



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:50 am BST

PDB ID : 1E1Q  
Title : BOVINE MITOCHONDRIAL F1-ATPASE AT 100K  
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2000-05-10  
Resolution : 2.61 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

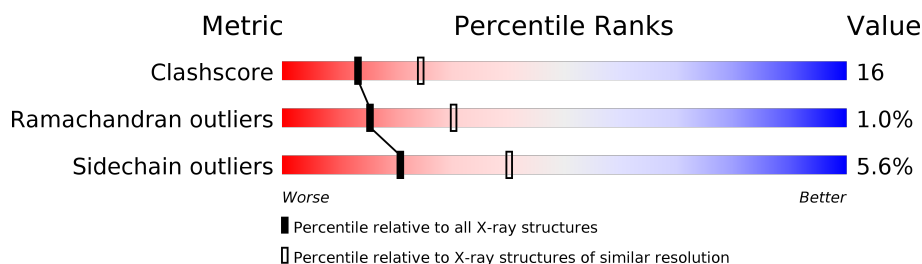
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23366 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

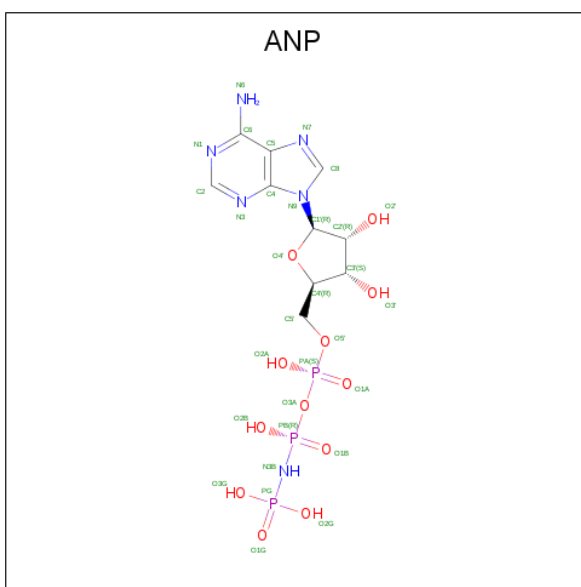
- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

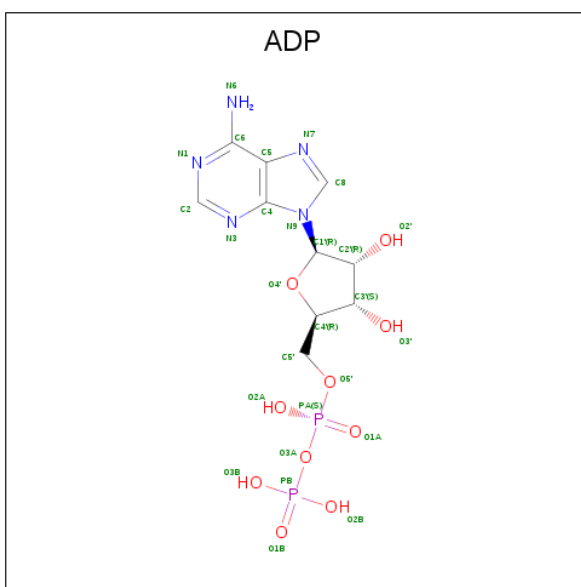


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

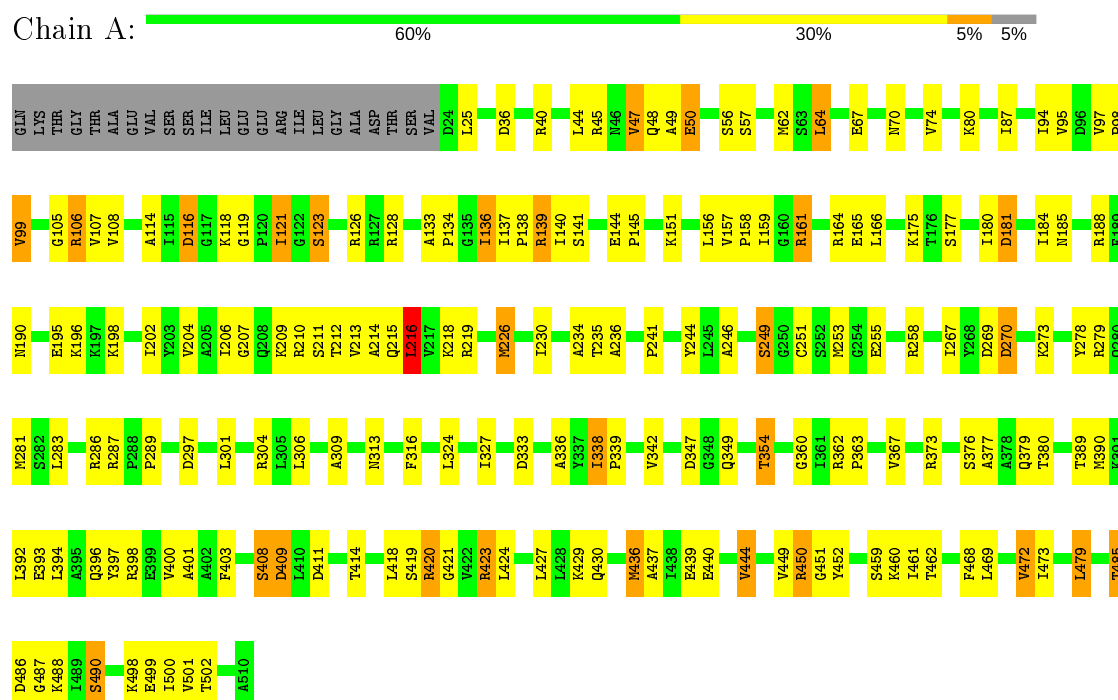
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	100	Total 100	O 100	0	0
8	B	83	Total 83	O 83	0	0
8	C	109	Total 109	O 109	0	0
8	D	92	Total 92	O 92	0	0
8	E	44	Total 44	O 44	0	0
8	F	107	Total 107	O 107	0	0
8	G	7	Total 7	O 7	0	0

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

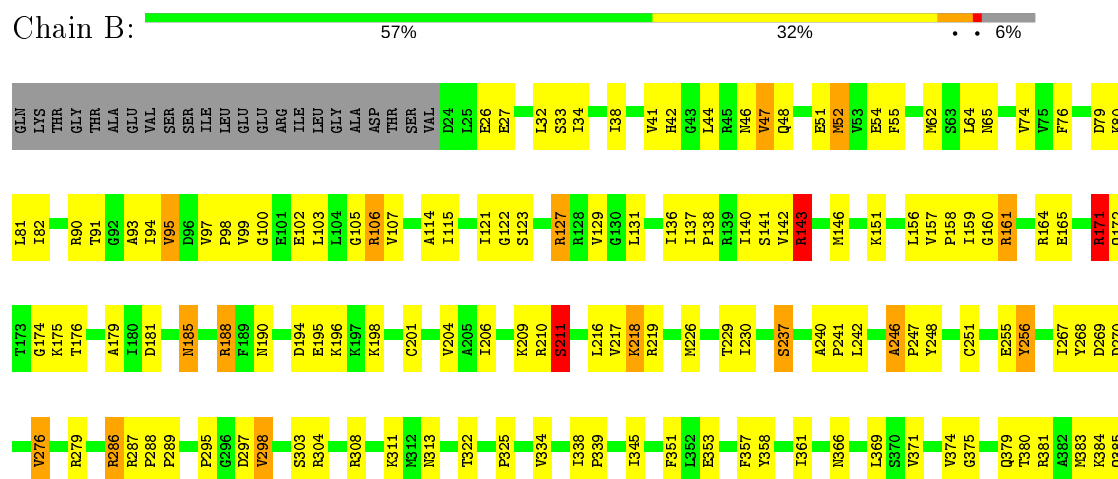
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

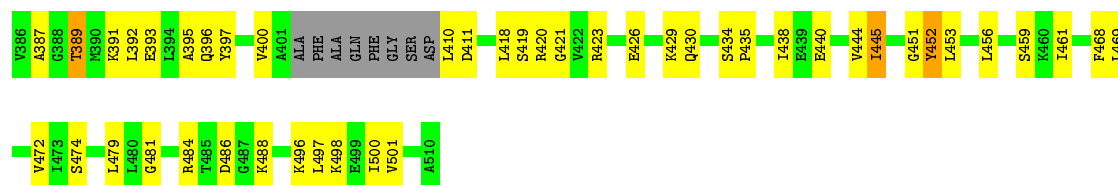
Note EDS was not executed.

#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



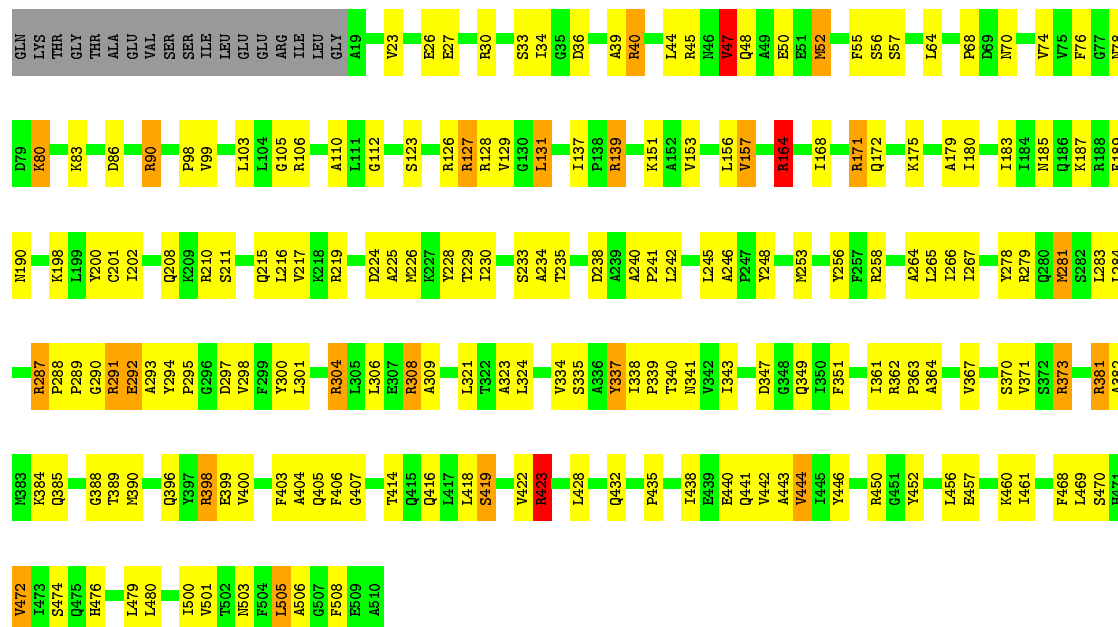
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE





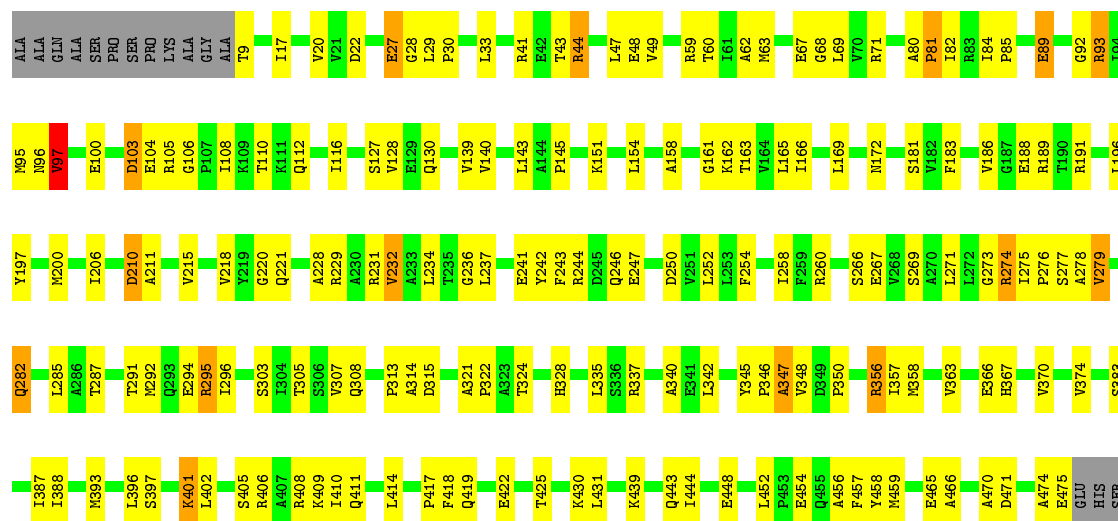
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

Chain C: 59% 32% 5%



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

Chain D: 60% 34% 6%



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



[illegible][illegible]

C78	I6	L10	I13	T20	S22	A28	A32	R36	E37	K39	P40	A41	R42	V43	Y44	GLY	VAL	GLY	SER	LEU	ALA	LEU	THR	GLU	LYS	ASP	ILE	LYS	THR	PRO	GLU	ASP	LVS	LVS	LYS	HIS	ILE	GLY	VAL
I81	H82	S83	R90	SER	GLU	ALA	ASN	LEU	ALA	ALA	GLY	LVS	VAL	VAL	GLY	ASP	LVS	ARG	HIS	SER	LEU	ARG	THR	THR	PHE	LVS	GLU	VAL	GLY	ARG	PRO	THR	PHE	GLY	ASP	ALA	SER		

ILE	TYR
ALA	GLN
LEU	GLU
GLU	TYR
LEU	SER
LEU	L209
ASN	A210
SER	N211
GLY	
TYR	S220
GLU	E224
PHE	
ASP	R228
GLU	N229
GLY	
SER	N232
ILE	
ILE	S236
PHE	K237
ASN	N238
ANG	A239
PHE	S240
ARG	E241
SER	N242
VAL	N243
ILE	
SER	L246
TYR	
LYS	F250
THR	
GLU	R254
GLU	
LYS	T259
PRQ	
ILE	L262
PHE	N263
SER	
LEU	T266
ASP	
THR	L272
ILE	
ILE	
SER	
SER	
ALA	
GLU	
SER	
MET	
SER	
SER	
ILE	
TYR	
ASP	
ASP	
ILE	
ASP	
ALA	
ASP	
VAL	
LEU	
ARG	
ASN	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	280.80 Å   107.40 Å   139.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.61	Depositor
% Data completeness (in resolution range)	95.0 (20.00-2.61)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.232 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ANP, MG, 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	A	0.59	0/3766	1.24	28/5080 (0.6%)
1	B	0.60	0/3704	1.24	23/4995 (0.5%)
1	C	0.63	0/3799	1.33	28/5126 (0.5%)
2	D	0.59	0/3596	1.28	26/4879 (0.5%)
2	E	0.55	0/3587	1.18	20/4867 (0.4%)
2	F	0.63	0/3587	1.29	26/4867 (0.5%)
3	G	0.45	0/949	0.97	4/1266 (0.3%)
All	All	0.59	0/22988	1.25	155/31080 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	274	ARG	NE-CZ-NH1	14.94	127.77	120.30
1	C	304	ARG	NE-CZ-NH2	13.00	126.80	120.30
1	C	423	ARG	NE-CZ-NH2	-12.63	113.98	120.30
1	C	219	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	A	210	ARG	CD-NE-CZ	11.64	139.89	123.60
2	E	229	ARG	NE-CZ-NH2	-11.18	114.71	120.30
2	D	59	ARG	NE-CZ-NH2	-10.87	114.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	ARG	NE-CZ-NH2	-10.30	115.15	120.30
2	D	105	ARG	NE-CZ-NH2	-10.29	115.16	120.30
2	F	274	ARG	CD-NE-CZ	10.15	137.82	123.60
1	A	304	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	B	171	ARG	NE-CZ-NH1	9.87	125.24	120.30
2	E	195	ASP	CB-CG-OD1	9.81	127.13	118.30
2	D	41	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	C	423	ARG	CD-NE-CZ	9.55	136.97	123.60
2	F	41	ARG	CG-CD-NE	9.21	131.14	111.80
2	D	93	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	C	308	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	A	423	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	A	258	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	C	423	ARG	NE-CZ-NH1	8.65	124.63	120.30
3	G	254	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	C	139	ARG	NE-CZ-NH1	-8.51	116.04	120.30
1	B	106	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	C	287	ARG	NE-CZ-NH1	-8.32	116.14	120.30
2	F	229	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	A	216	LEU	CA-CB-CG	8.23	134.22	115.30
2	D	97	VAL	CB-CA-C	-8.21	95.79	111.40
2	D	44	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	258	ARG	CD-NE-CZ	8.02	134.82	123.60
1	A	279	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	52	MET	CA-CB-CG	7.99	126.88	113.30
2	E	71	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	B	279	ARG	NE-CZ-NH1	7.96	124.28	120.30
2	F	41	ARG	NE-CZ-NH1	7.91	124.25	120.30
2	F	244	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	B	188	ARG	NE-CZ-NH1	-7.63	116.49	120.30
1	C	127	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	B	181	ASP	CB-CG-OD1	7.59	125.13	118.30
2	D	295	ARG	NE-CZ-NH1	7.57	124.09	120.30
2	E	229	ARG	NH1-CZ-NH2	7.49	127.64	119.40
1	C	164	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	F	71	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	B	304	ARG	NE-CZ-NH2	7.38	123.99	120.30
2	E	83	ARG	CD-NE-CZ	7.33	133.85	123.60
2	D	44	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	128	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	C	291	ARG	CD-NE-CZ	7.16	133.63	123.60
1	A	40	ARG	CD-NE-CZ	7.15	133.61	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	228	ARG	NE-CZ-NH2	7.10	123.85	120.30
2	F	281	TYR	CB-CG-CD2	-7.02	116.78	121.00
2	D	22	ASP	CB-CG-OD1	7.00	124.60	118.30
2	E	83	ARG	NE-CZ-NH2	-6.91	116.85	120.30
2	E	83	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	270	ASP	CA-CB-CG	6.87	128.52	113.40
2	F	356	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	398	ARG	NE-CZ-NH1	-6.85	116.88	120.30
2	E	288	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	47	VAL	CB-CA-C	-6.73	98.61	111.40
1	B	279	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	287	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	C	40	ARG	NE-CZ-NH2	-6.64	116.98	120.30
3	G	254	ARG	NH1-CZ-NH2	6.63	126.70	119.40
2	D	105	ARG	NE-CZ-NH1	6.61	123.60	120.30
2	D	241	GLU	OE1-CD-OE2	-6.61	115.37	123.30
1	C	126	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	E	64	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	276	VAL	CA-CB-CG2	6.53	120.69	110.90
2	D	197	TYR	CB-CG-CD1	6.49	124.90	121.00
1	A	106	ARG	CD-NE-CZ	6.47	132.66	123.60
2	F	274	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	E	295	ARG	CG-CD-NE	6.46	125.37	111.80
1	B	161	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	269	ASP	CB-CG-OD2	6.37	124.03	118.30
1	C	90	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	F	372	ARG	CD-NE-CZ	6.31	132.43	123.60
2	D	103	ASP	CB-CG-OD1	6.27	123.94	118.30
3	G	254	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	B	185	ASN	CA-CB-CG	6.22	127.08	113.40
2	F	233	ALA	CB-CA-C	6.19	119.39	110.10
1	C	281	MET	CA-CB-CG	6.19	123.82	113.30
1	C	304	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	C	373	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	D	105	ARG	CD-NE-CZ	6.05	132.07	123.60
1	B	256	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	B	127	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	161	ARG	NE-CZ-NH1	5.97	123.28	120.30
2	F	281	TYR	CB-CG-CD1	5.96	124.58	121.00
2	D	191	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	D	244	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	116	ASP	CB-CG-OD1	5.94	123.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ARG	NE-CZ-NH1	-5.94	117.33	120.30
2	F	241	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	C	139	ARG	NH1-CZ-NH2	5.92	125.91	119.40
2	F	77	ASP	CB-CG-OD1	5.92	123.63	118.30
2	F	191	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	F	287	THR	CA-CB-CG2	-5.90	104.14	112.40
2	D	41	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	B	246	ALA	N-CA-CB	5.86	118.31	110.10
1	A	450	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	F	372	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	279	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	47	VAL	N-CA-CB	5.78	124.22	111.50
2	D	41	ARG	CD-NE-CZ	5.77	131.68	123.60
2	E	359	ASP	CB-CG-OD1	5.74	123.47	118.30
2	E	319	ASP	CB-CG-OD2	5.72	123.44	118.30
2	D	337	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	287	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	234	ALA	N-CA-CB	5.68	118.05	110.10
1	B	171	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	C	40	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	F	139	VAL	CB-CA-C	-5.61	100.75	111.40
2	F	245	ASP	CB-CG-OD2	-5.59	113.26	118.30
2	D	229	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	211	SER	N-CA-CB	5.57	118.86	110.50
2	F	244	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	219	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	279	ARG	CD-NE-CZ	5.55	131.37	123.60
1	B	219	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	D	229	ARG	NE-CZ-NH2	5.53	123.06	120.30
2	D	295	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	F	244	ARG	CD-NE-CZ	5.49	131.28	123.60
2	E	229	ARG	NE-CZ-NH1	-5.48	117.56	120.30
2	E	326	PHE	CB-CG-CD2	5.46	124.62	120.80
2	F	256	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	106	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	47	VAL	CB-CA-C	-5.41	101.11	111.40
1	C	287	ARG	CD-NE-CZ	-5.41	116.03	123.60
1	A	181	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	161	ARG	NE-CZ-NH2	-5.41	117.60	120.30
2	E	41	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	246	ALA	CB-CA-C	5.32	118.08	110.10
2	D	356	ARG	CD-NE-CZ	5.28	130.99	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	191	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	171	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	340	THR	N-CA-CB	5.23	120.23	110.30
2	D	274	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	B	286	ARG	CD-NE-CZ	5.20	130.88	123.60
2	F	83	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	304	ARG	NH1-CZ-NH2	5.16	125.07	119.40
2	E	139	VAL	CB-CA-C	-5.13	101.65	111.40
1	B	93	ALA	N-CA-CB	-5.13	102.92	110.10
2	E	93	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	336	ALA	CB-CA-C	5.08	117.72	110.10
1	B	211	SER	CA-CB-OG	5.08	124.93	111.20
2	F	93	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	139	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	248	TYR	CB-CG-CD2	-5.04	117.98	121.00
2	D	71	ARG	NE-CZ-NH1	-5.03	117.78	120.30
2	E	222	MET	CG-SD-CE	5.03	108.25	100.20
1	B	143	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	226	MET	CA-CB-CG	5.01	121.82	113.30
2	E	337	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	F	337	ARG	NE-CZ-NH2	5.01	122.81	120.30
2	D	97	VAL	CG1-CB-CG2	5.00	118.90	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	97	VAL	Mainchain
2	E	223	ASN	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3814	136	0
1	B	3656	0	3765	142	0
1	C	3748	0	3845	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3539	0	3592	119	0
2	E	3530	0	3587	145	0
2	F	3530	0	3586	94	0
3	G	945	0	1019	30	0
4	A	31	0	13	1	0
4	B	31	0	13	2	0
4	C	31	0	13	2	0
4	F	31	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	D	27	0	12	1	0
7	E	5	0	0	1	0
8	A	100	0	0	6	0
8	B	83	0	0	6	0
8	C	109	0	0	3	0
8	D	92	0	0	4	0
8	E	44	0	0	4	0
8	F	107	0	0	3	0
8	G	7	0	0	0	0
All	All	23366	0	23272	741	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 16.

All (741) 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:D:282:GLN:H	2:D:282:GLN:HE21	0.96	0.96
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.52	0.91
2:D:139:VAL:HB	8:D:2027:HOH:O	1.72	0.90
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.54	0.89
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.56	0.88
2:F:282:GLN:H	2:F:282:GLN:HE21	0.89	0.88
2:E:449:TYR:HB3	2:E:452:LEU:HD12	1.56	0.87
2:F:282:GLN:H	2:F:282:GLN:NE2	1.71	0.87
1:A:389:THR:HB	1:A:449:VAL:HG21	1.58	0.84
2:F:282:GLN:N	2:F:282:GLN:HE21	1.74	0.83
2:D:282:GLN:H	2:D:282:GLN:NE2	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.61	0.82
2:E:388:ILE:HG23	2:E:393:MET:HB2	1.61	0.82
2:F:16:VAL:C	2:F:17:ILE:HD12	2.00	0.82
2:F:12:ARG:HE	2:F:74:LYS:HE3	1.44	0.82
1:A:218:LYS:HD2	2:D:128:VAL:HG21	1.62	0.81
1:C:295:PRO:O	1:C:298:VAL:HG23	1.82	0.80
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.61	0.80
2:D:393:MET:HG3	2:D:396:LEU:HD12	1.64	0.80
1:B:209:LYS:HG3	8:B:2030:HOH:O	1.82	0.79
2:E:419:GLN:HA	2:E:429:GLY:HA3	1.65	0.78
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.66	0.76
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.68	0.76
1:A:144:GLU:HB2	1:A:161:ARG:HG3	1.67	0.76
1:A:202:ILE:HG12	1:A:230:ILE:HD12	1.68	0.76
2:E:170:ILE:HD13	2:E:215:VAL:HG21	1.66	0.75
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.67	0.75
2:D:242:TYR:CE1	2:D:246:GLN:HG3	2.22	0.75
1:C:472:VAL:HG23	1:C:480:LEU:HD11	1.70	0.74
1:B:444:VAL:HG23	1:B:445:ILE:HD13	1.69	0.73
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.68	0.73
1:C:292:GLU:O	1:C:293:ALA:HB3	1.88	0.73
2:F:223:ASN:H	2:F:223:ASN:HD22	1.37	0.72
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.71	0.72
1:C:210:ARG:HG2	1:C:235:THR:HG21	1.71	0.72
1:A:94:ILE:HG12	1:A:95:VAL:H	1.54	0.72
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.25	0.72
2:F:287:THR:O	2:F:291:THR:HG23	1.90	0.71
1:B:171:ARG:HH11	1:B:171:ARG:HB2	1.55	0.71
2:E:223:ASN:ND2	2:E:223:ASN:H	1.88	0.71
1:B:453:LEU:HD13	1:B:461:ILE:HD12	1.73	0.71
1:B:374:VAL:HG23	1:B:374:VAL:O	1.89	0.71
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.73	0.71
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.72	0.71
2:E:404:VAL:O	2:E:408:ARG:HG3	1.91	0.70
2:F:252:LEU:HD23	2:F:305:THR:HB	1.73	0.70
1:B:366:ASN:ND2	1:B:369:LEU:HD12	2.05	0.70
1:B:334:VAL:HG11	1:B:351:PHE:HE2	1.56	0.70
2:D:388:ILE:HG21	2:D:396:LEU:HD11	1.72	0.70
2:F:396:LEU:HD13	2:F:400:ASP:HB3	1.73	0.70
2:E:223:ASN:H	2:E:223:ASN:HD22	1.40	0.70
1:A:196:LYS:H	1:A:196:LYS:HD2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:ILE:HD13	2:F:69:LEU:HD13	1.75	0.69
1:A:151:LYS:HE2	1:A:427:LEU:O	1.93	0.68
1:B:171:ARG:HB2	1:B:171:ARG:NH1	2.08	0.68
1:C:400:VAL:HG12	1:C:418:LEU:HD21	1.76	0.68
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.23	0.68
1:C:404:ALA:C	1:C:406:PHE:H	1.95	0.68
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.76	0.68
2:E:183:PHE:HB3	2:E:217:LEU:HD23	1.74	0.68
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.75	0.68
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.75	0.67
2:F:228:ALA:O	2:F:232:VAL:HG22	1.95	0.67
2:E:280:GLY:HA2	3:G:262:LEU:HD21	1.75	0.67
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.75	0.67
1:A:97:VAL:HG11	1:A:249:SER:HB3	1.76	0.67
1:B:497:LEU:HA	1:B:500:ILE:HD12	1.75	0.67
2:D:282:GLN:N	2:D:282:GLN:HE21	1.82	0.67
3:G:20:THR:HG22	3:G:236:SER:HB3	1.76	0.67
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.77	0.66
1:A:390:MET:HE2	1:A:424:LEU:HD22	1.77	0.66
1:B:361:ILE:CD1	1:B:429:LYS:HE2	2.26	0.66
1:A:44:LEU:O	1:A:47:VAL:HG22	1.96	0.66
1:C:338:ILE:HD12	1:C:338:ILE:H	1.61	0.65
2:E:139:VAL:HG13	2:E:414:LEU:HB3	1.78	0.65
2:E:163:THR:HG23	7:E:602:PO4:O2	1.96	0.65
1:C:202:ILE:HB	1:C:266:ILE:HG13	1.79	0.65
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.78	0.65
1:A:390:MET:CE	1:A:424:LEU:HD22	2.27	0.65
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.31	0.65
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.62	0.65
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.64
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.62	0.64
2:F:188:GLU:O	2:F:221:GLN:HB3	1.98	0.64
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.79	0.64
2:F:336:SER:HB3	2:F:339:ILE:HG13	1.79	0.64
1:A:469:LEU:O	1:A:473:ILE:HG13	1.98	0.64
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.13	0.64
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.80	0.64
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.78	0.64
2:D:143:LEU:CD1	2:D:350:PRO:HB3	2.28	0.63
2:E:282:GLN:H	2:E:282:GLN:NE2	1.96	0.63
2:E:390:ILE:HG21	3:G:28:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASP:HB3	8:A:2073:HOH:O	1.98	0.63
1:A:360:GLY:O	1:A:429:LYS:HE2	1.98	0.63
2:F:188:GLU:O	2:F:222:MET:HG2	1.99	0.63
1:A:87:ILE:HD12	1:A:87:ILE:H	1.64	0.62
1:B:456:LEU:HD23	1:B:461:ILE:HD13	1.81	0.62
2:D:258:ILE:HD11	2:D:292:MET:SD	2.39	0.62
2:D:408:ARG:NH1	2:D:454:GLU:OE1	2.30	0.62
1:C:423:ARG:HD3	1:C:461:ILE:HD11	1.81	0.62
2:E:282:GLN:H	2:E:282:GLN:HE21	1.45	0.62
1:A:408:SER:O	1:A:409:ASP:HB2	1.98	0.62
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.82	0.62
1:B:201:CYS:O	1:B:229:THR:HA	1.99	0.62
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.15	0.62
2:D:93:ARG:NH2	2:D:106:GLY:O	2.24	0.62
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.83	0.61
1:B:171:ARG:HH22	2:E:356:ARG:HH21	1.47	0.61
1:A:151:LYS:NZ	1:A:430:GLN:HB2	2.15	0.61
2:E:89:GLU:OE2	2:E:110:THR:HG22	2.01	0.61
1:A:158:PRO:HG3	1:A:379:GLN:NE2	2.16	0.61
2:E:149:GLY:HA2	2:E:304:ILE:O	2.00	0.61
1:B:185:ASN:HB2	1:B:435:PRO:HB2	1.83	0.61
1:B:453:LEU:HD13	1:B:461:ILE:HG23	1.83	0.60
1:B:141:SER:O	1:B:143:ARG:NH1	2.33	0.60
2:E:29:LEU:HD23	2:E:52:HIS:ND1	2.15	0.60
1:A:392:LEU:O	1:A:396:GLN:HG3	2.02	0.60
1:B:211:SER:HA	2:E:126:MET:HE2	1.82	0.60
1:C:157:VAL:HG12	1:C:371:VAL:C	2.21	0.60
1:A:121:ILE:HD11	8:A:2011:HOH:O	2.01	0.60
1:B:381:ARG:O	1:B:385:GLN:HG3	2.02	0.60
1:B:62:MET:HG3	1:B:95:VAL:HG21	1.83	0.60
2:F:111:LYS:HB2	2:F:112:GLN:OE1	2.01	0.60
1:B:400:VAL:HG12	1:B:418:LEU:HD21	1.83	0.60
2:F:405:SER:O	2:F:409:LYS:HG3	2.02	0.60
2:D:314:ALA:O	2:D:315:ASP:HB2	2.02	0.60
1:C:99:VAL:HG13	1:C:253:MET:HA	1.83	0.60
1:C:110:ALA:HB2	1:C:246:ALA:HB2	1.84	0.59
1:B:303:SER:HB2	2:F:222:MET:HB2	1.83	0.59
1:C:23:VAL:HG12	1:C:23:VAL:O	2.02	0.59
2:F:406:ARG:HH21	2:F:447:GLY:HA3	1.68	0.59
1:A:157:VAL:N	1:A:158:PRO:HD3	2.17	0.59
1:B:140:ILE:HB	1:B:313:ASN:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ALA:O	1:C:324:LEU:HD23	2.03	0.59
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.85	0.59
2:F:357:ILE:HG23	2:F:362:ILE:HG21	1.84	0.59
2:D:388:ILE:HD13	2:D:396:LEU:HD11	1.83	0.59
2:E:221:GLN:N	2:E:224:GLU:OE2	2.36	0.59
1:B:185:ASN:HB2	1:B:435:PRO:CB	2.33	0.59
1:A:44:LEU:HB3	1:A:47:VAL:HG22	1.85	0.59
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.32	0.59
2:E:422:GLU:HG2	2:E:427:HIS:O	2.02	0.59
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.38	0.59
2:D:366:GLU:O	2:D:370:VAL:HG23	2.03	0.58
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.85	0.58
1:A:151:LYS:HZ1	1:A:430:GLN:HB2	1.68	0.58
1:B:361:ILE:HD12	1:B:429:LYS:HE2	1.85	0.58
3:G:81:ILE:HG13	3:G:224:GLU:HA	1.85	0.58
2:F:223:ASN:N	2:F:223:ASN:HD22	2.00	0.58
1:A:106:ARG:NH2	1:A:119:GLY:O	2.30	0.58
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.34	0.58
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.85	0.58
1:C:187:LYS:CE	1:C:224:ASP:HB3	2.31	0.58
2:F:207:ASN:ND2	2:F:210:ASP:HB2	2.19	0.58
2:E:224:GLU:O	2:E:229:ARG:NH1	2.37	0.57
1:A:218:LYS:CD	2:D:128:VAL:HG21	2.34	0.57
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.87	0.57
1:C:418:LEU:O	1:C:422:VAL:HG23	2.03	0.57
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.85	0.57
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.87	0.57
1:C:127:ARG:HH21	1:C:131:LEU:HD12	1.70	0.57
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.39	0.57
2:F:130:GLN:HB3	2:F:357:ILE:CD1	2.33	0.57
2:D:308:GLN:HG3	8:D:2031:HOH:O	2.03	0.57
2:E:415:SER:HB2	2:E:459:MET:SD	2.45	0.57
1:B:103:LEU:HB2	1:B:230:ILE:HD13	1.87	0.57
1:C:105:GLY:HA2	1:C:226:MET:O	2.04	0.57
2:E:10:THR:HG23	2:E:76:LEU:HD23	1.87	0.57
1:A:144:GLU:CB	1:A:161:ARG:HG3	2.35	0.57
2:E:387:ILE:H	2:E:387:ILE:HD12	1.70	0.57
1:A:138:PRO:HB3	1:A:316:PHE:CZ	2.40	0.56
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.87	0.56
2:D:80:ALA:HB1	2:D:81:PRO:HD2	1.87	0.56
1:A:48:GLN:HG2	2:E:70:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:ASN:HB2	2:D:100:GLU:O	2.05	0.56
2:E:434:LEU:O	2:E:438:ILE:HG12	2.06	0.56
1:A:49:ALA:O	1:A:50:GLU:HB2	2.06	0.56
1:C:438:ILE:O	1:C:442:VAL:HG23	2.06	0.56
2:D:345:TYR:HA	2:D:346:PRO:C	2.25	0.56
1:A:157:VAL:N	1:A:158:PRO:CD	2.69	0.56
1:B:287:ARG:NE	8:B:2051:HOH:O	2.38	0.56
1:C:175:LYS:HE2	4:C:600:ANP:O1B	2.06	0.56
2:F:130:GLN:HB3	2:F:357:ILE:HD12	1.88	0.56
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.88	0.55
2:D:439:LYS:O	2:D:443:GLN:HG3	2.05	0.55
2:E:263:GLN:O	2:E:267:GLU:HG3	2.06	0.55
2:F:174:ALA:O	2:F:177:HIS:HB3	2.06	0.55
1:B:102:GLU:HG3	1:B:122:GLY:C	2.27	0.55
1:B:127:ARG:HE	1:B:131:LEU:HD12	1.71	0.55
2:E:319:ASP:O	2:E:322:PRO:HD2	2.07	0.55
2:F:345:TYR:HA	2:F:346:PRO:C	2.26	0.55
1:C:335:SER:O	2:D:314:ALA:HB1	2.07	0.55
2:E:360:PRO:HG3	2:E:368:TYR:CD2	2.41	0.55
1:B:334:VAL:HG11	1:B:351:PHE:CE2	2.40	0.55
2:E:257:ASN:HB2	2:E:309:ALA:O	2.07	0.55
2:E:384:LEU:O	2:E:388:ILE:HG12	2.07	0.55
2:F:455:GLN:O	2:F:469:LYS:HE2	2.06	0.55
2:D:277:SER:OG	2:D:278:ALA:N	2.36	0.54
2:E:167:MET:HE3	2:E:420:VAL:HG11	1.89	0.54
1:B:146:MET:HG3	1:B:322:THR:HG21	1.90	0.54
2:D:397:SER:O	2:D:401:LYS:HG2	2.08	0.54
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.08	0.54
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.88	0.54
2:D:63:MET:CE	2:D:97:VAL:HG11	2.37	0.54
1:A:313:ASN:OD1	1:A:316:PHE:HD1	1.91	0.54
1:C:172:GLN:HE21	4:C:600:ANP:HNB1	1.56	0.54
1:B:158:PRO:O	1:B:375:GLY:HA3	2.07	0.54
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.88	0.54
1:C:404:ALA:C	1:C:406:PHE:N	2.61	0.54
1:A:190:ASN:HA	1:A:198:LYS:HG2	1.90	0.54
1:A:278:TYR:HA	1:A:281:MET:CE	2.38	0.54
1:B:419:SER:O	1:B:423:ARG:HG2	2.08	0.53
1:B:62:MET:HG3	1:B:95:VAL:CG2	2.39	0.53
2:E:105:ARG:HD3	8:E:2014:HOH:O	2.09	0.53
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLU:O	1:A:444:VAL:HG13	2.07	0.53
2:F:151:LYS:HZ1	2:F:293:GLN:HB3	1.72	0.53
1:B:32:LEU:CG	1:B:42:HIS:HB2	2.39	0.53
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.43	0.53
2:D:181:SER:O	2:D:215:VAL:HA	2.08	0.53
2:F:443:GLN:HE21	2:F:449:TYR:HE2	1.56	0.53
3:G:239:ALA:O	3:G:243:ILE:HG13	2.09	0.53
1:B:164:ARG:HD3	1:B:164:ARG:N	2.24	0.53
1:B:251:CYS:HB2	1:B:268:TYR:OH	2.09	0.53
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.90	0.53
2:E:29:LEU:HD23	2:E:52:HIS:CE1	2.43	0.53
1:B:383:MET:SD	1:B:387:ALA:HB2	2.49	0.53
1:C:45:ARG:NH2	1:C:68:PRO:O	2.42	0.53
2:D:89:GLU:H	2:D:89:GLU:CD	2.11	0.53
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.41	0.52
2:E:243:PHE:HB2	2:E:251:VAL:HG21	1.91	0.52
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.90	0.52
1:A:362:ARG:HA	1:A:363:PRO:C	2.28	0.52
1:A:215:GLN:O	1:A:218:LYS:HB3	2.09	0.52
2:D:405:SER:O	2:D:409:LYS:HG3	2.10	0.52
2:D:419:GLN:O	2:D:422:GLU:HG3	2.09	0.52
2:E:48:GLU:OE2	2:E:231:ARG:NH2	2.42	0.52
2:E:243:PHE:HB2	2:E:251:VAL:CG2	2.40	0.52
1:A:468:PHE:O	1:A:472:VAL:HG13	2.09	0.52
1:A:498:LYS:O	1:A:502:THR:HG23	2.10	0.52
1:C:34:ILE:HD13	1:C:39:ALA:HB2	1.90	0.52
1:C:460:LYS:HE2	8:C:2103:HOH:O	2.08	0.52
2:E:170:ILE:HG21	2:E:215:VAL:CG2	2.39	0.52
3:G:228:ARG:O	3:G:232:MET:HG2	2.10	0.52
1:A:62:MET:CE	1:A:64:LEU:HD21	2.39	0.52
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.92	0.52
2:D:243:PHE:O	2:D:247:GLU:HB2	2.09	0.52
2:E:388:ILE:HD12	2:E:396:LEU:HD11	1.92	0.52
1:C:153:VAL:HA	1:C:157:VAL:HG23	1.91	0.52
2:E:314:ALA:O	2:E:315:ASP:HB2	2.08	0.52
1:B:48:GLN:HG3	1:B:51:GLU:OE1	2.09	0.52
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.91	0.52
2:D:417:PRO:HA	2:D:459:MET:HE1	1.92	0.52
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.43	0.52
2:E:282:GLN:N	2:E:282:GLN:HE21	2.07	0.52
1:B:451:GLY:C	1:B:453:LEU:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:HB3	1:B:46:ASN:ND2	2.24	0.52
2:D:456:ALA:HB1	2:D:466:ALA:O	2.09	0.52
3:G:38:LEU:HD11	3:G:42:ARG:NH2	2.25	0.52
1:B:129:VAL:O	1:B:308:ARG:NH1	2.39	0.52
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.92	0.51
1:B:161:ARG:HA	1:B:322:THR:OG1	2.10	0.51
2:E:334:VAL:HG21	2:E:352:ASP:HB3	1.92	0.51
2:F:185:GLY:HA3	2:F:219:TYR:CD1	2.44	0.51
2:D:9:THR:HG22	2:D:27:GLU:OE1	2.10	0.51
2:F:245:ASP:C	2:F:247:GLU:H	2.13	0.51
1:A:479:LEU:O	1:A:479:LEU:HD22	2.10	0.51
1:A:204:VAL:HG12	1:A:206:ILE:HD11	1.90	0.51
2:E:276:PRO:HD2	3:G:266:ILE:CD1	2.40	0.51
1:A:137:ILE:N	1:A:138:PRO:CD	2.73	0.51
2:D:340:ALA:HB2	2:D:347:ALA:HB2	1.91	0.51
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.46	0.51
2:F:189:ARG:HB2	2:F:192:GLU:HG3	1.92	0.51
1:B:174:GLY:HA2	4:B:600:ANP:PA	2.51	0.51
1:C:292:GLU:O	1:C:293:ALA:CB	2.54	0.51
1:A:99:VAL:CG2	1:A:253:MET:HA	2.40	0.51
1:C:501:VAL:O	1:C:505:LEU:HB2	2.10	0.51
1:B:141:SER:OG	1:B:143:ARG:NH1	2.44	0.51
1:B:423:ARG:O	1:B:426:GLU:N	2.43	0.51
2:E:374:VAL:O	2:E:377:ILE:HG22	2.11	0.50
1:C:183:ILE:HD11	1:C:267:ILE:CD1	2.41	0.50
1:B:468:PHE:O	1:B:472:VAL:HG22	2.11	0.50
3:G:39:LYS:N	3:G:40:PRO:HD2	2.26	0.50
1:C:50:GLU:OE2	2:D:67:GLU:HG2	2.10	0.50
2:D:474:ALA:O	2:D:475:GLU:HB2	2.12	0.50
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.94	0.50
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.92	0.50
2:D:417:PRO:CA	2:D:459:MET:HE1	2.42	0.50
1:A:376:SER:O	1:A:377:ALA:C	2.50	0.50
1:B:479:LEU:CD1	1:B:497:LEU:HD13	2.42	0.50
1:C:27:GLU:O	1:C:90:ARG:HG3	2.11	0.50
2:F:63:MET:HE3	2:F:97:VAL:HG11	1.93	0.50
1:A:389:THR:HG22	1:A:393:GLU:OE2	2.11	0.50
2:D:63:MET:HE1	2:D:97:VAL:HG11	1.92	0.50
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.93	0.50
1:C:382:ALA:HA	1:C:385:GLN:OE1	2.11	0.50
2:D:402:LEU:HD21	2:D:406:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LYS:HD2	1:A:196:LYS:N	2.25	0.49
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.77	0.49
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.94	0.49
2:E:210:ASP:O	2:E:212:THR:N	2.39	0.49
2:E:281:TYR:HB3	2:E:282:GLN:HE21	1.77	0.49
1:C:347:ASP:C	1:C:373:ARG:HG3	2.32	0.49
2:E:393:MET:HG3	2:E:396:LEU:HD11	1.93	0.49
2:F:336:SER:CB	2:F:339:ILE:HG13	2.42	0.49
1:A:439:GLU:H	1:A:439:GLU:CD	2.16	0.49
1:B:32:LEU:HG	1:B:42:HIS:HB2	1.94	0.49
1:B:410:LEU:O	1:B:411:ASP:HB3	2.12	0.49
1:C:40:ARG:NH1	1:C:70:ASN:OD1	2.45	0.49
2:E:357:ILE:HB	2:E:362:ILE:HG21	1.93	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.12	0.49
1:C:440:GLU:O	1:C:444:VAL:HG13	2.11	0.49
2:E:52:HIS:HB3	8:E:2006:HOH:O	2.12	0.49
1:A:180:ILE:O	1:A:184:ILE:HG12	2.13	0.49
1:B:393:GLU:HA	1:B:396:GLN:OE1	2.11	0.49
1:C:399:GLU:CG	2:D:342:LEU:HD22	2.43	0.49
1:C:443:ALA:O	1:C:446:TYR:HB3	2.12	0.49
2:E:366:GLU:O	2:E:370:VAL:HG23	2.12	0.49
1:B:240:ALA:N	1:B:241:PRO:CD	2.75	0.49
2:D:172:ASN:ND2	2:D:431:LEU:HD11	2.27	0.49
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.42	0.49
2:E:387:ILE:HD12	2:E:387:ILE:N	2.28	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.93	0.49
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.95	0.49
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.92	0.49
1:A:213:VAL:O	1:A:216:LEU:HB3	2.13	0.49
1:B:151:LYS:HG3	1:B:430:GLN:OE1	2.13	0.49
2:E:144:ALA:N	2:E:145:PRO:HD3	2.27	0.49
2:F:134:VAL:HA	2:F:141:ASP:OD1	2.12	0.49
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.94	0.49
1:B:209:LYS:HB3	2:E:294:GLU:OE2	2.12	0.49
2:E:66:THR:HB	2:E:69:LEU:HD12	1.94	0.49
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.95	0.49
1:B:210:ARG:O	1:B:211:SER:C	2.51	0.49
1:B:41:VAL:HG11	1:B:44:LEU:HD11	1.93	0.49
1:C:295:PRO:HD2	1:C:298:VAL:CG2	2.42	0.49
2:E:103:ASP:O	2:E:104:GLU:HB2	2.12	0.49
2:E:440:GLY:O	2:E:444:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.95	0.48
1:B:136:ILE:HG23	2:F:194:ASN:HA	1.94	0.48
1:C:300:TYR:CZ	1:C:304:ARG:HD3	2.49	0.48
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.95	0.48
1:A:67:GLU:HB2	1:A:70:ASN:O	2.12	0.48
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.95	0.48
3:G:210:ALA:O	3:G:211:ASN:C	2.51	0.48
1:A:338:ILE:N	1:A:339:PRO:CD	2.75	0.48
1:B:159:ILE:HG22	1:B:160:GLY:N	2.27	0.48
1:C:367:VAL:HG21	1:C:398:ARG:NH2	2.27	0.48
2:D:20:VAL:HG21	2:D:271:LEU:HB2	1.95	0.48
2:D:166:ILE:HG13	2:D:307:VAL:HG11	1.96	0.48
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.43	0.48
1:B:188:ARG:HH11	1:B:188:ARG:HG2	1.78	0.48
3:G:13:ILE:HD13	3:G:242:MET:SD	2.53	0.48
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.96	0.48
1:C:258:ARG:NH1	1:C:308:ARG:O	2.46	0.48
2:F:52:HIS:CD2	2:F:58:VAL:HG12	2.49	0.48
1:A:420:ARG:HH21	1:A:451:GLY:CA	2.26	0.48
1:B:100:GLY:O	1:B:103:LEU:HD13	2.14	0.48
1:B:41:VAL:HG11	1:B:44:LEU:CD1	2.43	0.48
1:B:27:GLU:OE1	1:B:90:ARG:NH1	2.47	0.48
1:C:52:MET:HE1	1:C:76:PHE:HE2	1.79	0.48
2:D:324:THR:O	2:D:324:THR:HG22	2.14	0.48
2:E:387:ILE:HG23	2:E:391:LEU:HD12	1.95	0.48
2:F:139:VAL:HG23	8:F:2100:HOH:O	2.13	0.48
2:F:422:GLU:HG2	2:F:427:HIS:O	2.14	0.48
2:F:97:VAL:HG21	2:F:228:ALA:HB1	1.96	0.48
1:C:168:ILE:HG23	1:C:351:PHE:HD1	1.78	0.48
2:F:406:ARG:HH21	2:F:447:GLY:CA	2.27	0.48
3:G:23:MET:HB2	3:G:232:MET:HE2	1.96	0.48
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.94	0.48
1:A:48:GLN:HG2	2:E:70:VAL:HG22	1.95	0.47
1:A:87:ILE:HD12	1:A:87:ILE:N	2.27	0.47
1:B:486:ASP:C	1:B:488:LYS:N	2.67	0.47
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.48	0.47
1:B:218:LYS:HG3	2:E:128:VAL:HB	1.96	0.47
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.14	0.47
2:E:183:PHE:HB3	2:E:217:LEU:CD2	2.42	0.47
2:D:252:LEU:HD23	2:D:305:THR:HB	1.96	0.47
2:D:430:LYS:HD2	2:D:465:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:ILE:HB	2:D:85:PRO:HD2	1.95	0.47
2:E:370:VAL:HG21	2:E:438:ILE:CG2	2.44	0.47
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.97	0.47
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.96	0.47
1:A:94:ILE:HG21	1:A:128:ARG:NH1	2.29	0.47
1:B:175:LYS:NZ	8:B:2024:HOH:O	2.47	0.47
1:A:286:ARG:NH2	2:D:273:GLY:O	2.48	0.47
2:D:410:ILE:O	2:D:414:LEU:HG	2.14	0.47
2:E:405:SER:O	2:E:409:LYS:HG3	2.14	0.47
2:F:151:LYS:NZ	2:F:293:GLN:HB3	2.29	0.47
3:G:28:ALA:HA	3:G:229:MET:SD	2.54	0.47
2:D:285:LEU:C	2:D:285:LEU:HD23	2.34	0.47
1:B:102:GLU:HG3	1:B:122:GLY:O	2.15	0.47
2:F:89:GLU:CD	2:F:89:GLU:H	2.16	0.47
2:F:389:ALA:HB1	3:G:242:MET:CE	2.44	0.47
1:C:137:ILE:HG21	2:D:104:GLU:OE1	2.14	0.47
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.45	0.47
1:C:456:LEU:HG	1:C:457:GLU:N	2.30	0.47
1:A:195:GLU:HA	1:A:198:LYS:HD2	1.95	0.47
1:A:420:ARG:HH21	1:A:451:GLY:HA3	1.79	0.47
1:B:486:ASP:C	1:B:488:LYS:H	2.18	0.47
2:E:456:ALA:HB1	2:E:466:ALA:O	2.14	0.47
1:B:165:GLU:O	1:B:325:PRO:HD2	2.14	0.47
1:B:357:PHE:HD1	1:B:358:TYR:HD1	1.63	0.47
1:B:451:GLY:O	1:B:453:LEU:N	2.48	0.47
1:C:103:LEU:O	1:C:106:ARG:HB2	2.15	0.47
1:C:297:ASP:HA	2:D:267:GLU:HG2	1.96	0.47
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.97	0.47
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.48	0.47
1:A:354:THR:HG23	8:A:2028:HOH:O	2.15	0.47
2:D:279:VAL:O	2:D:279:VAL:HG12	2.15	0.47
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.79	0.47
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.44	0.47
3:G:81:ILE:HG22	3:G:82:HIS:N	2.30	0.47
1:A:164:ARG:HD2	1:A:309:ALA:HB3	1.97	0.47
1:A:373:ARG:NH2	2:E:189:ARG:NH2	2.62	0.47
1:A:380:THR:HG23	8:A:2021:HOH:O	2.15	0.47
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.97	0.47
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.80	0.46
1:C:74:VAL:HG11	1:C:281:MET:SD	2.56	0.46
2:E:95:MET:HE3	8:E:2012:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:MET:HG3	2:F:99:GLY:HA2	1.96	0.46
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.31	0.46
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.97	0.46
1:A:99:VAL:HG22	1:A:253:MET:HA	1.97	0.46
1:B:420:ARG:HH21	1:B:451:GLY:CA	2.28	0.46
1:C:404:ALA:O	1:C:406:PHE:N	2.48	0.46
1:A:144:GLU:HA	1:A:145:PRO:HD3	1.80	0.46
1:C:309:ALA:HB1	1:C:321:LEU:O	2.14	0.46
2:D:228:ALA:O	2:D:232:VAL:HG22	2.15	0.46
2:D:321:ALA:HB3	2:D:322:PRO:HD3	1.96	0.46
2:E:254:PHE:HA	2:E:307:VAL:O	2.15	0.46
2:E:97:VAL:HG21	2:E:228:ALA:HB1	1.96	0.46
1:A:48:GLN:HA	2:E:69:LEU:O	2.16	0.46
1:B:94:ILE:O	1:B:95:VAL:C	2.54	0.46
2:F:190:THR:HA	2:F:221:GLN:HG3	1.96	0.46
1:B:385:GLN:OE1	1:B:488:LYS:HG3	2.15	0.46
1:B:438:ILE:HG22	8:B:2080:HOH:O	2.16	0.46
2:D:383:SER:O	2:D:387:ILE:HD12	2.15	0.46
2:E:49:VAL:HA	2:E:60:THR:HG22	1.98	0.46
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.96	0.46
1:A:452:TYR:CD2	1:A:501:VAL:HG21	2.50	0.46
1:B:137:ILE:N	1:B:138:PRO:CD	2.78	0.46
1:B:389:THR:O	1:B:393:GLU:HG3	2.15	0.46
1:A:207:GLY:O	1:A:236:ALA:HB2	2.14	0.46
2:E:370:VAL:HG21	2:E:438:ILE:HG23	1.96	0.46
2:E:422:GLU:OE1	2:E:428:LEU:HA	2.16	0.46
2:E:449:TYR:CE2	2:E:463:ILE:HG12	2.50	0.46
2:F:360:PRO:HD3	2:F:368:TYR:CD1	2.51	0.46
1:A:297:ASP:HA	8:E:2026:HOH:O	2.15	0.46
1:A:338:ILE:N	1:A:339:PRO:HD2	2.31	0.46
2:E:80:ALA:HB1	2:E:81:PRO:CD	2.39	0.46
2:F:212:THR:O	2:F:214:LYS:HD2	2.15	0.46
2:F:80:ALA:HB1	2:F:81:PRO:HD3	1.97	0.46
1:B:103:LEU:N	1:B:103:LEU:HD12	2.30	0.46
1:B:171:ARG:HH11	1:B:171:ARG:CB	2.24	0.46
2:E:421:ALA:HB1	2:E:425:THR:HG21	1.97	0.46
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.46	0.46
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.97	0.45
1:A:188:ARG:NH2	1:A:436:MET:HA	2.31	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
2:D:410:ILE:HG13	2:D:444:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:38:LEU:HD11	3:G:42:ARG:CZ	2.46	0.45
1:C:361:ILE:O	1:C:364:ALA:HA	2.16	0.45
2:D:313:PRO:O	2:D:314:ALA:C	2.54	0.45
2:E:152:ILE:HA	2:E:331:ALA:O	2.17	0.45
1:B:286:ARG:HA	2:E:275:ILE:CD1	2.47	0.45
2:E:36:LEU:O	2:E:46:VAL:HA	2.16	0.45
2:F:393:MET:SD	2:F:404:VAL:HG11	2.56	0.45
1:A:157:VAL:O	1:A:159:ILE:HD13	2.15	0.45
1:A:450:ARG:HD2	8:A:2095:HOH:O	2.16	0.45
2:D:95:MET:HG3	2:D:108:ILE:CD1	2.45	0.45
2:F:282:GLN:HA	2:F:283:PRO:HD3	1.87	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.16	0.45
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.46	0.45
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.51	0.45
1:B:127:ARG:NE	1:B:131:LEU:HD12	2.31	0.45
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.47	0.45
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.98	0.45
2:F:389:ALA:HB1	3:G:242:MET:HE1	1.97	0.45
1:C:48:GLN:HA	2:D:69:LEU:O	2.17	0.45
2:F:17:ILE:HD12	2:F:17:ILE:N	2.31	0.45
2:F:229:ARG:HA	2:F:232:VAL:CG2	2.47	0.45
1:A:403:PHE:CD1	3:G:22:SER:HB2	2.52	0.45
1:A:204:VAL:CG1	1:A:206:ILE:HD11	2.46	0.45
1:B:107:VAL:HG12	1:B:115:ILE:HD11	1.99	0.45
1:C:52:MET:HA	1:C:52:MET:HE3	1.98	0.45
1:A:400:VAL:HG12	1:A:418:LEU:CD2	2.44	0.45
1:B:392:LEU:O	1:B:395:ALA:HB3	2.17	0.45
1:C:76:PHE:HB3	1:C:242:LEU:HD21	1.99	0.45
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.41	0.45
2:F:337:ARG:HH11	2:F:337:ARG:HG3	1.81	0.45
1:A:249:SER:O	1:A:253:MET:HG3	2.15	0.45
1:C:234:ALA:HA	1:C:238:ASP:OD2	2.17	0.45
2:D:140:VAL:HG23	8:D:2027:HOH:O	2.16	0.45
2:E:138:LYS:NZ	2:E:413:PHE:O	2.43	0.45
1:A:419:SER:O	1:A:423:ARG:HD3	2.17	0.45
2:D:363:VAL:HB	2:D:367:HIS:ND1	2.32	0.45
2:F:241:GLU:CD	2:F:295:ARG:HH21	2.21	0.45
2:F:462:PRO:HD2	2:F:465:GLU:CD	2.37	0.45
1:A:204:VAL:HG12	1:A:206:ILE:CD1	2.47	0.44
1:C:384:LYS:HE3	8:C:2089:HOH:O	2.17	0.44
2:E:116:ILE:HA	2:E:238:THR:OG1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:292:MET:SD	2:E:293:GLN:NE2	2.90	0.44
3:G:237:LYS:O	3:G:241:GLU:HG3	2.16	0.44
3:G:259:THR:HG22	3:G:263:ILE:HD12	1.99	0.44
1:A:164:ARG:N	1:A:164:ARG:HD3	2.32	0.44
1:A:486:ASP:OD2	1:A:490:SER:HB3	2.17	0.44
1:B:54:GLU:HG3	1:B:91:THR:HG22	1.99	0.44
2:D:103:ASP:O	2:D:104:GLU:HB2	2.17	0.44
2:E:94:ILE:HD11	2:E:197:TYR:CG	2.52	0.44
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.98	0.44
1:B:99:VAL:O	1:B:123:SER:OG	2.36	0.44
1:C:33:SER:OG	1:C:40:ARG:HB2	2.18	0.44
1:C:414:THR:O	1:C:418:LEU:HG	2.17	0.44
2:E:189:ARG:NH1	2:E:192:GLU:OE1	2.51	0.44
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.99	0.44
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.47	0.44
2:F:34:ASN:O	2:F:49:VAL:HG23	2.18	0.44
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.52	0.44
2:D:161:GLY:O	2:D:162:LYS:C	2.55	0.44
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.18	0.44
2:E:96:ASN:HB2	2:E:102:ILE:CG2	2.47	0.44
2:E:96:ASN:HB2	2:E:102:ILE:HG23	1.99	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.44
2:D:84:ILE:HD12	2:D:95:MET:HE1	2.00	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.63	0.44
2:F:203:SER:OG	2:F:205:VAL:HG13	2.16	0.44
2:F:29:LEU:HA	2:F:30:PRO:HD3	1.78	0.44
1:C:215:GLN:HG3	2:F:356:ARG:HH12	1.83	0.44
2:F:357:ILE:HG23	2:F:362:ILE:CG2	2.47	0.44
2:F:437:THR:O	2:F:441:PHE:HD2	2.00	0.44
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.48	0.44
1:B:142:VAL:HG13	8:B:2021:HOH:O	2.17	0.44
1:B:251:CYS:O	1:B:255:GLU:HG3	2.18	0.44
1:B:55:PHE:CE2	1:B:82:ILE:HD13	2.53	0.44
2:E:319:ASP:O	2:E:320:PRO:C	2.54	0.44
2:F:319:ASP:O	2:F:322:PRO:HD2	2.17	0.44
1:A:105:GLY:HA2	1:A:226:MET:O	2.17	0.44
1:C:419:SER:O	1:C:423:ARG:HG2	2.17	0.44
1:C:503:ASN:O	1:C:506:ALA:HB3	2.18	0.44
1:C:52:MET:CE	1:C:76:PHE:HE2	2.30	0.44
2:D:48:GLU:OE2	2:D:231:ARG:NE	2.32	0.44
2:E:310:ILE:CD1	2:E:329:LEU:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HD11	2:E:193:GLY:HA3	1.99	0.44
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.45	0.44
1:C:185:ASN:OD1	1:C:435:PRO:HB2	2.18	0.44
2:D:151:LYS:HE2	2:D:328:HIS:O	2.18	0.44
1:A:166:LEU:HB3	1:A:349:GLN:HG3	2.00	0.43
1:A:278:TYR:HA	1:A:281:MET:HE2	2.00	0.43
1:A:485:THR:C	1:A:487:GLY:H	2.21	0.43
1:C:151:LYS:HG2	1:C:441:GLN:HG2	1.99	0.43
2:D:266:SER:HB3	2:D:282:GLN:NE2	2.33	0.43
2:D:411:GLN:O	2:D:414:LEU:HB2	2.18	0.43
1:A:211:SER:O	1:A:214:ALA:HB3	2.17	0.43
1:B:237:SER:HB3	8:B:2033:HOH:O	2.18	0.43
1:B:379:GLN:HB3	1:B:384:LYS:HE2	2.00	0.43
2:D:374:VAL:HG13	2:D:410:ILE:HG21	2.00	0.43
2:D:452:LEU:HD22	2:D:470:ALA:CB	2.48	0.43
2:E:421:ALA:HB1	2:E:425:THR:CG2	2.48	0.43
2:E:81:PRO:HG2	2:E:115:ALA:HB1	2.00	0.43
1:C:225:ALA:HA	1:C:228:TYR:CE2	2.53	0.43
1:C:476:HIS:CD2	1:C:500:ILE:HD11	2.53	0.43
1:C:78:ASN:OD1	1:C:80:LYS:HB3	2.17	0.43
1:C:98:PRO:CG	1:C:112:GLY:HA3	2.49	0.43
1:A:36:ASP:OD1	2:D:274:ARG:NH2	2.51	0.43
2:F:226:PRO:HA	2:F:229:ARG:HH21	1.82	0.43
2:F:33:LEU:O	2:F:81:PRO:HB3	2.18	0.43
1:A:108:VAL:HG12	1:A:114:ALA:HA	1.99	0.43
1:B:140:ILE:HG22	1:B:311:LYS:HG3	2.00	0.43
1:B:295:PRO:O	1:B:298:VAL:HG22	2.19	0.43
1:C:389:THR:HG22	2:D:425:THR:O	2.18	0.43
2:E:449:TYR:HB3	2:E:452:LEU:CD1	2.37	0.43
1:A:327:ILE:HD11	1:A:342:VAL:HG21	2.01	0.43
1:B:366:ASN:HD21	1:B:369:LEU:HD12	1.81	0.43
1:C:362:ARG:HA	1:C:363:PRO:C	2.39	0.43
2:E:151:LYS:HE3	2:E:296:ILE:HG22	2.01	0.43
2:E:388:ILE:CD1	2:E:396:LEU:HD11	2.48	0.43
3:G:78:CYS:SG	3:G:228:ARG:NH2	2.90	0.43
1:A:286:ARG:HH11	1:A:286:ARG:HG2	1.83	0.43
1:B:106:ARG:NH1	1:B:121:ILE:HD13	2.33	0.43
1:C:240:ALA:N	1:C:241:PRO:CD	2.81	0.43
2:E:352:ASP:O	2:E:354:THR:HG23	2.19	0.43
1:B:33:SER:HB2	2:E:52:HIS:O	2.18	0.43
2:E:89:GLU:H	2:E:89:GLU:CD	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:14:LYS:HG2	3:G:243:ILE:HD13	2.00	0.43
1:C:290:GLY:O	1:C:291:ARG:C	2.57	0.43
1:C:248:TYR:OH	1:C:301:LEU:HD12	2.19	0.43
2:F:220:GLY:HA3	2:F:232:VAL:HG11	2.00	0.43
1:A:486:ASP:C	1:A:488:LYS:H	2.22	0.43
1:B:269:ASP:HA	1:B:270:ASP:HA	1.74	0.43
1:B:297:ASP:HA	8:F:2061:HOH:O	2.19	0.43
1:C:36:ASP:HB3	1:C:284:LEU:HD13	2.01	0.43
2:D:27:GLU:HB2	2:D:28:GLY:H	1.68	0.43
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.49	0.43
1:C:164:ARG:HD2	1:C:306:LEU:O	2.18	0.43
1:C:381:ARG:HD2	1:C:381:ARG:N	2.33	0.43
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.84	0.43
1:B:176:THR:O	1:B:179:ALA:N	2.49	0.43
2:F:163:THR:HG21	2:F:192:GLU:OE1	2.19	0.43
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.74	0.42
1:B:194:ASP:C	1:B:196:LYS:H	2.22	0.42
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.88	0.42
1:C:201:CYS:O	1:C:229:THR:HA	2.18	0.42
1:C:338:ILE:HD12	1:C:338:ILE:N	2.32	0.42
2:D:17:ILE:HD13	2:D:17:ILE:HG21	1.75	0.42
2:D:49:VAL:HA	2:D:60:THR:HG22	2.01	0.42
2:E:142:LEU:HG	2:E:143:LEU:CD2	2.49	0.42
2:F:83:ARG:NH2	2:F:113:PHE:HB2	2.34	0.42
3:G:10:LEU:HD21	3:G:246:LEU:HB2	2.01	0.42
1:B:204:VAL:HG12	1:B:206:ILE:HG13	2.00	0.42
1:C:200:TYR:O	1:C:264:ALA:HA	2.19	0.42
2:D:165:LEU:O	2:D:169:LEU:HG	2.18	0.42
2:E:298:THR:HA	2:E:303:SER:HB2	2.01	0.42
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.54	0.42
1:B:171:ARG:HH22	2:E:356:ARG:NH2	2.13	0.42
2:F:170:ILE:O	2:F:174:ALA:HB3	2.18	0.42
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.02	0.42
1:B:76:PHE:O	1:B:242:LEU:HD21	2.19	0.42
1:C:233:SER:OG	1:C:235:THR:HG23	2.19	0.42
1:C:287:ARG:HA	1:C:288:PRO:HD3	1.78	0.42
1:C:444:VAL:CG1	1:C:469:LEU:HD13	2.49	0.42
2:F:370:VAL:HG22	2:F:442:GLN:HG2	2.01	0.42
1:B:288:PRO:HB3	2:F:276:PRO:HG3	2.02	0.42
1:C:338:ILE:O	1:C:341:ASN:HB2	2.20	0.42
2:D:237:LEU:HD21	2:D:295:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLY:C	1:B:453:LEU:N	2.72	0.42
2:E:246:GLN:HA	2:E:246:GLN:HE21	1.85	0.42
1:A:159:ILE:CD1	1:A:165:GLU:HG2	2.49	0.42
1:A:138:PRO:HB3	1:A:316:PHE:CE1	2.55	0.42
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.54	0.42
1:B:481:GLY:HA2	1:B:484:ARG:NH1	2.35	0.42
1:C:343:ILE:HG22	2:D:158:ALA:HB1	2.02	0.42
2:D:188:GLU:O	2:D:221:GLN:HB3	2.20	0.42
2:E:125:GLU:HA	2:E:300:LYS:HE3	2.02	0.42
1:A:175:LYS:HB2	1:A:175:LYS:HE3	1.77	0.42
1:A:389:THR:CB	1:A:449:VAL:HG21	2.38	0.42
1:C:127:ARG:NH2	1:C:131:LEU:HD12	2.35	0.42
1:C:179:ALA:HB1	1:C:267:ILE:HG12	2.01	0.42
1:C:55:PHE:O	1:C:56:SER:C	2.58	0.42
1:C:370:SER:O	1:C:371:VAL:HG12	2.20	0.42
1:C:156:LEU:HD11	1:C:428:LEU:HD11	2.02	0.42
2:D:181:SER:HB2	2:D:215:VAL:HG22	2.02	0.42
1:A:177:SER:OG	4:A:600:ANP:H8	2.20	0.42
1:B:105:GLY:HA2	1:B:226:MET:O	2.20	0.42
1:C:99:VAL:HG11	1:C:256:TYR:HB2	2.02	0.42
2:D:29:LEU:HA	2:D:30:PRO:HD2	1.85	0.42
2:D:313:PRO:O	2:D:315:ASP:N	2.53	0.42
2:E:120:ALA:O	2:E:121:PRO:C	2.58	0.42
2:E:25:PHE:HB2	2:E:29:LEU:HD12	2.02	0.42
2:E:393:MET:HG3	2:E:396:LEU:CD1	2.50	0.42
2:F:82:ILE:O	2:F:115:ALA:HA	2.20	0.42
1:A:411:ASP:OD2	1:A:414:THR:HG23	2.20	0.41
1:B:137:ILE:HB	1:B:138:PRO:HD3	2.01	0.41
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.55	0.41
1:C:103:LEU:HB2	1:C:230:ILE:HD13	2.01	0.41
1:B:62:MET:HB2	1:B:76:PHE:CE2	2.54	0.41
1:B:80:LYS:HG3	1:B:81:LEU:N	2.34	0.41
2:D:163:THR:O	2:D:166:ILE:HG22	2.20	0.41
2:D:370:VAL:O	2:D:374:VAL:HG23	2.20	0.41
2:F:247:GLU:HB3	2:F:249:GLN:HG2	2.02	0.41
2:F:439:LYS:HE3	2:F:443:GLN:OE1	2.20	0.41
1:A:390:MET:HE3	1:A:424:LEU:HD22	2.02	0.41
1:B:157:VAL:N	1:B:158:PRO:CD	2.84	0.41
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.55	0.41
2:E:330:ASP:O	2:E:356:ARG:HG3	2.19	0.41
2:D:287:THR:O	2:D:291:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:409:LYS:HD3	2:D:457:PHE:CE1	2.55	0.41
2:E:32:ILE:O	2:E:33:LEU:HB2	2.20	0.41
1:A:188:ARG:HH21	1:A:437:ALA:N	2.18	0.41
1:C:295:PRO:HD2	1:C:298:VAL:HG22	2.01	0.41
2:E:147:ALA:HB2	2:E:357:ILE:HD13	2.02	0.41
2:E:422:GLU:O	2:E:424:PHE:N	2.53	0.41
1:C:265:LEU:HD11	1:C:324:LEU:HG	2.03	0.41
1:C:367:VAL:HG21	1:C:398:ARG:HH21	1.85	0.41
2:D:82:ILE:HB	2:D:116:ILE:HG12	2.03	0.41
2:F:229:ARG:HA	2:F:232:VAL:HG22	2.03	0.41
2:F:139:VAL:HG11	2:F:348:VAL:HB	2.03	0.41
1:B:211:SER:HA	2:E:126:MET:CE	2.47	0.41
1:C:505:LEU:O	1:C:508:PHE:HB3	2.20	0.41
2:D:346:PRO:HG3	2:D:418:PHE:CZ	2.56	0.41
2:E:36:LEU:HB2	2:E:47:LEU:HB2	2.03	0.41
1:B:345:ILE:O	2:F:189:ARG:NE	2.53	0.41
2:D:340:ALA:HB2	2:D:347:ALA:CB	2.51	0.41
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.55	0.41
2:E:298:THR:HA	2:E:303:SER:CB	2.51	0.41
2:E:25:PHE:O	2:E:56:SER:HB3	2.21	0.41
2:F:274:ARG:HA	8:F:2064:HOH:O	2.20	0.41
3:G:32:ALA:O	3:G:36:ARG:HG3	2.20	0.41
1:A:134:PRO:HG2	1:A:139:ARG:NH2	2.36	0.41
1:A:251:CYS:O	1:A:255:GLU:HG3	2.21	0.41
1:A:283:LEU:CD2	1:A:289:PRO:HB3	2.50	0.41
1:B:172:GLN:HA	4:B:600:ANP:HNB1	1.85	0.41
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.34	0.41
2:D:186:VAL:HG12	2:D:260:ARG:HB2	2.03	0.41
2:D:275:ILE:HG23	2:D:276:PRO:HD2	2.02	0.41
2:F:438:ILE:O	2:F:442:GLN:HG3	2.21	0.41
1:A:180:ILE:O	1:A:181:ASP:C	2.59	0.41
1:A:235:THR:HB	8:A:2038:HOH:O	2.21	0.41
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.89	0.41
1:B:423:ARG:HD2	1:B:461:ILE:HD11	2.02	0.41
1:C:432:GLN:NE2	8:C:2097:HOH:O	2.53	0.41
2:D:188:GLU:OE1	2:D:188:GLU:HA	2.21	0.41
2:D:92:GLY:HA2	2:D:206:ILE:HG12	2.02	0.41
2:D:210:ASP:HB2	2:D:211:ALA:H	1.69	0.41
2:D:189:ARG:O	2:D:221:GLN:OE1	2.38	0.41
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.56	0.41
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HB	1:A:98:PRO:CD	2.47	0.40
1:B:38:ILE:HD11	1:B:74:VAL:HG22	2.02	0.40
1:C:36:ASP:OD2	2:F:274:ARG:HD2	2.20	0.40
1:C:419:SER:HB3	1:C:423:ARG:HH12	1.85	0.40
2:D:196:LEU:HG	2:D:200:MET:HE2	2.03	0.40
2:D:47:LEU:HD23	2:D:62:ALA:HA	2.03	0.40
2:E:96:ASN:HD22	2:E:100:GLU:HB2	1.85	0.40
2:E:282:GLN:HA	2:E:283:PRO:HD3	1.80	0.40
2:F:89:GLU:OE2	2:F:110:THR:HG22	2.21	0.40
1:B:374:VAL:CG2	1:B:374:VAL:O	2.61	0.40
2:D:183:PHE:CD2	2:D:254:PHE:HB2	2.56	0.40
2:D:9:THR:HA	2:D:27:GLU:OE1	2.20	0.40
2:E:144:ALA:N	2:E:145:PRO:CD	2.84	0.40
2:E:162:LYS:NZ	2:E:256:ASP:OD2	2.40	0.40
2:E:126:MET:HE1	2:E:297:THR:HG21	2.04	0.40
2:E:467:VAL:O	2:E:468:ALA:C	2.60	0.40
1:A:485:THR:C	1:A:487:GLY:N	2.75	0.40
1:B:140:ILE:CG2	1:B:311:LYS:HG3	2.51	0.40
1:C:74:VAL:CG1	1:C:241:PRO:CG	2.99	0.40
1:C:450:ARG:HA	1:C:450:ARG:HD3	1.76	0.40
2:D:348:VAL:HG21	8:D:2027:HOH:O	2.22	0.40
1:A:212:THR:HG23	2:D:356:ARG:HH12	1.86	0.40
1:C:406:PHE:HE2	2:D:393:MET:HB2	1.86	0.40
2:E:321:ALA:N	2:E:322:PRO:HD2	2.36	0.40
2:E:412:ARG:O	2:E:415:SER:OG	2.36	0.40
1:A:327:ILE:HD12	1:A:338:ILE:HG22	2.03	0.40
1:C:139:ARG:HH11	1:C:139:ARG:HD3	1.59	0.40
1:B:194:ASP:OD2	1:B:196:LYS:HB2	2.21	0.40
1:B:496:LYS:HG2	1:B:500:ILE:HD11	2.02	0.40
1:A:80:LYS:HE3	2:D:33:LEU:HD12	2.02	0.40
1:C:403:PHE:CG	2:D:408:ARG:NH2	2.89	0.40
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.22	0.40
3:G:39:LYS:HB2	3:G:40:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	452 (93%)	25 (5%)	8 (2%)	9	18
1	B	475/510 (93%)	434 (91%)	38 (8%)	3 (1%)	25	45
1	C	490/510 (96%)	457 (93%)	28 (6%)	5 (1%)	15	30
2	D	465/482 (96%)	429 (92%)	32 (7%)	4 (1%)	17	33
2	E	464/482 (96%)	419 (90%)	40 (9%)	5 (1%)	14	27
2	F	464/482 (96%)	431 (93%)	31 (7%)	2 (0%)	34	55
3	G	116/272 (43%)	107 (92%)	6 (5%)	3 (3%)	5	8
All	All	2959/3248 (91%)	2729 (92%)	200 (7%)	30 (1%)	15	30

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	ASP
2	E	211	ALA
1	B	452	TYR
1	C	337	TYR
1	C	388	GLY
2	E	357	ILE
2	F	247	GLU
3	G	210	ALA
1	A	25	LEU
1	B	195	GLU
1	C	405	GLN
1	C	407	GLY
2	E	423	VAL
1	A	118	LYS
1	A	123	SER
1	A	141	SER
1	C	292	GLU
2	D	347	ALA

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Mol	Chain	Res	Type
2	D	448	GLU
2	E	455	GLN
2	F	246	GLN
1	A	401	ALA
1	A	485	THR
3	G	211	ASN
1	B	95	VAL
1	A	500	ILE
3	G	81	ILE
2	D	81	PRO
2	E	279	VAL
2	D	279	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	365 (93%)	28 (7%)	14	28
1	B	388/412 (94%)	371 (96%)	17 (4%)	28	52
1	C	397/412 (96%)	368 (93%)	29 (7%)	14	27
2	D	377/386 (98%)	358 (95%)	19 (5%)	24	46
2	E	376/386 (97%)	355 (94%)	21 (6%)	21	40
2	F	376/386 (97%)	359 (96%)	17 (4%)	27	50
3	G	102/230 (44%)	97 (95%)	5 (5%)	25	46
All	All	2409/2624 (92%)	2273 (94%)	136 (6%)	21	40

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	47	VAL
1	A	50	GLU
1	A	56	SER
1	A	57	SER

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Mol	Chain	Res	Type
1	A	64	LEU
1	A	99	VAL
1	A	121	ILE
1	A	123	SER
1	A	136	ILE
1	A	140	ILE
1	A	216	LEU
1	A	249	SER
1	A	270	ASP
1	A	338	ILE
1	A	354	THR
1	A	408	SER
1	A	420	ARG
1	A	436	MET
1	A	444	VAL
1	A	459	SER
1	A	460	LYS
1	A	461	ILE
1	A	462	THR
1	A	472	VAL
1	A	479	LEU
1	A	490	SER
1	A	499	GLU
1	B	52	MET
1	B	143	ARG
1	B	171	ARG
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	237	SER
1	B	276	VAL
1	B	298	VAL
1	B	371	VAL
1	B	380	THR
1	B	389	THR
1	B	434	SER
1	B	445	ILE
1	B	459	SER
1	B	474	SER
1	C	47	VAL
1	C	52	MET

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Mol	Chain	Res	Type
1	C	57	SER
1	C	64	LEU
1	C	80	LYS
1	C	83	LYS
1	C	123	SER
1	C	131	LEU
1	C	157	VAL
1	C	164	ARG
1	C	171	ARG
1	C	189	PHE
1	C	208	GLN
1	C	211	SER
1	C	217	VAL
1	C	334	VAL
1	C	349	GLN
1	C	381	ARG
1	C	390	MET
1	C	398	ARG
1	C	416	GLN
1	C	419	SER
1	C	423	ARG
1	C	444	VAL
1	C	470	SER
1	C	472	VAL
1	C	474	SER
1	C	479	LEU
1	C	505	LEU
2	D	27	GLU
2	D	43	THR
2	D	44	ARG
2	D	89	GLU
2	D	97	VAL
2	D	112	GLN
2	D	127	SER
2	D	130	GLN
2	D	154	LEU
2	D	210	ASP
2	D	232	VAL
2	D	250	ASP
2	D	269	SER
2	D	282	GLN
2	D	303	SER

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Mol	Chain	Res	Type
2	D	335	LEU
2	D	358	MET
2	D	401	LYS
2	D	471	ASP
2	E	43	THR
2	E	67	GLU
2	E	112	GLN
2	E	132	ILE
2	E	139	VAL
2	E	164	VAL
2	E	188	GLU
2	E	191	ARG
2	E	223	ASN
2	E	225	PRO
2	E	232	VAL
2	E	252	LEU
2	E	277	SER
2	E	282	GLN
2	E	297	THR
2	E	306	SER
2	E	358	MET
2	E	365	SER
2	E	377	ILE
2	E	395	GLU
2	E	431	LEU
2	F	41	ARG
2	F	51	GLN
2	F	67	GLU
2	F	76	LEU
2	F	95	MET
2	F	96	ASN
2	F	97	VAL
2	F	110	THR
2	F	124	VAL
2	F	166	ILE
2	F	223	ASN
2	F	232	VAL
2	F	237	LEU
2	F	258	ILE
2	F	282	GLN
2	F	292	MET
2	F	405	SER

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Mol	Chain	Res	Type
3	G	77	LEU
3	G	83	SER
3	G	220	SER
3	G	236	SER
3	G	262	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	A	471	HIS
1	B	46	ASN
1	B	65	ASN
1	B	503	ASN
1	C	172	GLN
1	C	260	ASN
1	C	263	HIS
1	C	349	GLN
2	D	39	GLN
2	D	198	HIS
2	D	221	GLN
2	D	282	GLN
2	E	223	ASN
2	E	246	GLN
2	E	263	GLN
2	E	282	GLN
2	E	293	GLN
2	E	308	GLN
2	E	367	HIS
2	E	379	GLN
2	E	411	GLN
2	E	419	GLN
2	F	96	ASN
2	F	223	ASN
2	F	282	GLN
2	F	443	GLN
3	G	82	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ANP	F	600	5	29,33,33	1.48	5 (17%)	31,52,52	1.78	5 (16%)
6	ADP	D	600	5	24,29,29	0.92	2 (8%)	29,45,45	1.27	3 (10%)
7	PO4	E	602	-	4,4,4	0.76	0	6,6,6	0.51	0
4	ANP	B	600	5	29,33,33	1.63	7 (24%)	31,52,52	2.74	7 (22%)
4	ANP	A	600	5	29,33,33	1.46	5 (17%)	31,52,52	1.59	6 (19%)
4	ANP	C	600	5	29,33,33	1.59	6 (20%)	31,52,52	1.60	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	F	600	5	-	4/14/38/38	0/3/3/3
4	ANP	A	600	5	-	3/14/38/38	0/3/3/3
6	ADP	D	600	5	-	5/12/32/32	0/3/3/3
4	ANP	B	600	5	-	3/14/38/38	0/3/3/3
4	ANP	C	600	5	-	3/14/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	ANP	PG-O3G	-4.32	1.45	1.56
4	C	600	ANP	PG-O3G	-3.98	1.46	1.56
4	F	600	ANP	PG-O3G	-3.67	1.46	1.56
4	C	600	ANP	PB-O3A	-3.61	1.54	1.59
4	A	600	ANP	PG-O3G	-3.44	1.47	1.56
4	A	600	ANP	PB-O2B	-3.36	1.47	1.56
4	B	600	ANP	PG-O1G	3.35	1.51	1.46
4	C	600	ANP	PG-O2G	-3.32	1.47	1.56
4	F	600	ANP	PB-O1B	3.29	1.51	1.46
4	A	600	ANP	PG-O2G	-3.28	1.47	1.56
4	C	600	ANP	PB-O2B	-3.15	1.48	1.56
4	A	600	ANP	PB-O3A	3.03	1.62	1.59
4	F	600	ANP	PB-O2B	-3.01	1.48	1.56
4	A	600	ANP	C2-N1	2.80	1.39	1.33
4	F	600	ANP	PG-O2G	-2.80	1.49	1.56
4	B	600	ANP	PG-O2G	-2.58	1.49	1.56
4	B	600	ANP	C2'-C1'	-2.49	1.50	1.53
4	B	600	ANP	PB-O3A	2.43	1.62	1.59
4	F	600	ANP	C2-N1	2.38	1.38	1.33
4	B	600	ANP	PG-N3B	-2.37	1.57	1.63
4	C	600	ANP	C2-N1	2.33	1.38	1.33
4	C	600	ANP	PB-N3B	2.25	1.69	1.63
4	B	600	ANP	C2-N1	2.16	1.37	1.33
6	D	600	ADP	PB-O2B	-2.09	1.46	1.54
6	D	600	ADP	PB-O3B	-2.07	1.46	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ANP	O1B-PB-N3B	12.61	130.33	111.77
4	F	600	ANP	C5-C6-N6	6.45	130.15	120.35
4	A	600	ANP	O2B-PB-O1B	4.58	119.52	109.92
4	B	600	ANP	O2G-PG-O1G	-4.17	102.97	113.45
4	A	600	ANP	C5-C6-N6	3.38	125.48	120.35
4	C	600	ANP	O2B-PB-O3A	3.35	115.81	104.64
4	C	600	ANP	O3G-PG-O2G	3.31	116.45	107.64
4	F	600	ANP	N6-C6-N1	-3.22	111.89	118.57
4	F	600	ANP	O3G-PG-O2G	3.20	116.17	107.64
4	F	600	ANP	O1G-PG-N3B	-3.11	107.19	111.77
4	B	600	ANP	O3G-PG-O2G	2.86	115.25	107.64
6	D	600	ADP	C1'-N9-C4	-2.85	121.64	126.64
4	C	600	ANP	O2G-PG-O1G	-2.77	106.50	113.45
4	B	600	ANP	C5-C6-N6	2.74	124.52	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ANP	C3'-C2'-C1'	2.70	105.04	100.98
4	C	600	ANP	C4-C5-N7	2.69	112.21	109.40
4	A	600	ANP	O1B-PB-N3B	2.69	115.73	111.77
4	A	600	ANP	O3G-PG-O2G	2.55	114.44	107.64
4	C	600	ANP	C3'-C2'-C1'	2.55	104.81	100.98
4	B	600	ANP	C2'-C3'-C4'	2.49	107.48	102.64
6	D	600	ADP	O2B-PB-O3A	2.48	112.96	104.64
4	C	600	ANP	O3A-PB-N3B	-2.33	100.13	106.59
4	C	600	ANP	C2'-C3'-C4'	2.30	107.10	102.64
4	F	600	ANP	O2B-PB-O3A	2.26	112.17	104.64
6	D	600	ADP	O3B-PB-O2B	2.21	116.07	107.64
4	A	600	ANP	O2G-PG-O1G	-2.17	107.99	113.45
4	C	600	ANP	O1G-PG-N3B	-2.11	108.66	111.77
4	B	600	ANP	O3A-PB-N3B	-2.09	100.80	106.59
4	A	600	ANP	O4'-C1'-C2'	-2.06	103.92	106.93

There are no chirality outliers.

All (18) torsion outliers are listed below:

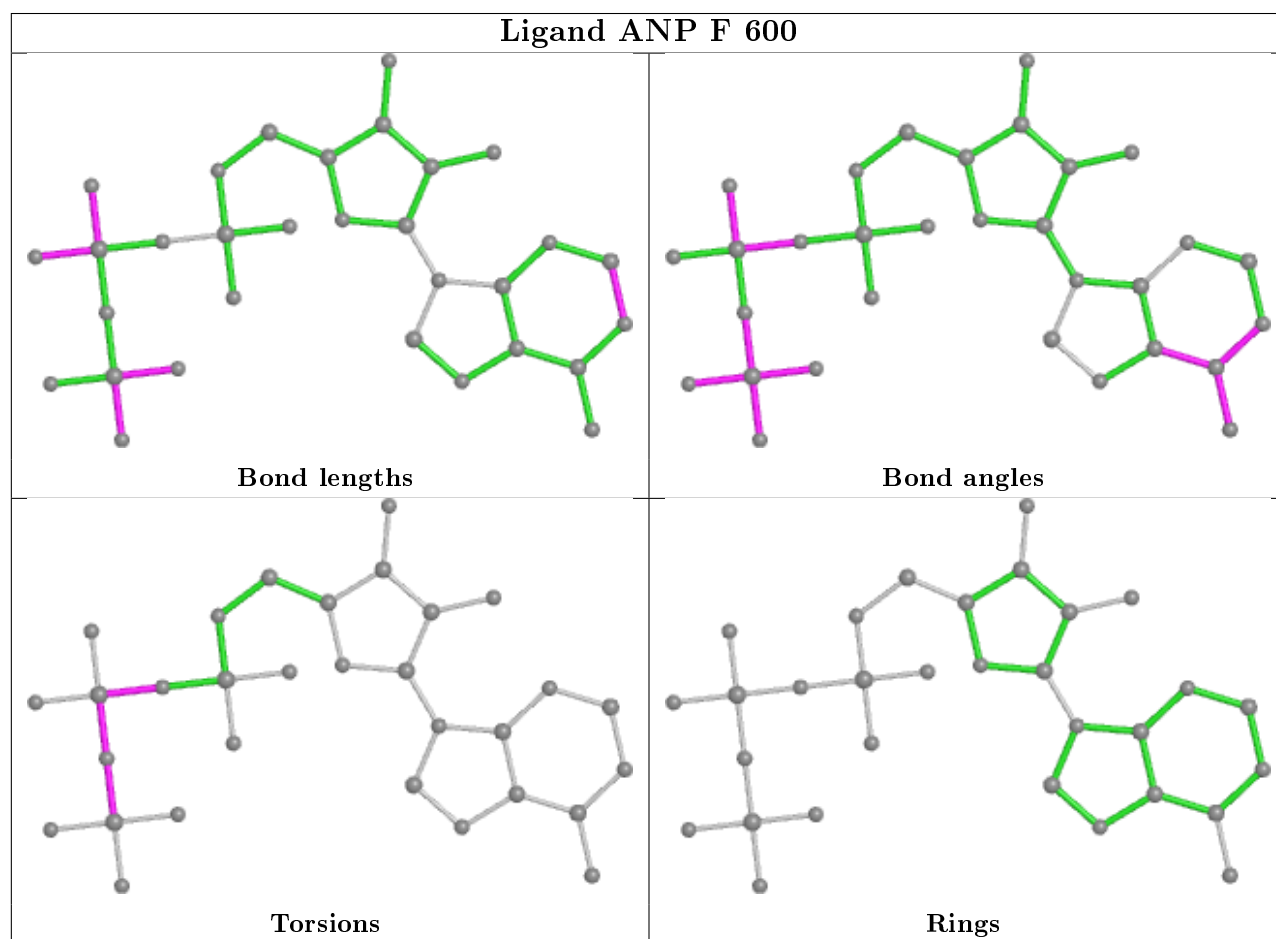
Mol	Chain	Res	Type	Atoms
4	F	600	ANP	PB-N3B-PG-O1G
4	F	600	ANP	PG-N3B-PB-O1B
4	F	600	ANP	PA-O3A-PB-O1B
4	F	600	ANP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O2B
6	D	600	ADP	C5'-O5'-PA-O3A
4	B	600	ANP	PB-N3B-PG-O1G
4	B	600	ANP	PG-N3B-PB-O1B
4	B	600	ANP	PA-O3A-PB-O1B
4	A	600	ANP	PB-N3B-PG-O1G
4	A	600	ANP	PG-N3B-PB-O1B
4	C	600	ANP	PB-N3B-PG-O1G
4	C	600	ANP	PG-N3B-PB-O1B
4	C	600	ANP	PG-N3B-PB-O3A
6	D	600	ADP	C3'-C4'-C5'-O5'
6	D	600	ADP	O4'-C4'-C5'-O5'
6	D	600	ADP	PA-O3A-PB-O3B
4	A	600	ANP	PG-N3B-PB-O3A

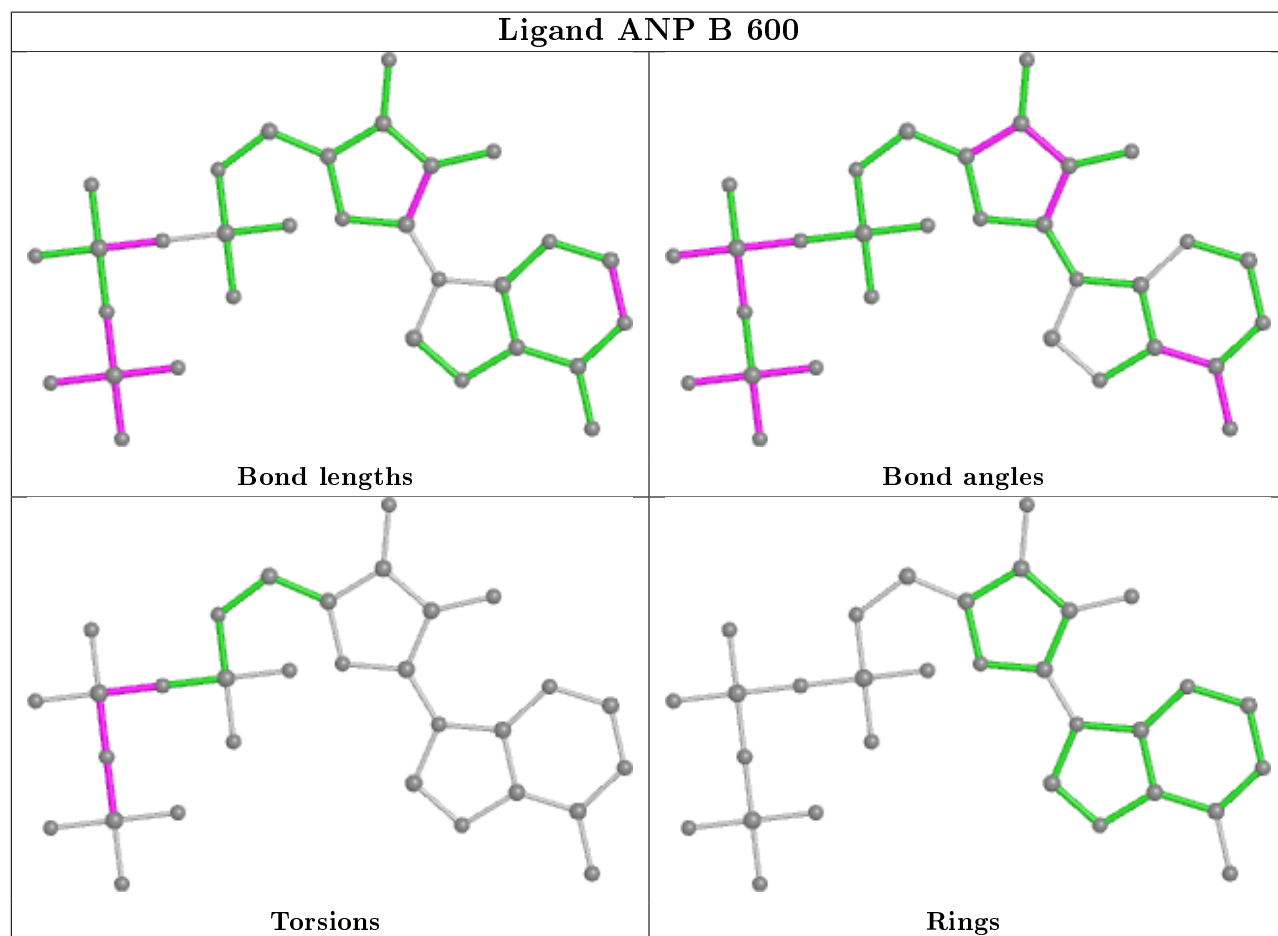
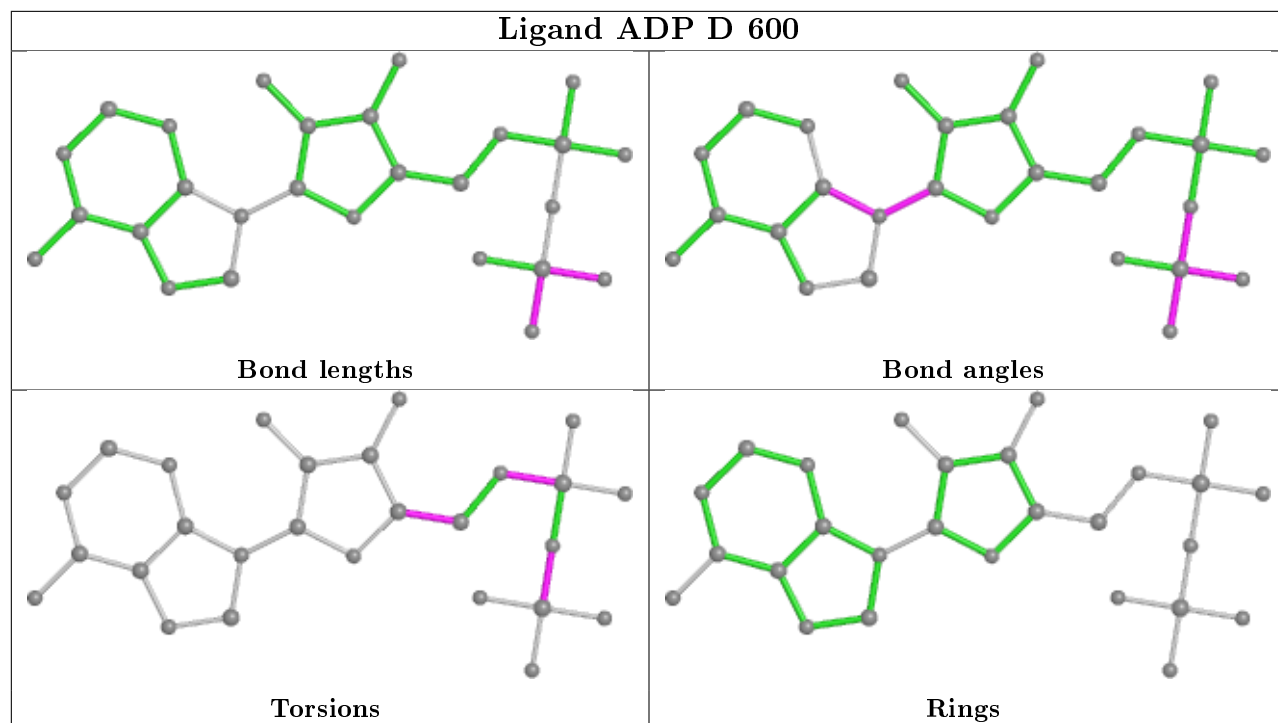
There are no ring outliers.

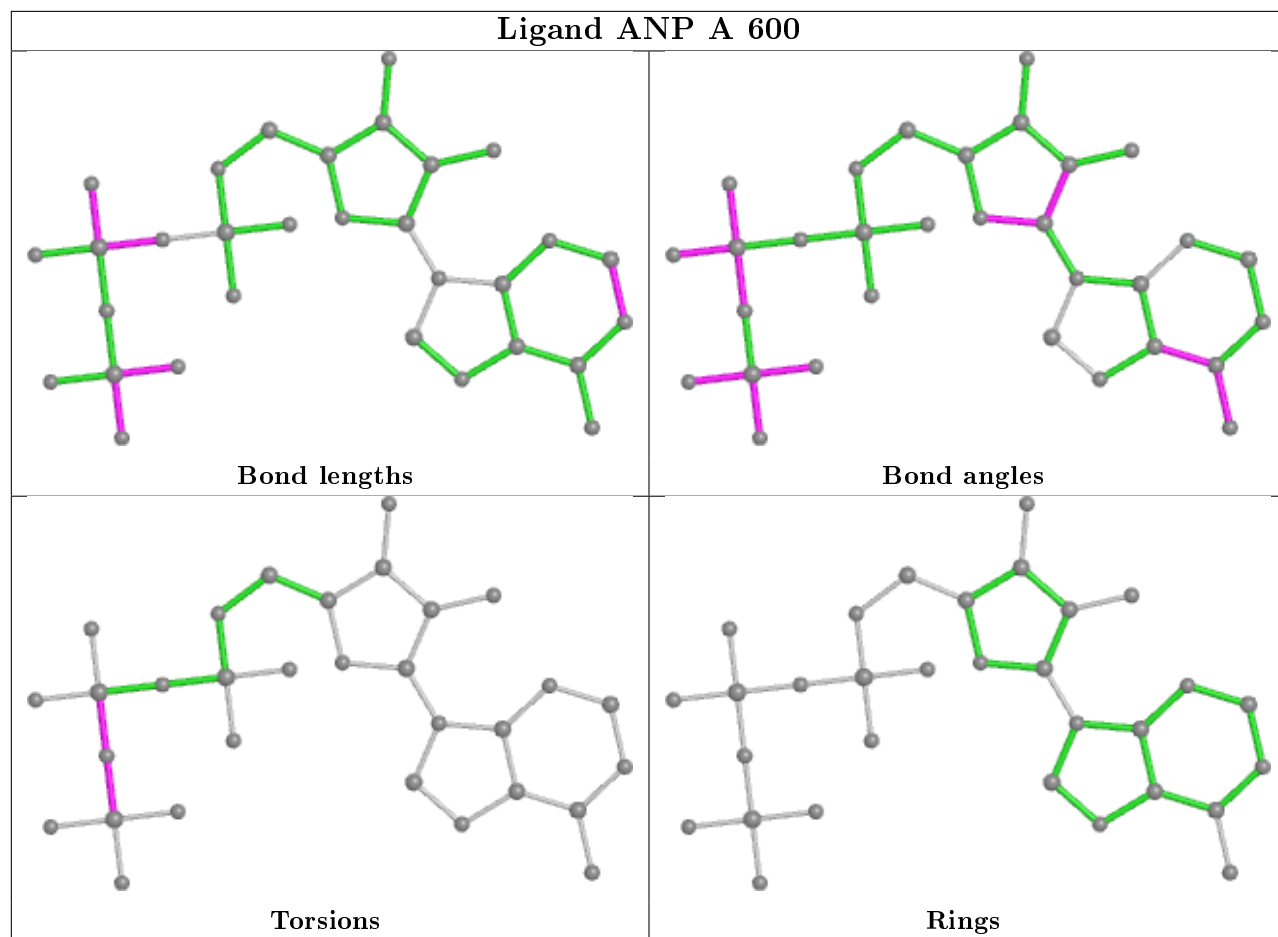
5 monomers are involved in 7 short contacts:

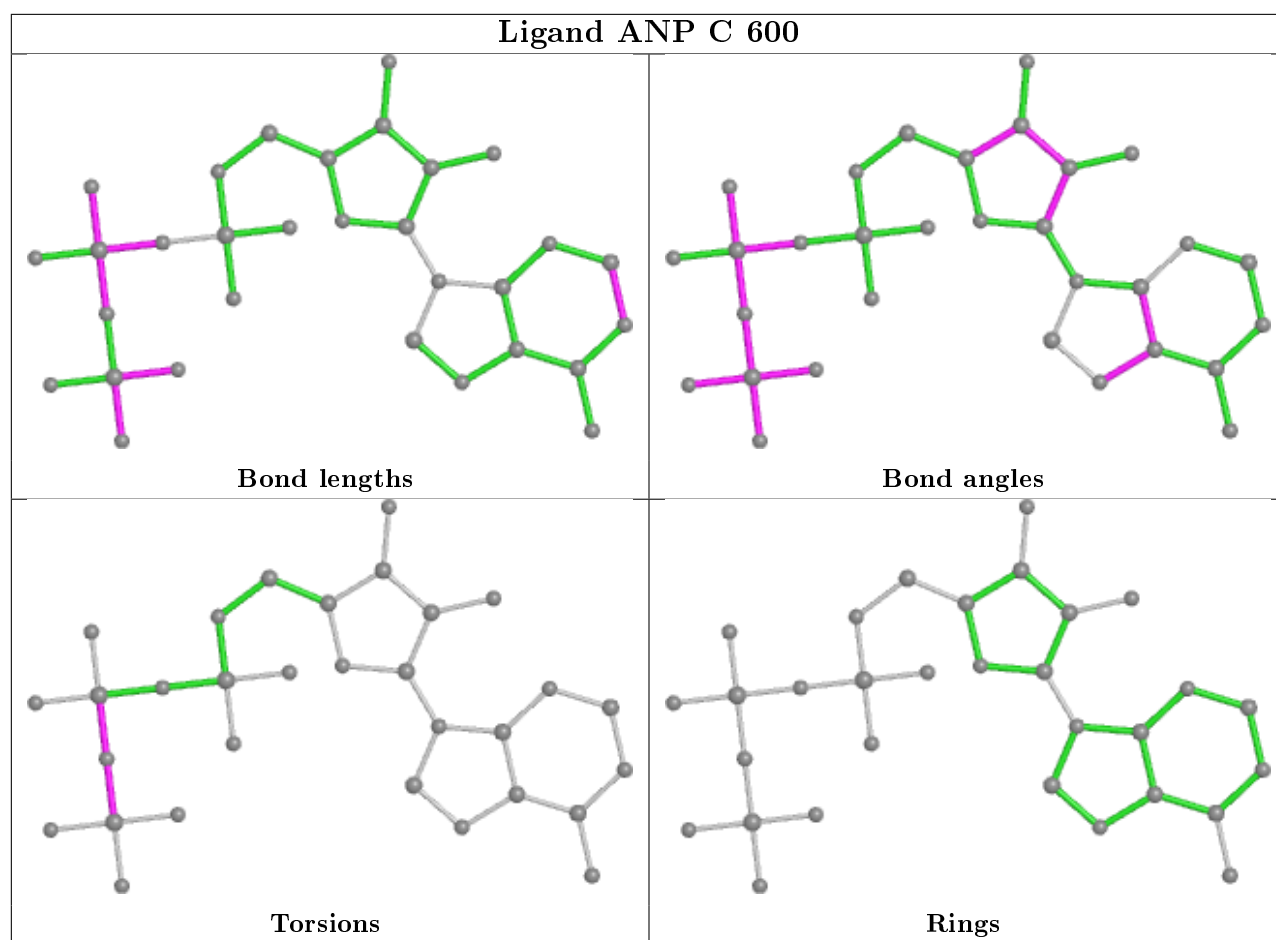
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	ADP	1	0
7	E	602	PO4	1	0
4	B	600	ANP	2	0
4	A	600	ANP	1	0
4	C	600	ANP	2	0

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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.