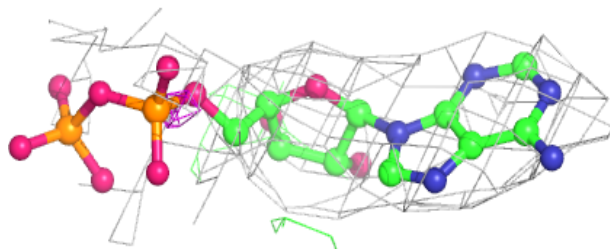
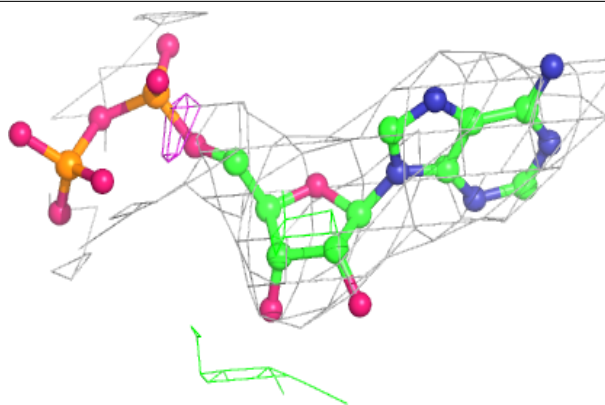
**Electron density around ADP O 602:**

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

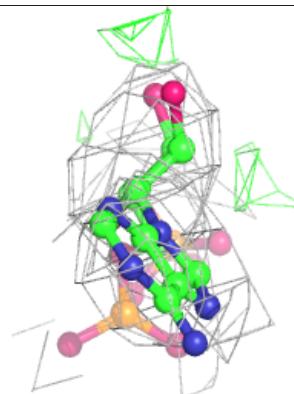
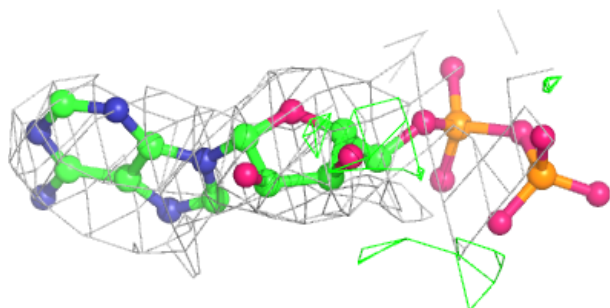
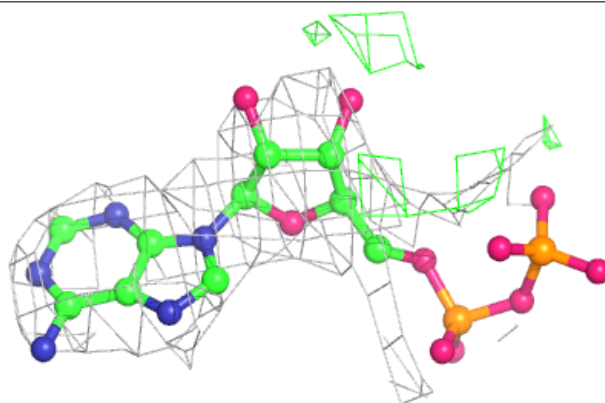


**Electron density around ADP n 602:**

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

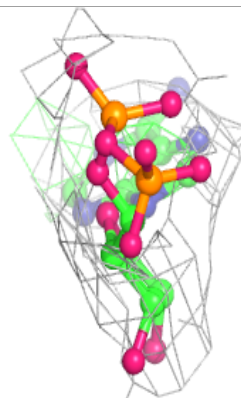
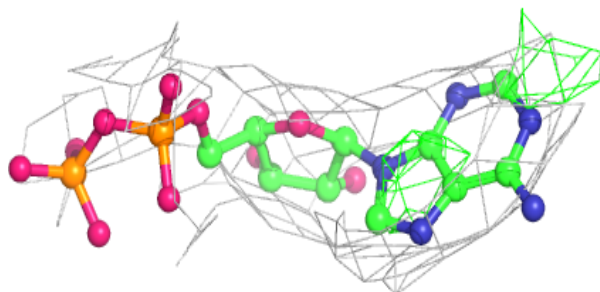
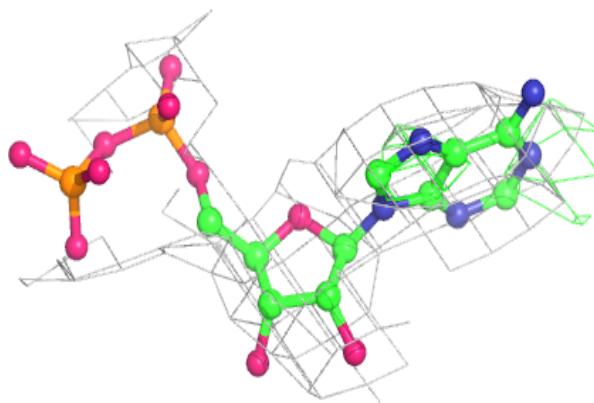
**Electron density around ADP i 602:**

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

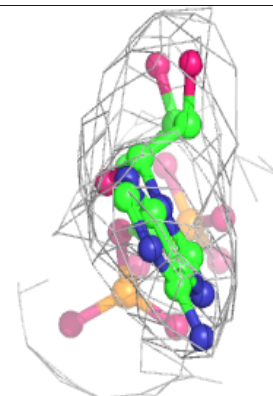
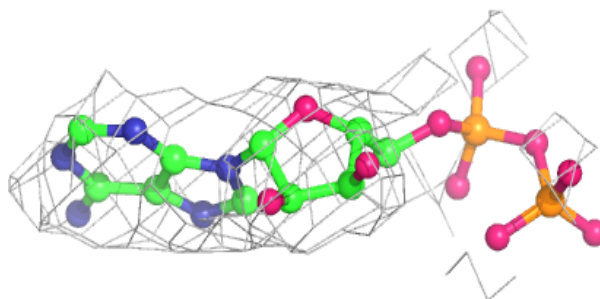
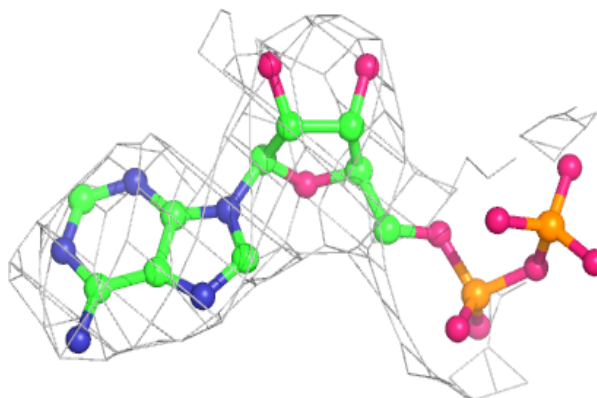


**Electron density around ADP p 602:**

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

**Electron density around ADP e 602:**

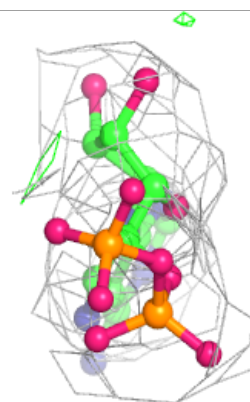
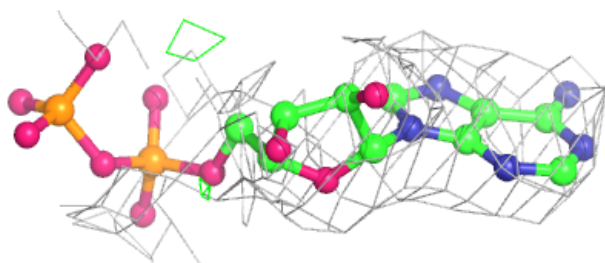
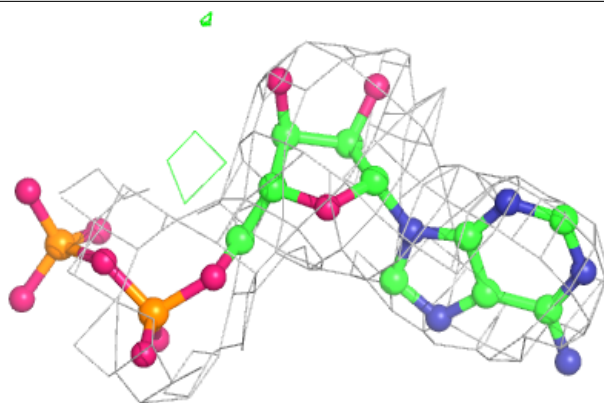
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



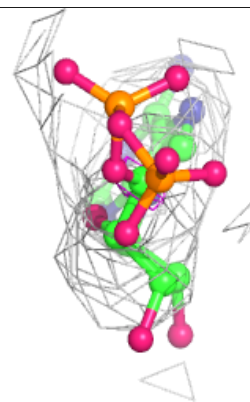
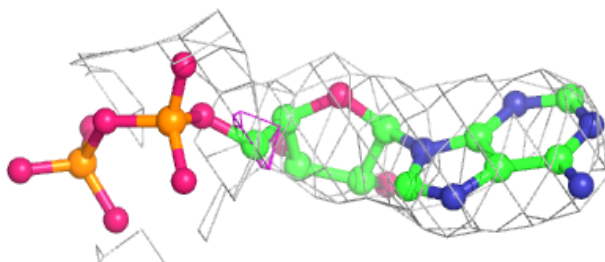
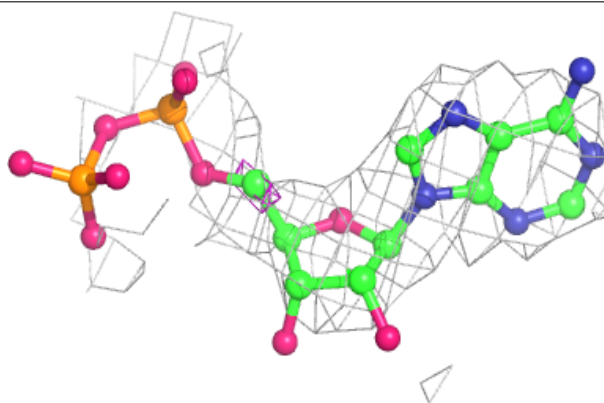


**Electron density around ADP B 602:**

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

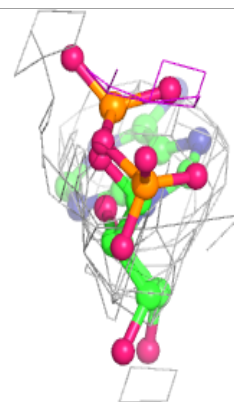
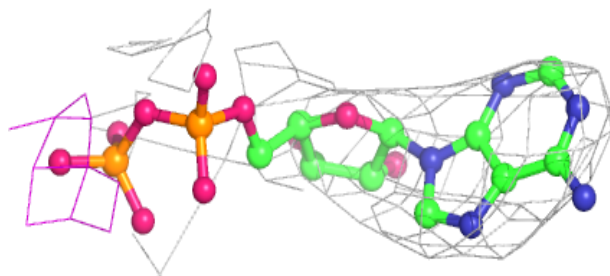
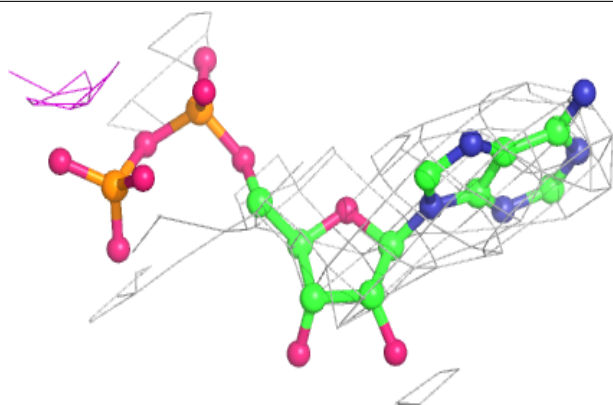
**Electron density around ADP I 602:**

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

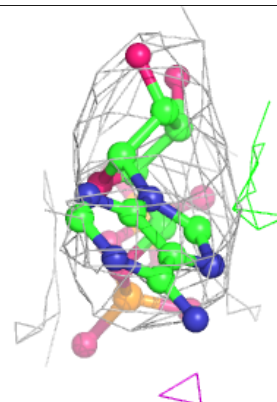
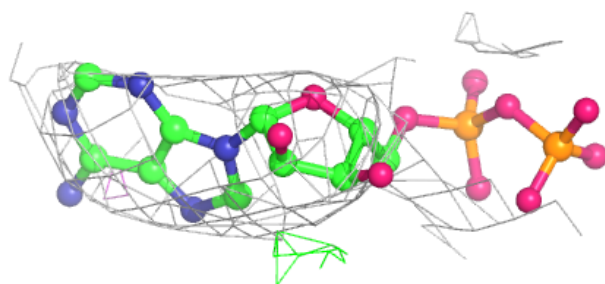
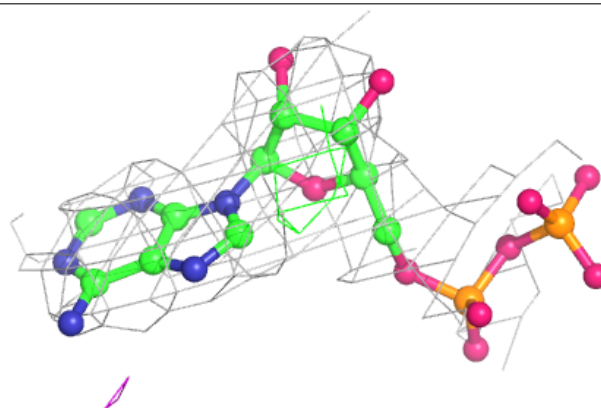


**Electron density around ADP h 602:**

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

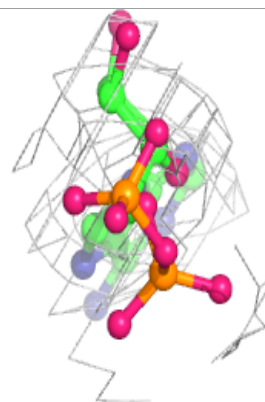
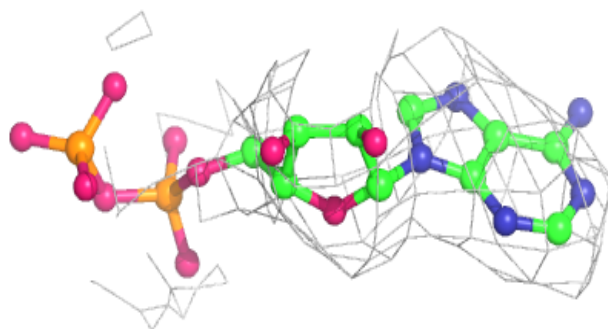
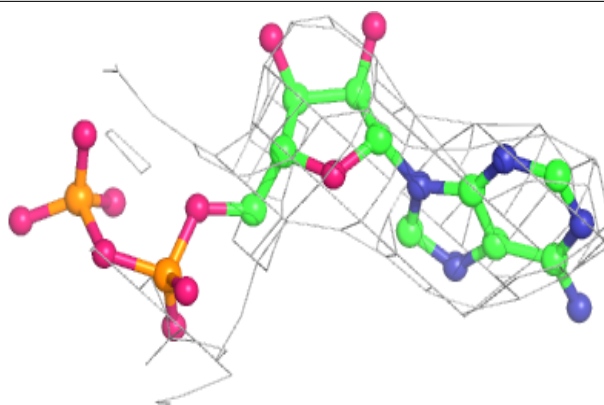
**Electron density around ADP K 1102:**

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

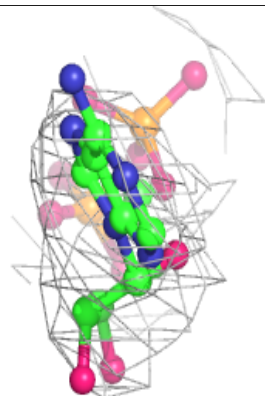
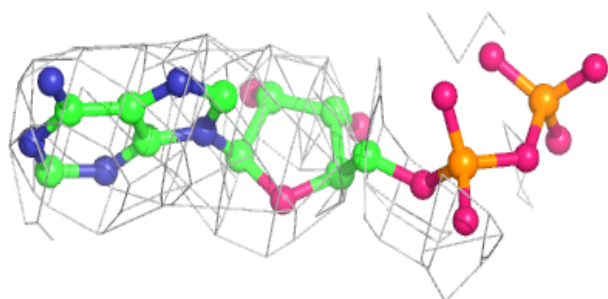
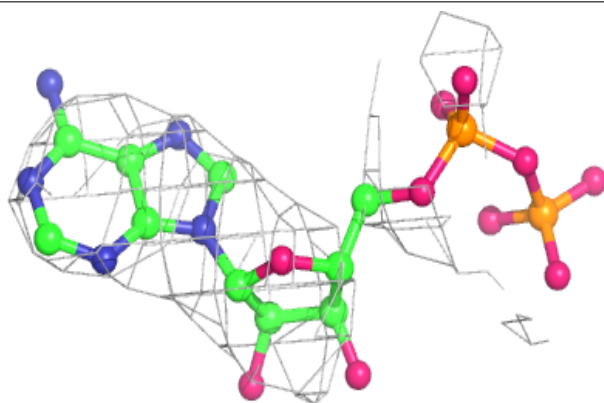


**Electron density around ADP G 602:**

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

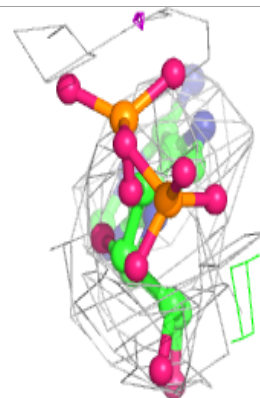
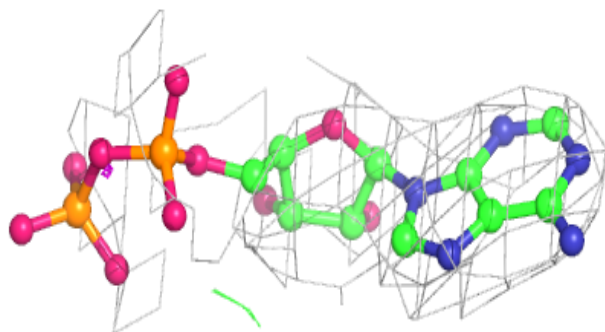
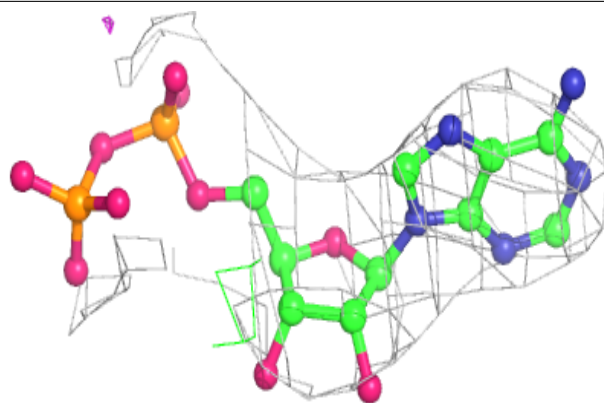
**Electron density around ADP E 602:**

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

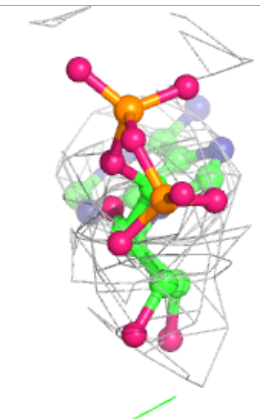
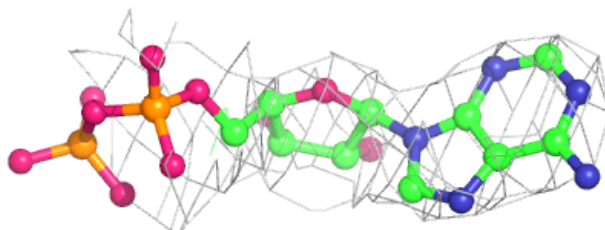
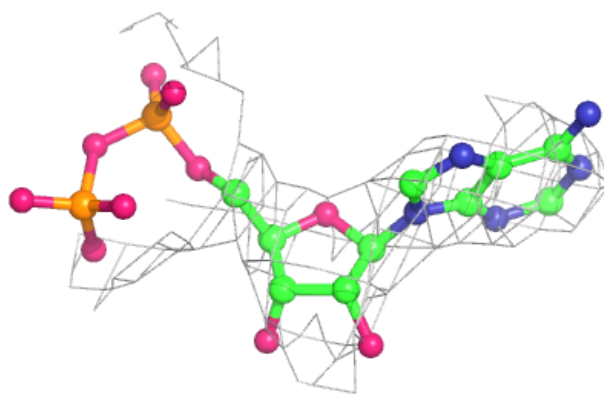


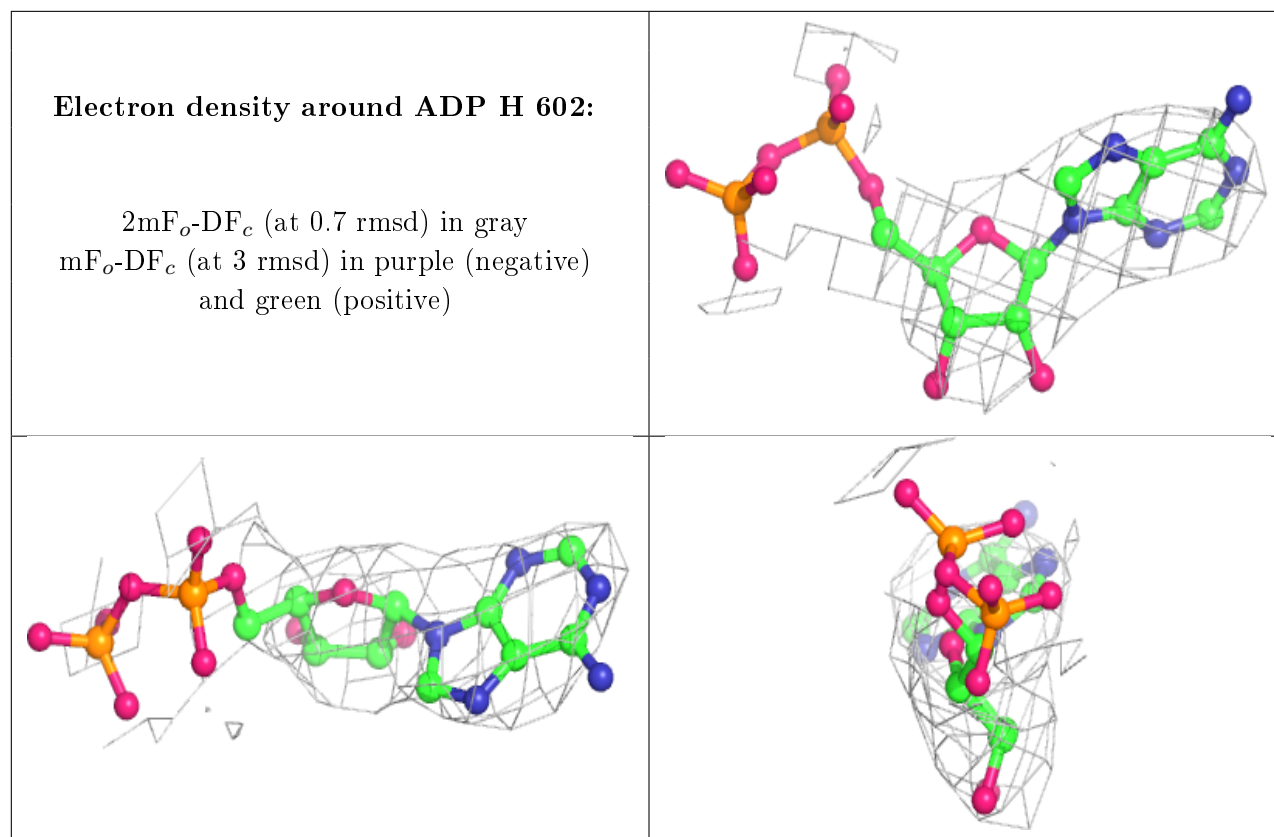
**Electron density around ADP o 602:**

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

**Electron density around ADP D 602:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.