



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 06:58 PM JST

PDB ID : 7COQ  
Title : Hexameric Ring Complex of Engineered V1-ATPase bound to AMP-PNP:  
A3(De)3\_(ANP)1cat  
Authors : Kosugi, T.; Tanabe, M.; Koga, N.  
Deposited on : 2020-08-05  
Resolution : 3.44 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:

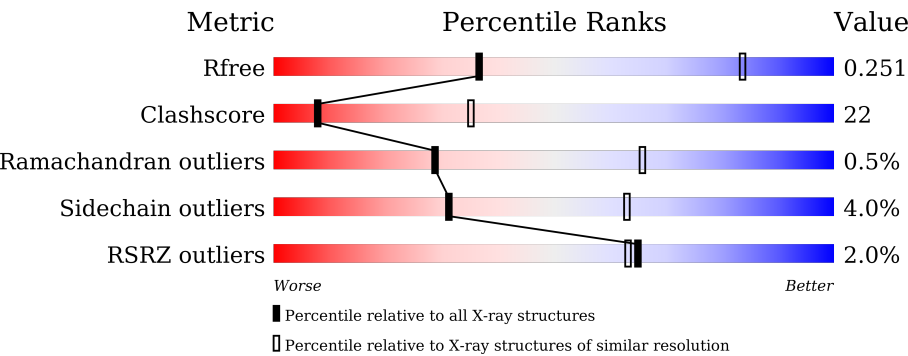
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.44 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	596	<div><div></div><div>69%28%..</div></div>
1	B	596	<div><div>3%</div><div>57%38%..</div></div>
1	C	596	<div><div>2%</div><div>62%35%..</div></div>
2	D	458	<div><div>3%</div><div>53%38%.6%</div></div>
2	E	458	<div><div>4%</div><div>49%44%5%. </div></div>
2	F	458	<div><div>%</div><div>52%43%..</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24060 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	B	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	C	584	Total	C	N	O	S	0	0	0
			4549	2858	764	901	26			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	432	Total	C	N	O	S	0	0	0
			3369	2134	576	646	13			
2	E	449	Total	C	N	O	S	0	0	0
			3509	2224	601	670	14			
2	F	445	Total	C	N	O	S	0	0	0
			3477	2204	597	662	14			

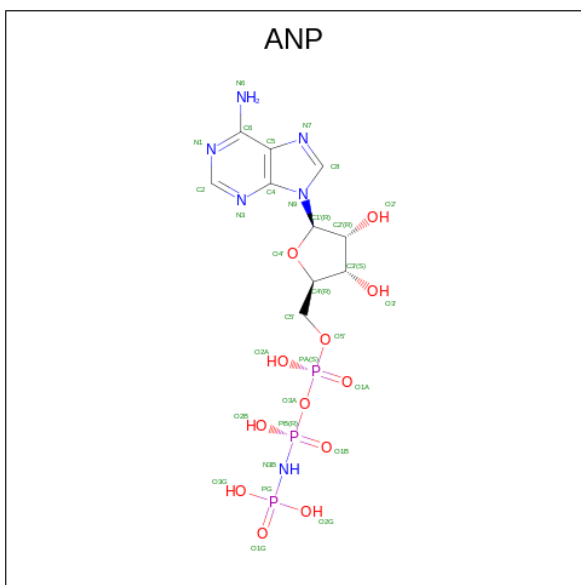
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLY	SER	engineered mutation	UNP Q08637
D	152	PRO	GLY	engineered mutation	UNP Q08637
D	153	PRO	SER	engineered mutation	UNP Q08637
D	155	ALA	LEU	engineered mutation	UNP Q08637
D	156	GLY	PRO	engineered mutation	UNP Q08637
D	157	LYS	HIS	engineered mutation	UNP Q08637
D	158	SER	LYS	engineered mutation	UNP Q08637
D	159	ALA	GLU	engineered mutation	UNP Q08637
D	248	GLU	THR	engineered mutation	UNP Q08637
D	339	SER	GLN	engineered mutation	UNP Q08637
E	151	GLY	SER	engineered mutation	UNP Q08637
E	152	PRO	GLY	engineered mutation	UNP Q08637
E	153	PRO	SER	engineered mutation	UNP Q08637
E	155	ALA	LEU	engineered mutation	UNP Q08637
E	156	GLY	PRO	engineered mutation	UNP Q08637
E	157	LYS	HIS	engineered mutation	UNP Q08637
E	158	SER	LYS	engineered mutation	UNP Q08637
E	159	ALA	GLU	engineered mutation	UNP Q08637
E	248	GLU	THR	engineered mutation	UNP Q08637
E	339	SER	GLN	engineered mutation	UNP Q08637
F	151	GLY	SER	engineered mutation	UNP Q08637
F	152	PRO	GLY	engineered mutation	UNP Q08637
F	153	PRO	SER	engineered mutation	UNP Q08637
F	155	ALA	LEU	engineered mutation	UNP Q08637
F	156	GLY	PRO	engineered mutation	UNP Q08637
F	157	LYS	HIS	engineered mutation	UNP Q08637
F	158	SER	LYS	engineered mutation	UNP Q08637
F	159	ALA	GLU	engineered mutation	UNP Q08637
F	248	GLU	THR	engineered mutation	UNP Q08637
F	339	SER	GLN	engineered mutation	UNP Q08637

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- 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>) (labeled as "Ligand of Interest" by depositor).

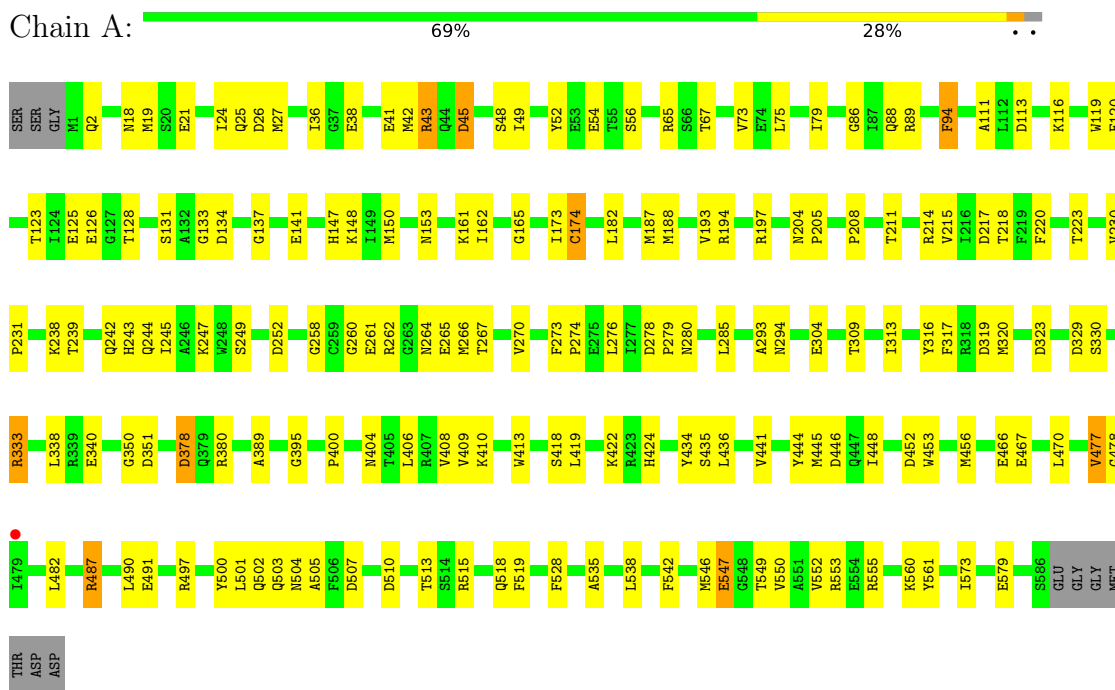


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

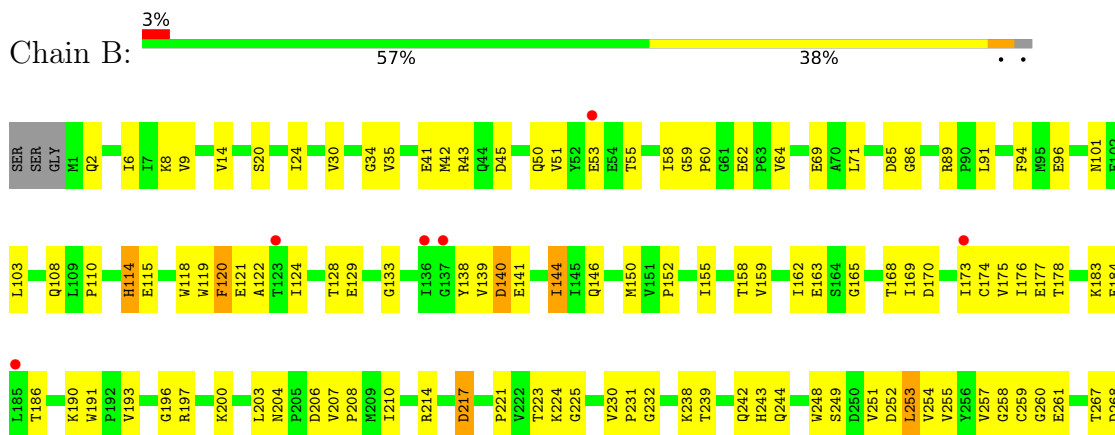
### 3 Residue-property plots [i](#)

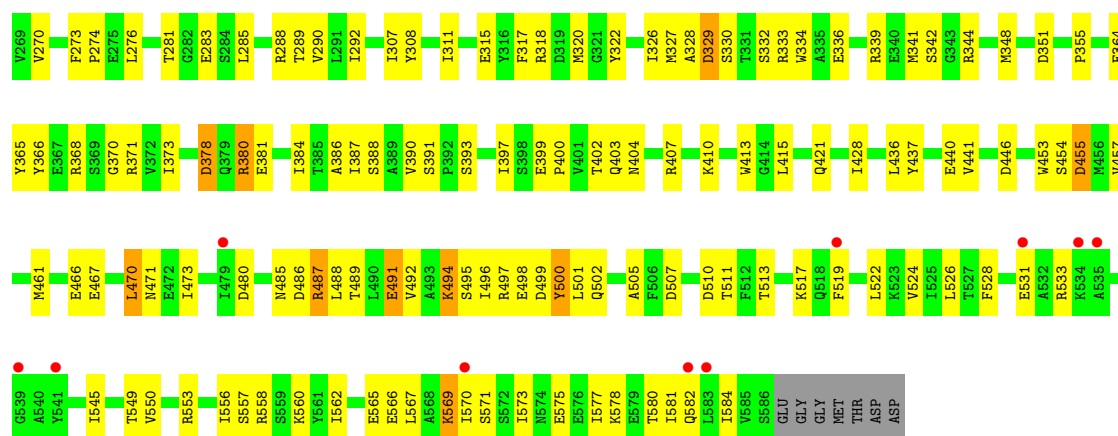
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: V-type sodium ATPase catalytic subunit A

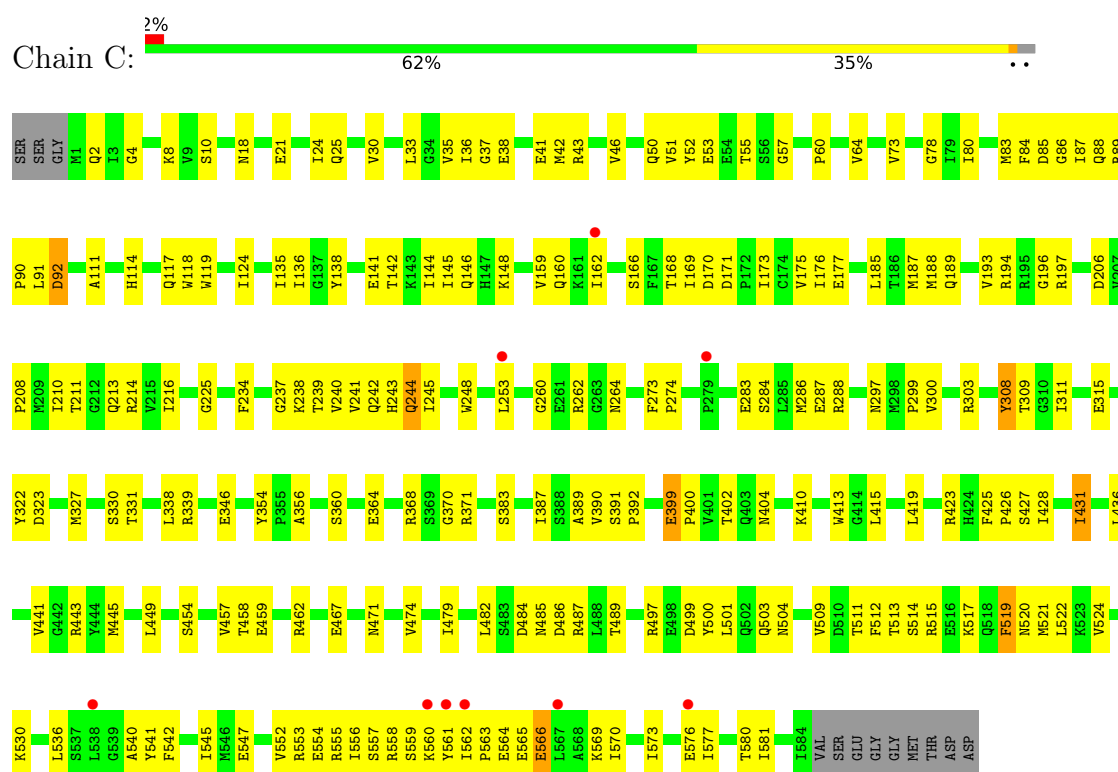


- Molecule 1: V-type sodium ATPase catalytic subunit A

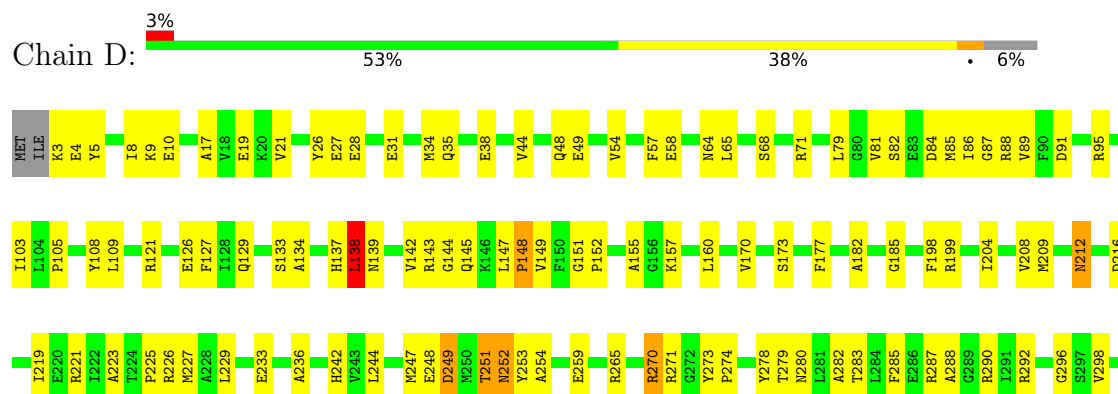


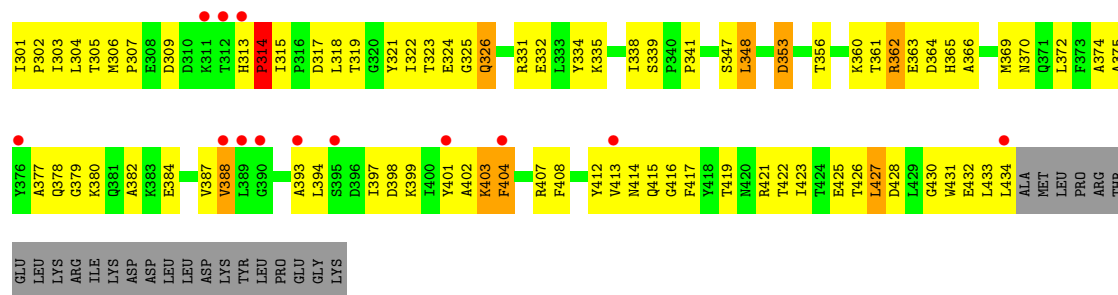


• Molecule 1: V-type sodium ATPase catalytic subunit A

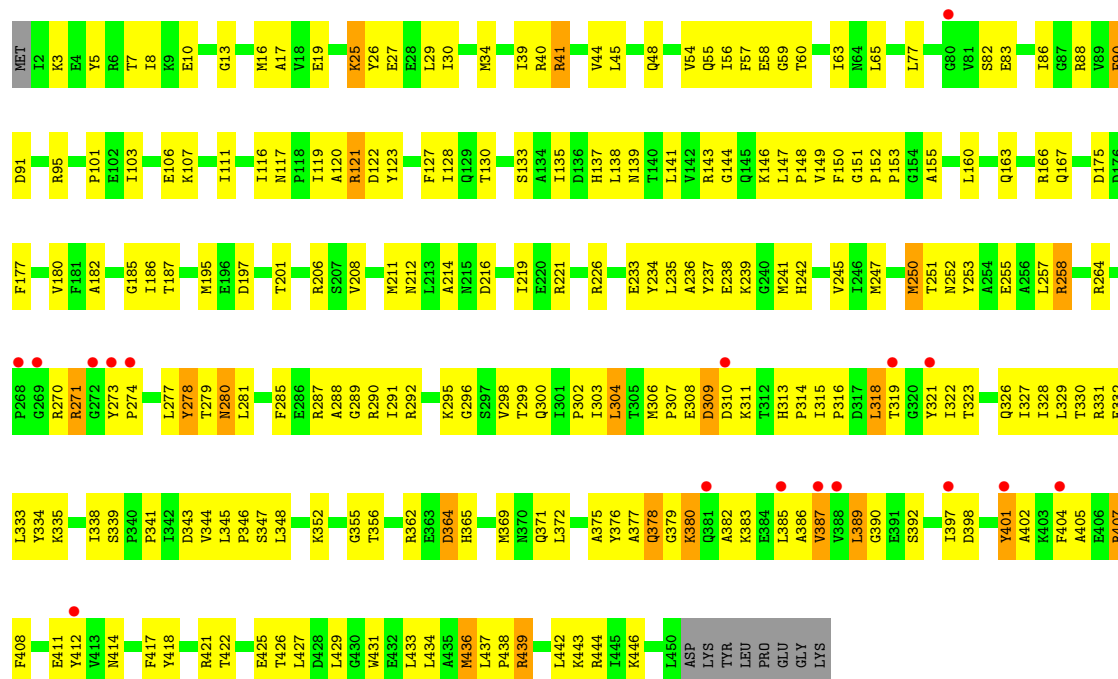


• Molecule 2: V-type sodium ATPase subunit B

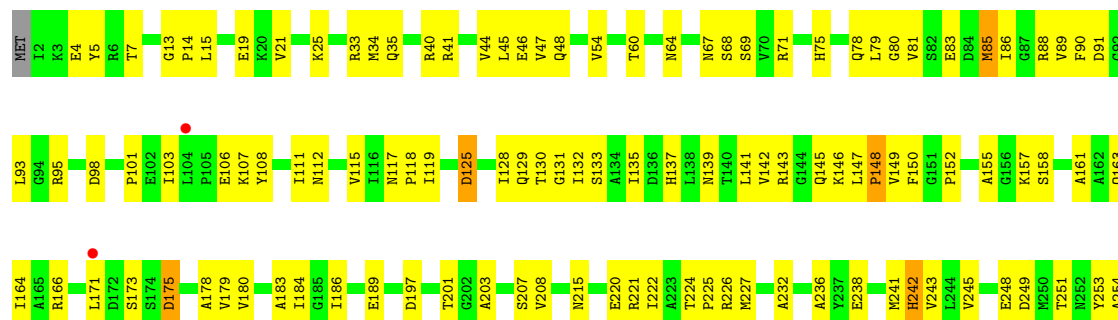




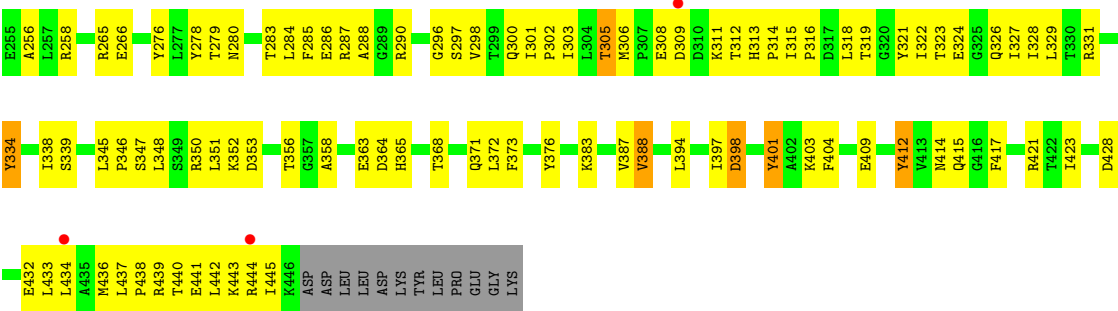
• Molecule 2: V-type sodium ATPase subunit B



• Molecule 2: V-type sodium ATPase subunit B







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.44Å 124.49Å 131.34Å 90.00° 93.03° 90.00°	Depositor
Resolution (Å)	46.34 – 3.44 46.34 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.34-3.44) 99.8 (46.34-3.44)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.18_3845)	Depositor
R, $R_{free}$	0.213 , 0.248 0.213 , 0.251	Depositor DCC
$R_{free}$ test set	2379 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.3	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: ANP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.31	1/4638 (0.0%)	0.49	0/6275
1	B	0.33	0/4638	0.54	1/6275 (0.0%)
1	C	0.34	0/4625	0.56	1/6257 (0.0%)
2	D	0.44	1/3429 (0.0%)	0.73	8/4637 (0.2%)
2	E	0.43	0/3570	0.72	8/4826 (0.2%)
2	F	0.40	0/3538	0.61	1/4782 (0.0%)
All	All	0.37	2/24438 (0.0%)	0.60	19/33052 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	252	ASN	CG-ND2	9.99	1.57	1.32
1	A	547	GLU	CB-CG	-5.50	1.41	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	138	LEU	CB-CG-CD2	16.26	138.64	111.00
1	B	253	LEU	CB-CG-CD1	-10.52	93.12	111.00
2	E	304	LEU	CB-CG-CD1	-8.57	96.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	258	ARG	NE-CZ-NH2	7.66	124.13	120.30
2	E	318	LEU	CA-CB-CG	-7.27	98.57	115.30
2	E	389	LEU	CA-CB-CG	6.59	130.46	115.30
2	D	251	THR	C-N-CA	-6.23	106.12	121.70
2	D	404	PHE	CB-CG-CD1	6.17	125.12	120.80
2	D	403	LYS	CB-CG-CD	6.14	127.58	111.60
2	D	252	ASN	N-CA-CB	6.09	121.56	110.60
2	D	404	PHE	CB-CG-CD2	-6.05	116.56	120.80
2	E	364	ASP	CB-CG-OD1	-5.93	112.96	118.30
2	D	314	PRO	CA-N-CD	-5.78	103.42	111.50
1	C	431	ILE	CG1-CB-CG2	-5.56	99.16	111.40
2	E	258	ARG	NE-CZ-NH1	-5.32	117.64	120.30
2	E	387	VAL	CG1-CB-CG2	-5.23	102.54	110.90
2	F	305	THR	CA-CB-CG2	-5.17	105.16	112.40
2	D	427	LEU	CB-CG-CD2	-5.06	102.40	111.00
2	E	304	LEU	CB-CG-CD2	5.03	119.54	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	363	GLU	Peptide
2	E	378	GLN	Sidechain

## 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	4562	0	4528	121	2
1	B	4562	0	4528	195	1
1	C	4549	0	4513	181	0
2	D	3369	0	3377	179	0
2	E	3509	0	3537	227	1
2	F	3477	0	3507	181	0
3	C	1	0	0	0	0
4	C	31	0	13	8	0
All	All	24060	0	24003	1037	2

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 22.

All (1037) 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:E:333:LEU:HB3	2:E:338:ILE:HD11	1.30	1.12
1:B:403:GLN:NE2	2:F:308:GLU:OE2	1.87	1.06
2:D:185:GLY:O	2:D:252:ASN:ND2	1.96	0.98
1:B:366:TYR:HH	1:B:388:SER:HG	0.98	0.95
1:B:470:LEU:HD23	1:B:470:LEU:H	1.30	0.94
2:E:251:THR:HG23	2:E:304:LEU:HB2	1.49	0.94
2:D:307:PRO:HG3	2:D:313:HIS:HB2	1.48	0.94
2:D:157:LYS:NZ	2:D:305:THR:OG1	2.02	0.93
1:B:281:THR:HG23	1:B:283:GLU:H	1.37	0.89
2:D:177:PHE:HE2	2:D:244:LEU:HB2	1.39	0.88
1:C:426:PRO:HG3	1:C:503:GLN:H	1.39	0.88
1:B:122:ALA:HB1	1:B:162:ILE:HD12	1.55	0.86
2:E:285:PHE:HD2	2:E:322:ILE:CD1	1.89	0.86
2:D:382:ALA:HB2	2:D:401:TYR:HB3	1.58	0.86
2:E:389:LEU:HD12	2:E:392:SER:HB2	1.57	0.85
2:F:131:GLY:O	2:F:415:GLN:NE2	2.09	0.85
2:D:251:THR:HG23	2:D:314:PRO:HG2	1.59	0.84
2:E:278:TYR:HB3	2:E:318:LEU:HD21	1.60	0.84
1:A:351:ASP:OD1	2:E:258:ARG:NH2	2.10	0.83
2:E:55:GLN:OE1	2:E:264:ARG:NH1	2.11	0.83
1:A:549:THR:HG23	1:A:553:ARG:HD3	1.62	0.82
2:E:270:ARG:NH1	2:E:278:TYR:OH	2.12	0.82
2:E:328:ILE:HG12	2:E:347:SER:HB3	1.58	0.81
1:B:528:PHE:HA	1:B:577:ILE:HD13	1.62	0.80
1:B:232:GLY:HA3	1:B:238:LYS:HD2	1.63	0.80
1:B:214:ARG:NH2	1:B:510:ASP:OD1	2.14	0.80
1:C:160:GLN:NE2	1:C:177:GLU:OE1	2.15	0.80
2:E:437:LEU:HD22	2:E:438:PRO:HD2	1.63	0.80
2:E:379:GLY:HA3	2:E:405:ALA:HB2	1.63	0.80
2:D:382:ALA:CB	2:D:401:TYR:HB3	2.12	0.80
2:F:313:HIS:CD2	2:F:316:PRO:HD2	2.17	0.79
2:E:412:TYR:HA	2:E:421:ARG:HH12	1.47	0.79
2:E:13:GLY:O	2:E:60:THR:OG1	2.01	0.79
2:E:338:ILE:HG22	2:E:414:ASN:HB2	1.65	0.79
1:B:144:ILE:HD11	1:B:281:THR:HG21	1.66	0.79
1:A:528:PHE:HE2	1:A:549:THR:HG1	1.31	0.78
1:B:467:GLU:O	1:B:471:ASN:ND2	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:PHE:CE1	2:D:433:LEU:HB3	2.18	0.78
2:E:365:HIS:HB2	2:E:427:LEU:HD21	1.65	0.78
2:F:34:MET:SD	2:F:40:ARG:NH1	2.57	0.78
2:D:365:HIS:HB2	2:D:427:LEU:HD11	1.66	0.78
2:F:288:ALA:HB2	2:F:300:GLN:HG3	1.65	0.78
1:C:210:ILE:HD11	1:C:515:ARG:HH21	1.49	0.78
2:F:4:GLU:OE2	2:F:71:ARG:NH2	2.17	0.77
2:F:356:THR:OG1	2:F:365:HIS:ND1	2.16	0.77
2:F:183:ALA:HB1	2:F:186:ILE:HD11	1.65	0.77
2:D:399:LYS:HA	2:D:402:ALA:HB3	1.67	0.77
1:B:206:ASP:OD1	1:B:371:ARG:NH1	2.18	0.76
1:C:208:PRO:HG3	1:C:441:VAL:HG22	1.68	0.76
1:B:566:GLU:OE1	1:B:569:LYS:NZ	2.18	0.76
1:A:133:GLY:O	1:A:380:ARG:NH2	2.18	0.76
2:E:166:ARG:O	2:E:206:ARG:NH1	2.17	0.76
1:A:214:ARG:NH2	1:A:510:ASP:OD1	2.16	0.76
1:C:542:PHE:HA	1:C:545:ILE:HB	1.67	0.76
1:B:159:VAL:HA	1:B:176:ILE:HG22	1.68	0.75
2:D:356:THR:HG23	2:D:365:HIS:CD2	2.21	0.75
1:B:507:ASP:HB3	1:B:510:ASP:HB3	1.68	0.75
1:B:545:ILE:O	1:B:549:THR:OG1	2.04	0.75
2:D:143:ARG:NH2	2:D:170:VAL:HG21	2.02	0.75
2:F:146:LYS:HE3	2:F:288:ALA:HB3	1.68	0.75
2:F:89:VAL:HB	2:F:98:ASP:HB3	1.68	0.75
1:B:549:THR:HG22	1:B:553:ARG:HG3	1.68	0.75
2:E:411:GLU:O	2:E:421:ARG:NH2	2.20	0.75
1:C:390:VAL:HG21	1:C:402:THR:HG22	1.68	0.74
2:E:285:PHE:HD2	2:E:322:ILE:HD13	1.51	0.74
2:F:141:LEU:HD11	2:F:301:ILE:HD11	1.68	0.74
2:E:160:LEU:O	2:E:163:GLN:HB3	1.88	0.74
2:E:285:PHE:CD2	2:E:322:ILE:HD11	2.23	0.73
1:B:253:LEU:HD11	1:B:317:PHE:CD2	2.24	0.73
1:C:238:LYS:NZ	4:C:602:ANP:O1B	2.21	0.73
2:D:199:ARG:HG2	2:D:204:ILE:HD12	1.70	0.73
1:B:85:ASP:OD1	1:B:86:GLY:N	2.21	0.73
1:C:245:ILE:HD11	1:C:387:ILE:HG13	1.71	0.73
2:E:429:LEU:O	2:E:433:LEU:HB2	1.89	0.73
1:B:522:LEU:HG	1:B:526:LEU:HD11	1.70	0.72
1:C:560:LYS:HE2	1:C:560:LYS:HA	1.71	0.72
2:F:133:SER:OG	2:F:421:ARG:NH1	2.23	0.72
2:F:254:ALA:HB3	2:F:315:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:ALA:HB3	2:D:314:PRO:HG3	1.71	0.72
2:F:137:HIS:ND1	2:F:412:TYR:OH	2.23	0.72
2:F:401:TYR:OH	2:F:441:GLU:HG2	1.90	0.72
2:E:313:HIS:HB3	2:E:314:PRO:HD2	1.71	0.72
1:B:155:ILE:HD11	1:B:183:LYS:HG3	1.71	0.72
2:E:375:ALA:HA	2:E:378:GLN:OE1	1.88	0.72
2:F:338:ILE:HG13	2:F:414:ASN:HB3	1.72	0.72
1:A:258:GLY:HA2	1:A:329:ASP:O	1.90	0.71
2:E:146:LYS:HE3	2:E:302:PRO:HG3	1.71	0.71
1:B:9:VAL:HG23	1:B:14:VAL:HG22	1.71	0.71
1:C:400:PRO:O	1:C:404:ASN:ND2	2.18	0.71
2:D:380:LYS:HA	2:D:384:GLU:HB2	1.72	0.71
1:C:264:ASN:ND2	2:F:324:GLU:OE2	2.22	0.71
1:C:425:PHE:HB3	4:C:602:ANP:C5	2.20	0.71
2:E:86:ILE:HA	2:E:208:VAL:HG23	1.72	0.71
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.08	0.71
1:B:168:THR:HG23	1:B:170:ASP:H	1.54	0.71
2:F:44:VAL:HG22	2:F:54:VAL:HG12	1.72	0.71
1:C:330:SER:H	1:C:389:ALA:HB3	1.55	0.71
2:D:147:LEU:O	2:D:301:ILE:HA	1.90	0.71
2:F:64:ASN:OD1	2:F:67:ASN:ND2	2.23	0.71
2:F:434:LEU:HD12	2:F:437:LEU:HD23	1.71	0.71
1:C:536:LEU:HA	1:C:540:ALA:HB3	1.71	0.71
2:E:151:GLY:O	2:E:306:MET:N	2.23	0.71
1:B:244:GLN:OE1	1:B:248:TRP:NE1	2.23	0.70
2:F:306:MET:HG3	2:F:316:PRO:HG3	1.73	0.70
2:D:198:PHE:HB3	2:D:204:ILE:HG13	1.73	0.70
2:F:184:ILE:HD11	2:F:225:PRO:HD3	1.73	0.70
1:A:238:LYS:NZ	1:A:329:ASP:OD2	2.22	0.70
2:D:315:ILE:HB	2:D:318:LEU:HB2	1.72	0.70
1:B:207:VAL:HG13	1:B:224:LYS:HB2	1.72	0.70
1:C:297:ASN:HD21	2:F:286:GLU:HB3	1.57	0.70
2:E:107:LYS:NZ	2:E:238:GLU:OE1	2.16	0.70
1:C:146:GLN:O	1:C:322:TYR:OH	2.09	0.70
1:C:214:ARG:HG3	1:C:503:GLN:OE1	1.91	0.70
1:C:399:GLU:OE1	1:C:402:THR:HG23	1.92	0.70
2:D:393:ALA:O	2:D:394:LEU:HG	1.92	0.70
2:D:148:PRO:HD2	2:D:326:GLN:HA	1.72	0.70
2:E:146:LYS:HD3	2:E:300:GLN:HG3	1.73	0.70
2:F:112:ASN:O	2:F:287:ARG:NH1	2.25	0.70
2:E:322:ILE:HD12	2:E:322:ILE:C	2.12	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:VAL:HG11	1:B:573:ILE:HD12	1.74	0.69
1:C:262:ARG:NH1	2:F:323:THR:O	2.25	0.69
1:B:242:GLN:NE2	1:B:329:ASP:OD1	2.24	0.69
2:E:150:PHE:CE2	2:E:304:LEU:HD11	2.28	0.69
2:E:285:PHE:CD2	2:E:322:ILE:CD1	2.75	0.69
2:E:386:ALA:HA	2:E:389:LEU:HB3	1.73	0.69
1:B:467:GLU:HA	1:B:470:LEU:HD11	1.72	0.69
2:E:141:LEU:HD21	2:E:299:THR:HG21	1.74	0.69
2:D:339:SER:H	2:D:414:ASN:CB	2.06	0.69
2:E:106:GLU:OE2	2:E:234:TYR:OH	2.09	0.68
1:A:555:ARG:HD3	1:A:573:ILE:HG12	1.76	0.68
2:E:383:LYS:O	2:E:387:VAL:HG23	1.93	0.68
2:F:125:ASP:OD1	2:F:290:ARG:NH1	2.26	0.68
2:D:221:ARG:O	2:D:225:PRO:HD2	1.93	0.68
2:D:248:GLU:OE1	2:D:249:ASP:HB2	1.93	0.68
2:D:339:SER:H	2:D:414:ASN:HB3	1.58	0.68
1:A:262:ARG:NH1	1:A:265:GLU:OE1	2.26	0.68
1:B:214:ARG:HB3	1:B:500:TYR:CE1	2.28	0.68
2:D:319:THR:O	2:D:323:THR:HG23	1.93	0.68
2:E:285:PHE:HD2	2:E:322:ILE:HD11	1.59	0.68
2:F:221:ARG:O	2:F:225:PRO:HD2	1.94	0.68
1:C:514:SER:H	1:C:560:LYS:NZ	1.91	0.67
1:C:234:PHE:HB3	2:F:321:TYR:CD1	2.29	0.67
2:E:29:LEU:HD21	2:E:77:LEU:HD13	1.76	0.67
1:C:410:LYS:HB3	1:C:436:LEU:HB2	1.77	0.67
1:C:78:GLY:N	1:C:141:GLU:OE1	2.17	0.67
2:D:428:ASP:HA	2:D:431:TRP:HD1	1.59	0.66
2:E:362:ARG:HB3	2:E:364:ASP:OD1	1.95	0.66
1:C:346:GLU:O	2:D:265:ARG:NH2	2.25	0.66
1:A:214:ARG:NH1	1:A:513:THR:OG1	2.28	0.66
1:C:513:THR:HG23	1:C:517:LYS:HD2	1.77	0.66
2:D:177:PHE:CE2	2:D:244:LEU:HB2	2.27	0.66
1:C:552:VAL:HA	1:C:555:ARG:HD3	1.78	0.66
1:B:69:GLU:OE1	1:B:190:LYS:NZ	2.28	0.66
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.76	0.66
2:F:132:ILE:HB	2:F:135:ILE:HB	1.78	0.66
2:F:148:PRO:HD2	2:F:326:GLN:HA	1.77	0.66
1:B:2:GLN:HE22	1:B:20:SER:H	1.44	0.66
1:C:30:VAL:HG23	1:C:64:VAL:HG22	1.77	0.66
2:D:253:TYR:OH	2:D:280:ASN:OD1	2.14	0.65
1:A:173:ILE:HD13	1:A:187:MET:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:602:ANP:O2G	4:C:602:ANP:O2B	2.15	0.65
2:E:371:GLN:OE1	2:E:443:LYS:N	2.17	0.65
2:F:4:GLU:OE1	2:F:69:SER:OG	2.14	0.65
1:B:129:GLU:N	1:B:129:GLU:OE1	2.27	0.65
1:B:528:PHE:HD1	1:B:577:ILE:HD12	1.61	0.65
1:B:176:ILE:HD11	1:B:183:LYS:HB2	1.77	0.65
1:C:114:HIS:ND1	1:C:170:ASP:OD1	2.20	0.65
1:C:297:ASN:HD22	2:F:115:VAL:HG13	1.61	0.65
2:E:137:HIS:HE1	2:E:372:LEU:HD23	1.61	0.65
1:B:85:ASP:OD2	1:B:89:ARG:NH2	2.29	0.65
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.77	0.65
2:F:394:LEU:HA	2:F:398:ASP:HB2	1.78	0.65
2:D:148:PRO:HB3	2:D:302:PRO:HG2	1.80	0.64
2:E:236:ALA:O	2:E:296:GLY:HA3	1.97	0.64
2:D:387:VAL:O	2:D:388:VAL:HG12	1.98	0.64
1:C:449:LEU:HD13	1:C:519:PHE:HD2	1.63	0.64
1:B:244:GLN:NE2	1:B:505:ALA:O	2.31	0.64
2:D:338:ILE:HA	2:D:414:ASN:HB3	1.80	0.64
2:D:138:LEU:HD22	2:D:139:ASN:H	1.63	0.64
2:D:398:ASP:O	2:D:401:TYR:HB2	1.98	0.64
2:E:40:ARG:NH1	2:E:59:GLY:O	2.29	0.64
2:F:179:VAL:O	2:F:207:SER:OG	2.13	0.64
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.79	0.63
1:C:262:ARG:NH2	4:C:602:ANP:O1G	2.31	0.63
1:C:499:ASP:OD1	1:C:553:ARG:HB3	1.98	0.63
1:C:10:SER:HB2	2:F:46:GLU:HG3	1.79	0.63
2:D:356:THR:HG22	2:D:366:ALA:HB2	1.79	0.63
2:E:251:THR:HG22	2:E:315:ILE:HD12	1.79	0.63
2:E:137:HIS:CE1	2:E:372:LEU:HD23	2.33	0.63
2:E:332:GLU:OE2	2:E:332:GLU:N	2.29	0.63
2:F:143:ARG:HD3	2:F:242:HIS:CD2	2.33	0.63
1:B:307:ILE:HB	1:B:365:TYR:CE2	2.33	0.63
1:B:318:ARG:HD3	1:B:384:ILE:HG13	1.79	0.63
2:E:377:ALA:O	2:E:380:LYS:HB3	1.99	0.63
2:F:148:PRO:HG3	2:F:323:THR:HG21	1.80	0.63
1:C:426:PRO:HG3	1:C:503:GLN:N	2.11	0.63
2:F:353:ASP:HA	2:F:356:THR:HG22	1.80	0.63
1:B:466:GLU:C	1:B:470:LEU:HD21	2.18	0.63
2:E:10:GLU:HG2	2:E:17:ALA:HB3	1.81	0.63
2:D:285:PHE:HE2	2:D:319:THR:HG1	1.47	0.63
1:A:504:ASN:OD1	1:A:507:ASP:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HA	1:B:64:VAL:HG22	1.81	0.62
1:A:487:ARG:HG2	1:A:542:PHE:CE2	2.34	0.62
1:B:208:PRO:HA	1:B:223:THR:HA	1.79	0.62
2:E:7:THR:OG1	2:E:19:GLU:O	2.17	0.62
1:B:575:GLU:N	1:B:575:GLU:OE1	2.32	0.62
2:E:111:ILE:O	2:E:287:ARG:NH2	2.31	0.62
1:C:117:GLN:OE1	1:C:166:SER:OG	2.16	0.62
2:E:148:PRO:HB3	2:E:302:PRO:HG2	1.82	0.62
1:A:141:GLU:OE1	1:A:147:HIS:ND1	2.25	0.62
1:B:214:ARG:HB3	1:B:500:TYR:HE1	1.63	0.62
1:B:327:MET:HA	1:B:387:ILE:O	1.99	0.62
1:B:550:VAL:HG22	1:B:553:ARG:HH22	1.65	0.62
1:A:410:LYS:HB3	1:A:436:LEU:HB2	1.81	0.62
1:C:562:ILE:HG22	1:C:563:PRO:HD2	1.82	0.62
2:F:371:GLN:HE21	2:F:443:LYS:HG3	1.65	0.62
1:C:237:GLY:HA3	4:C:602:ANP:H2	1.80	0.61
2:F:137:HIS:HE2	2:F:368:THR:HG1	0.63	0.61
2:D:362:ARG:NH2	2:D:364:ASP:OD2	2.20	0.61
1:C:497:ARG:HA	1:C:501:LEU:HB2	1.81	0.61
1:C:514:SER:OG	1:C:560:LYS:NZ	2.32	0.61
1:B:62:GLU:OE2	2:E:25:LYS:NZ	2.31	0.61
1:B:333:ARG:NH1	1:B:391:SER:OG	2.34	0.61
1:A:120:PHE:HE2	1:A:162:ILE:HD11	1.64	0.61
1:B:230:VAL:HG13	1:B:238:LYS:HZ1	1.66	0.61
2:D:339:SER:HB2	2:D:417:PHE:CD1	2.35	0.61
2:F:313:HIS:HE2	2:F:315:ILE:HB	1.66	0.61
1:B:437:TYR:OH	2:F:189:GLU:OE1	2.15	0.61
2:D:397:ILE:HA	2:D:399:LYS:HE3	1.82	0.61
2:D:404:PHE:HE1	2:D:433:LEU:HB3	1.61	0.60
1:B:399:GLU:O	1:B:403:GLN:HG2	2.01	0.60
2:D:236:ALA:O	2:D:296:GLY:HA3	2.01	0.60
2:F:132:ILE:HA	2:F:415:GLN:NE2	2.16	0.60
2:F:166:ARG:NH1	2:F:197:ASP:OD2	2.35	0.60
1:A:266:MET:SD	1:A:293:ALA:HB1	2.41	0.60
2:D:212:ASN:HD21	2:D:216:ASP:HB2	1.66	0.60
2:F:339:SER:HB3	2:F:417:PHE:CE2	2.37	0.60
1:B:413:TRP:HB3	1:B:428:ILE:HD13	1.83	0.60
2:E:185:GLY:O	2:E:252:ASN:ND2	2.35	0.60
2:E:330:THR:HB	2:E:333:LEU:HD13	1.82	0.60
2:F:86:ILE:HD12	2:F:86:ILE:H	1.67	0.60
1:B:495:SER:O	1:B:499:ASP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HG12	1:C:176:ILE:HD12	1.84	0.60
1:C:160:GLN:HB3	1:C:175:VAL:HG13	1.83	0.60
2:E:41:ARG:H	2:E:41:ARG:HD2	1.67	0.60
2:F:155:ALA:HB3	2:F:334:TYR:OH	2.01	0.60
1:B:565:GLU:N	1:B:565:GLU:OE1	2.33	0.60
2:E:333:LEU:CB	2:E:338:ILE:HD11	2.19	0.60
2:F:288:ALA:HA	2:F:298:VAL:HG13	1.84	0.59
1:B:257:VAL:HG12	1:B:292:ILE:HB	1.85	0.59
2:D:121:ARG:NH1	2:D:288:ALA:O	2.35	0.59
2:E:57:PHE:HD1	2:E:219:ILE:HD12	1.66	0.59
1:C:283:GLU:HG2	1:C:287:GLU:HG3	1.83	0.59
2:D:226:ARG:NH2	2:D:253:TYR:OH	2.36	0.59
2:F:313:HIS:ND1	2:F:314:PRO:HD2	2.18	0.59
1:C:2:GLN:NE2	1:C:18:ASN:OD1	2.34	0.59
2:E:163:GLN:NE2	2:E:417:PHE:O	2.34	0.59
2:F:387:VAL:O	2:F:388:VAL:HG22	2.03	0.59
2:F:221:ARG:HD3	2:F:256:ALA:HB2	1.85	0.59
2:F:345:LEU:HB2	2:F:346:PRO:HD3	1.84	0.59
1:C:573:ILE:O	1:C:577:ILE:HG13	2.02	0.59
2:E:226:ARG:NH2	2:E:280:ASN:OD1	2.35	0.59
2:D:422:THR:HB	2:D:425:GLU:HG3	1.83	0.59
1:B:400:PRO:HA	1:B:403:GLN:HG3	1.85	0.59
1:C:517:LYS:NZ	1:C:560:LYS:HB2	2.18	0.59
1:B:513:THR:HG23	1:B:517:LYS:HD3	1.84	0.58
2:E:130:THR:HG21	2:E:135:ILE:HG21	1.85	0.58
2:E:401:TYR:CE1	2:E:437:LEU:HD21	2.38	0.58
1:A:41:GLU:OE2	1:A:43:ARG:NH1	2.35	0.58
1:B:50:GLN:NE2	1:B:341:MET:SD	2.68	0.58
2:F:376:TYR:OH	2:F:409:GLU:OE1	2.16	0.58
2:E:437:LEU:HD13	2:E:438:PRO:N	2.18	0.58
2:F:285:PHE:HE2	2:F:319:THR:HG23	1.69	0.58
2:E:401:TYR:CE1	2:E:437:LEU:HD11	2.39	0.58
2:E:408:PHE:HD2	2:E:433:LEU:HD23	1.66	0.58
2:F:131:GLY:HA2	2:F:421:ARG:O	2.02	0.58
2:D:382:ALA:O	2:D:394:LEU:HD22	2.02	0.58
2:E:313:HIS:HB3	2:E:314:PRO:CD	2.33	0.58
2:F:442:LEU:HD12	2:F:442:LEU:H	1.68	0.58
2:D:315:ILE:HD12	2:D:315:ILE:H	1.68	0.58
2:E:146:LYS:HE2	2:E:285:PHE:CG	2.39	0.58
1:A:546:MET:O	1:A:550:VAL:HG23	2.03	0.58
2:D:372:LEU:HA	2:D:375:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:352:LYS:O	2:E:356:THR:HG22	2.04	0.58
2:E:422:THR:O	2:E:426:THR:HG23	2.02	0.58
1:B:270:VAL:O	1:B:274:PRO:HD2	2.04	0.58
1:C:51:VAL:HG21	1:C:55:THR:CG2	2.34	0.58
2:D:309:ASP:N	2:D:309:ASP:OD1	2.34	0.58
2:F:371:GLN:NE2	2:F:443:LYS:HG3	2.19	0.58
1:A:79:ILE:HD11	1:A:313:ILE:HD13	1.85	0.58
2:E:45:LEU:HD21	2:E:264:ARG:NH1	2.19	0.58
1:B:446:ASP:OD1	1:B:453:TRP:N	2.37	0.57
1:C:300:VAL:HA	1:C:303:ARG:HG3	1.85	0.57
2:E:212:ASN:OD1	2:E:221:ARG:HA	2.03	0.57
2:F:13:GLY:O	2:F:60:THR:OG1	2.13	0.57
1:A:528:PHE:HE2	1:A:549:THR:OG1	1.87	0.57
1:C:514:SER:H	1:C:560:LYS:HZ1	1.50	0.57
2:E:407:ARG:NE	2:E:411:GLU:OE2	2.29	0.57
2:F:428:ASP:O	2:F:432:GLU:HG3	2.03	0.57
1:B:214:ARG:NH2	1:B:560:LYS:HB2	2.19	0.57
2:E:116:ILE:HG21	2:E:121:ARG:HE	1.69	0.57
2:E:315:ILE:HG13	2:E:316:PRO:HD3	1.86	0.57
2:D:149:VAL:CG1	2:D:303:ILE:HG13	2.35	0.57
2:F:117:ASN:OD1	2:F:119:ILE:HG12	2.03	0.57
1:A:43:ARG:HG3	2:E:10:GLU:HB2	1.86	0.57
1:B:467:GLU:OE1	1:B:497:ARG:NH2	2.34	0.57
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.86	0.57
2:F:183:ALA:HB1	2:F:186:ILE:CD1	2.34	0.57
1:A:406:LEU:HA	1:A:409:VAL:HG22	1.87	0.57
2:D:137:HIS:CE1	2:D:369:MET:HA	2.39	0.57
1:B:128:THR:H	1:B:159:VAL:HG22	1.70	0.57
1:C:467:GLU:CD	1:C:497:ARG:HH22	2.08	0.57
2:F:139:ASN:ND2	2:F:347:SER:HB3	2.20	0.57
2:D:127:PHE:HA	2:D:142:VAL:HA	1.87	0.57
2:D:134:ALA:C	2:D:138:LEU:HD11	2.25	0.57
2:D:280:ASN:O	2:D:283:THR:OG1	2.22	0.57
2:F:145:GLN:HG3	2:F:351:LEU:HD12	1.87	0.57
2:F:147:LEU:O	2:F:301:ILE:HA	2.03	0.57
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.70	0.56
1:C:415:LEU:HB3	1:C:427:SER:OG	2.05	0.56
1:B:571:SER:O	1:B:575:GLU:OE1	2.23	0.56
2:D:58:GLU:OE2	2:D:58:GLU:N	2.36	0.56
2:D:338:ILE:HA	2:D:414:ASN:HD22	1.70	0.56
2:E:57:PHE:CD1	2:E:219:ILE:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:LYS:HE3	2:F:305:THR:HG21	1.87	0.56
2:D:270:ARG:NH1	2:D:270:ARG:HB2	2.19	0.56
2:D:338:ILE:HG12	2:D:341:PRO:HA	1.86	0.56
2:F:175:ASP:N	2:F:175:ASP:OD1	2.37	0.56
1:C:315:GLU:OE2	1:C:368:ARG:NE	2.39	0.56
1:C:471:ASN:O	1:C:474:VAL:HG12	2.05	0.56
1:C:484:ASP:HB3	1:C:542:PHE:HE2	1.70	0.56
2:E:364:ASP:OD1	2:E:364:ASP:N	2.37	0.56
2:F:150:PHE:HB3	2:F:306:MET:SD	2.45	0.56
2:D:334:TYR:HA	2:D:338:ILE:HG23	1.85	0.56
2:F:88:ARG:NH1	2:F:101:PRO:O	2.39	0.56
1:A:86:GLY:N	1:A:294:ASN:OD1	2.39	0.56
2:E:152:PRO:HB2	2:E:153:PRO:HD2	1.88	0.56
2:E:153:PRO:HG2	2:E:331:ARG:HH12	1.71	0.56
1:C:273:PHE:HB3	1:C:286:MET:HG2	1.88	0.56
2:D:126:GLU:OE1	2:D:126:GLU:N	2.33	0.56
2:D:31:GLU:OE1	2:D:71:ARG:NH1	2.35	0.56
2:E:437:LEU:HD13	2:E:438:PRO:CD	2.36	0.56
1:B:8:LYS:HB2	2:E:48:GLN:HB2	1.87	0.56
1:B:124:ILE:O	1:B:162:ILE:HD11	2.06	0.56
1:C:482:LEU:O	1:C:487:ARG:NH2	2.39	0.56
1:B:24:ILE:HD11	1:B:42:MET:HB3	1.88	0.55
1:A:445:MET:HE3	1:A:515:ARG:CZ	2.36	0.55
2:D:82:SER:OG	2:D:84:ASP:OD2	2.24	0.55
2:E:378:GLN:NE2	2:E:401:TYR:CZ	2.74	0.55
1:C:485:ASN:O	1:C:489:THR:OG1	2.18	0.55
2:D:428:ASP:O	2:D:432:GLU:HG2	2.06	0.55
2:F:226:ARG:NH2	2:F:253:TYR:OH	2.39	0.55
2:E:386:ALA:HA	2:E:389:LEU:CB	2.37	0.55
1:C:520:ASN:O	1:C:524:VAL:HG13	2.07	0.55
2:E:128:ILE:HG13	2:E:143:ARG:HG3	1.88	0.55
2:D:144:GLY:HA2	2:D:298:VAL:O	2.06	0.55
2:E:133:SER:HB3	2:E:412:TYR:CE2	2.41	0.55
2:F:251:THR:CG2	2:F:315:ILE:HG21	2.37	0.55
2:E:122:ASP:N	2:E:290:ARG:O	2.27	0.55
1:B:251:VAL:O	1:B:288:ARG:NH1	2.40	0.55
1:B:365:TYR:HD1	1:B:366:TYR:CD1	2.24	0.55
1:C:264:ASN:HD21	2:F:146:LYS:NZ	2.05	0.55
2:D:133:SER:CB	2:D:421:ARG:HH11	2.20	0.55
2:D:364:ASP:OD1	2:D:364:ASP:N	2.37	0.55
1:A:482:LEU:HD23	1:A:482:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:MET:HA	1:B:344:ARG:HD3	1.90	0.54
1:B:581:ILE:HG13	1:B:582:GLN:N	2.22	0.54
1:C:33:LEU:H	1:C:33:LEU:HD12	1.71	0.54
2:F:313:HIS:NE2	2:F:315:ILE:HB	2.21	0.54
1:A:446:ASP:OD1	1:A:453:TRP:N	2.39	0.54
1:A:560:LYS:HG2	1:A:561:TYR:CD1	2.43	0.54
1:C:211:THR:HG23	1:C:245:ILE:HG22	1.88	0.54
2:D:87:GLY:HA2	2:D:204:ILE:O	2.07	0.54
2:D:133:SER:OG	2:D:421:ARG:NH1	2.40	0.54
2:F:86:ILE:HA	2:F:208:VAL:HG22	1.88	0.54
1:A:211:THR:OG1	1:A:217:ASP:OD1	2.18	0.54
1:B:378:ASP:HB2	1:B:380:ARG:HD2	1.89	0.54
2:E:147:LEU:HD11	2:E:327:ILE:HG13	1.89	0.54
1:B:110:PRO:HB3	1:B:114:HIS:CE1	2.43	0.54
1:B:281:THR:HG23	1:B:283:GLU:N	2.14	0.54
2:F:403:LYS:HD2	2:F:403:LYS:N	2.23	0.54
2:F:254:ALA:HB3	2:F:315:ILE:CD1	2.35	0.54
1:B:410:LYS:HE3	1:B:437:TYR:OH	2.08	0.54
1:B:158:THR:HG23	1:B:177:GLU:HB3	1.90	0.54
1:B:415:LEU:HD23	1:B:428:ILE:HG12	1.89	0.54
1:C:214:ARG:HD3	1:C:513:THR:HG21	1.90	0.54
2:D:282:ALA:HB2	2:D:322:ILE:HD13	1.90	0.54
1:C:38:GLU:OE2	1:C:194:ARG:NH2	2.41	0.53
2:D:127:PHE:HE1	2:D:360:LYS:O	1.90	0.53
2:E:216:ASP:O	2:E:221:ARG:NH1	2.41	0.53
2:E:233:GLU:OE2	2:E:287:ARG:HG2	2.07	0.53
1:B:494:LYS:O	1:B:498:GLU:HB2	2.08	0.53
2:E:285:PHE:CE2	2:E:322:ILE:HD11	2.44	0.53
1:B:221:PRO:HB2	1:B:441:VAL:HG21	1.90	0.53
1:B:244:GLN:NE2	1:B:505:ALA:HB1	2.22	0.53
1:B:410:LYS:HB3	1:B:436:LEU:HB3	1.90	0.53
2:E:345:LEU:HD23	2:E:346:PRO:HD3	1.90	0.53
1:C:53:GLU:HA	1:C:299:PRO:HG2	1.91	0.53
1:C:85:ASP:OD1	1:C:86:GLY:N	2.41	0.53
1:C:169:ILE:HG22	1:C:188:MET:HB2	1.91	0.53
1:C:560:LYS:HE2	1:C:560:LYS:CA	2.35	0.53
2:F:137:HIS:HD2	2:F:365:HIS:HD2	1.57	0.53
1:B:248:TRP:CZ2	1:B:511:THR:HG23	2.43	0.53
1:B:528:PHE:CD1	1:B:577:ILE:HD12	2.43	0.53
1:B:562:ILE:HD11	1:B:570:ILE:HG12	1.91	0.53
2:D:134:ALA:O	2:D:138:LEU:HD11	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:TYR:CD1	2:E:437:LEU:HD21	2.44	0.53
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.44	0.53
1:B:267:THR:HG21	2:E:121:ARG:HG2	1.91	0.53
4:C:602:ANP:O3'	2:F:348:LEU:HD21	2.09	0.53
2:F:279:THR:O	2:F:283:THR:HG23	2.09	0.53
1:A:148:LYS:H	1:A:320:MET:CE	2.20	0.53
1:B:404:ASN:OD1	1:B:407:ARG:NH1	2.42	0.53
1:C:323:ASP:OD2	1:C:383:SER:OG	2.27	0.53
1:C:484:ASP:HB3	1:C:542:PHE:CE2	2.44	0.53
2:D:143:ARG:HH11	2:D:242:HIS:CE1	2.25	0.53
2:E:237:TYR:OH	2:E:289:GLY:O	2.26	0.53
2:F:319:THR:O	2:F:323:THR:HG23	2.08	0.53
1:A:125:GLU:O	1:A:128:THR:OG1	2.24	0.53
2:E:250:MET:HB2	2:E:304:LEU:HB3	1.91	0.53
1:A:123:THR:HG23	1:A:137:GLY:HA2	1.91	0.52
1:C:83:MET:HG2	1:C:91:LEU:HD12	1.91	0.52
1:C:173:ILE:HD13	1:C:187:MET:HG2	1.90	0.52
2:E:397:ILE:O	2:E:401:TYR:HB2	2.10	0.52
1:B:41:GLU:OE1	1:B:43:ARG:NH2	2.43	0.52
1:B:71:LEU:HD22	1:B:193:VAL:HG11	1.91	0.52
1:B:371:ARG:NH2	1:B:381:GLU:OE1	2.38	0.52
1:A:89:ARG:HD2	1:A:94:PHE:HE2	1.75	0.52
1:A:350:GLY:C	2:E:258:ARG:HH21	2.12	0.52
1:C:565:GLU:N	1:C:565:GLU:OE2	2.42	0.52
2:D:126:GLU:OE2	2:D:290:ARG:NH1	2.43	0.52
1:B:326:ILE:HG23	1:B:386:ALA:HA	1.91	0.52
2:D:148:PRO:HG3	2:D:323:THR:OG1	2.10	0.52
2:D:332:GLU:O	2:D:335:LYS:HG2	2.09	0.52
2:F:5:TYR:CD2	2:F:21:VAL:HG12	2.45	0.52
1:B:152:PRO:O	1:B:155:ILE:HG22	2.09	0.52
2:D:212:ASN:ND2	2:D:216:ASP:HB2	2.24	0.52
2:E:422:THR:OG1	2:E:425:GLU:HG3	2.10	0.52
2:F:35:GLN:OE1	2:F:35:GLN:N	2.38	0.52
2:F:157:LYS:HD3	2:F:305:THR:HG22	1.91	0.52
2:F:222:ILE:HA	2:F:253:TYR:HE1	1.75	0.52
1:B:332:SER:O	1:B:336:GLU:HG3	2.09	0.52
1:C:214:ARG:NH1	1:C:513:THR:OG1	2.43	0.52
2:D:138:LEU:CG	2:D:139:ASN:H	2.23	0.52
1:A:477:VAL:HG12	1:A:478:GLY:H	1.75	0.52
1:C:504:ASN:HB3	1:C:511:THR:HA	1.91	0.52
1:A:252:ASP:OD2	1:A:323:ASP:N	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLU:N	1:C:283:GLU:OE1	2.42	0.52
1:C:524:VAL:HG12	1:C:573:ILE:HG12	1.91	0.52
2:F:372:LEU:HD23	2:F:404:PHE:HZ	1.74	0.52
1:B:562:ILE:HD11	1:B:570:ILE:CG1	2.40	0.51
1:C:425:PHE:HB3	4:C:602:ANP:C4	2.39	0.51
2:E:257:LEU:HD12	2:E:277:LEU:HD13	1.92	0.51
1:A:205:PRO:C	1:A:223:THR:HG21	2.31	0.51
2:D:34:MET:HE2	2:D:38:GLU:HB3	1.92	0.51
2:E:245:VAL:O	2:E:300:GLN:HA	2.10	0.51
1:A:270:VAL:O	1:A:274:PRO:HD2	2.11	0.51
1:B:91:LEU:HB3	2:E:119:ILE:HD13	1.91	0.51
1:B:485:ASN:O	1:B:488:LEU:HG	2.10	0.51
2:E:39:ILE:HD12	2:E:39:ILE:O	2.10	0.51
2:F:334:TYR:HD1	2:F:334:TYR:O	1.92	0.51
1:B:258:GLY:HA2	1:B:329:ASP:O	2.09	0.51
1:C:360:SER:OG	2:D:259:GLU:OE1	2.25	0.51
2:E:146:LYS:HE2	2:E:285:PHE:CD1	2.46	0.51
1:C:91:LEU:HD13	2:F:118:PRO:HD2	1.92	0.51
1:C:4:GLY:O	1:C:64:VAL:N	2.42	0.51
2:E:83:GLU:HG3	2:E:239:LYS:HE2	1.92	0.51
1:A:497:ARG:HA	1:A:501:LEU:HB2	1.93	0.51
1:B:497:ARG:HA	1:B:501:LEU:HB2	1.92	0.51
2:D:79:LEU:HB2	2:D:227:MET:SD	2.51	0.51
2:D:137:HIS:O	2:D:365:HIS:HE1	1.94	0.51
2:E:58:GLU:N	2:E:58:GLU:OE1	2.43	0.51
2:E:278:TYR:CD1	2:E:279:THR:HG23	2.46	0.51
2:F:137:HIS:HD2	2:F:365:HIS:CD2	2.29	0.51
2:F:150:PHE:O	2:F:328:ILE:HA	2.11	0.51
1:B:174:CYS:SG	1:B:175:VAL:N	2.84	0.50
1:B:486:ASP:OD1	1:B:486:ASP:N	2.37	0.50
2:E:250:MET:O	2:E:253:TYR:HB3	2.11	0.50
2:E:258:ARG:HB2	2:E:273:TYR:CD1	2.46	0.50
1:B:51:VAL:HG21	1:B:55:THR:HG22	1.93	0.50
1:B:403:GLN:HE22	2:F:308:GLU:CD	2.03	0.50
2:D:339:SER:HB2	2:D:417:PHE:CE1	2.46	0.50
2:E:234:TYR:HD1	2:E:235:LEU:HD23	1.76	0.50
2:F:148:PRO:HB3	2:F:302:PRO:HG2	1.93	0.50
1:A:18:ASN:N	1:A:45:ASP:OD1	2.42	0.50
1:A:126:GLU:OE2	1:A:161:LYS:HA	2.11	0.50
1:B:470:LEU:HA	1:B:473:ILE:HD12	1.92	0.50
1:C:37:GLY:HA2	1:C:51:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:ARG:HB2	2:D:270:ARG:HH11	1.77	0.50
2:D:339:SER:O	2:D:414:ASN:HA	2.12	0.50
2:F:178:ALA:HB2	2:F:241:MET:HE2	1.93	0.50
1:A:466:GLU:O	1:A:470:LEU:HG	2.12	0.50
1:B:580:THR:O	1:B:584:ILE:HG13	2.12	0.50
1:C:43:ARG:O	1:C:46:VAL:HG12	2.12	0.50
2:E:30:ILE:HD13	2:E:54:VAL:HG11	1.94	0.50
1:C:144:ILE:HB	1:C:145:ILE:HD12	1.92	0.50
1:C:509:VAL:HG12	1:C:557:SER:O	2.12	0.50
2:D:273:TYR:HB3	2:D:274:PRO:HD2	1.93	0.50
1:B:35:VAL:HG21	1:B:58:ILE:HD11	1.93	0.50
1:C:211:THR:HG21	1:C:216:ILE:HD12	1.94	0.50
1:C:264:ASN:HD21	2:F:146:LYS:HZ2	1.58	0.50
1:C:559:SER:OG	1:C:569:LYS:NZ	2.26	0.50
2:E:338:ILE:HD12	2:E:338:ILE:O	2.12	0.50
2:E:371:GLN:HG2	2:E:434:LEU:HD21	1.93	0.50
1:A:262:ARG:NE	2:D:321:TYR:O	2.45	0.50
1:B:210:ILE:O	1:B:249:SER:HA	2.12	0.50
1:C:364:GLU:O	1:C:368:ARG:HG3	2.12	0.50
2:D:317:ASP:O	2:D:321:TYR:HD1	1.94	0.50
2:E:304:LEU:HD12	2:E:304:LEU:C	2.32	0.50
2:F:150:PHE:HB2	2:F:328:ILE:HG22	1.94	0.50
1:B:122:ALA:CB	1:B:162:ILE:HD12	2.37	0.49
1:C:124:ILE:HG22	1:C:162:ILE:HD13	1.94	0.49
2:D:81:VAL:HA	2:D:85:MET:CE	2.42	0.49
2:E:88:ARG:NH2	2:E:101:PRO:O	2.43	0.49
2:E:155:ALA:HA	2:E:334:TYR:CD2	2.47	0.49
2:E:338:ILE:CG2	2:E:414:ASN:HB2	2.39	0.49
2:F:236:ALA:HB2	2:F:243:VAL:HG23	1.94	0.49
1:A:54:GLU:HG3	1:A:56:SER:H	1.76	0.49
1:B:124:ILE:HG22	1:B:162:ILE:CD1	2.42	0.49
1:B:239:THR:O	1:B:243:HIS:ND1	2.45	0.49
2:D:307:PRO:HG3	2:D:313:HIS:CB	2.32	0.49
2:D:377:ALA:O	2:D:380:LYS:HE2	2.11	0.49
1:B:553:ARG:HA	1:B:556:ILE:HD12	1.94	0.49
1:C:474:VAL:HG23	1:C:482:LEU:HD11	1.94	0.49
2:F:404:PHE:CD1	2:F:437:LEU:HD21	2.47	0.49
1:B:365:TYR:HD1	1:B:366:TYR:HD1	1.60	0.49
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.94	0.49
1:C:423:ARG:HG2	1:C:425:PHE:CE1	2.48	0.49
2:E:278:TYR:CB	2:E:318:LEU:HD21	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:TRP:O	1:B:457:VAL:HG23	2.13	0.49
1:C:38:GLU:OE1	1:C:52:TYR:OH	2.30	0.49
1:C:262:ARG:NH2	2:F:350:ARG:HH12	2.11	0.49
2:D:428:ASP:HA	2:D:431:TRP:CD1	2.43	0.49
1:A:419:LEU:HB3	1:A:424:HIS:HB3	1.94	0.49
1:A:507:ASP:HB3	1:A:510:ASP:HB3	1.95	0.49
2:D:91:ASP:OD1	2:D:91:ASP:N	2.38	0.49
2:D:325:GLY:HA2	2:D:348:LEU:CD1	2.43	0.49
2:E:319:THR:O	2:E:323:THR:N	2.46	0.49
2:F:137:HIS:CE1	2:F:368:THR:HG1	2.20	0.49
1:B:531:GLU:OE2	1:B:581:ILE:HD13	2.13	0.49
2:D:129:GLN:OE1	2:D:422:THR:HA	2.13	0.49
1:B:133:GLY:O	1:B:380:ARG:NH2	2.22	0.49
1:B:191:TRP:NE1	1:B:197:ARG:HG3	2.28	0.49
1:C:24:ILE:HG22	1:C:25:GLN:HG3	1.94	0.49
2:E:26:TYR:CD2	2:E:27:GLU:HG3	2.48	0.49
2:F:91:ASP:OD2	2:F:95:ARG:NH2	2.43	0.49
2:F:171:LEU:HD12	2:F:171:LEU:HA	1.64	0.49
2:F:251:THR:HG23	2:F:315:ILE:HG21	1.94	0.49
1:B:470:LEU:H	1:B:470:LEU:CD2	2.06	0.48
1:C:454:SER:O	1:C:458:THR:HG23	2.13	0.48
1:C:521:MET:CE	1:C:556:ILE:HB	2.43	0.48
2:D:138:LEU:CD2	2:D:139:ASN:H	2.24	0.48
2:E:29:LEU:HD11	2:E:77:LEU:N	2.28	0.48
2:E:138:LEU:HA	2:E:369:MET:HG3	1.94	0.48
2:E:195:MET:CE	2:E:211:MET:HG3	2.43	0.48
2:E:65:LEU:HD12	2:E:65:LEU:H	1.78	0.48
2:E:127:PHE:HB2	2:E:355:GLY:O	2.13	0.48
2:F:266:GLU:OE2	2:F:276:TYR:OH	2.10	0.48
1:C:445:MET:SD	1:C:515:ARG:NH1	2.86	0.48
2:E:398:ASP:N	2:E:398:ASP:OD1	2.43	0.48
2:F:364:ASP:O	2:F:368:THR:HG23	2.13	0.48
1:C:547:GLU:HA	1:C:547:GLU:OE1	2.13	0.48
2:E:278:TYR:HA	2:E:318:LEU:HD22	1.96	0.48
1:B:311:ILE:HG12	1:B:326:ILE:HD13	1.95	0.48
1:C:524:VAL:HG12	1:C:573:ILE:CG1	2.43	0.48
2:D:88:ARG:HH12	2:D:103:ILE:HD11	1.78	0.48
2:D:307:PRO:CG	2:D:313:HIS:HB2	2.34	0.48
2:D:380:LYS:CA	2:D:384:GLU:HB2	2.42	0.48
2:D:382:ALA:HB1	2:D:401:TYR:C	2.32	0.48
2:E:364:ASP:OD1	2:E:365:HIS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:433:LEU:O	2:F:436:MET:HG3	2.14	0.48
1:C:241:VAL:O	1:C:245:ILE:HG23	2.13	0.48
2:E:163:GLN:O	2:E:167:GLN:HG3	2.14	0.48
2:E:182:ALA:O	2:E:247:MET:HA	2.13	0.48
2:E:327:ILE:HA	2:E:347:SER:HB2	1.96	0.48
2:F:318:LEU:O	2:F:322:ILE:HG13	2.13	0.48
1:A:487:ARG:HG2	1:A:542:PHE:HE2	1.79	0.48
1:C:459:GLU:OE2	1:C:462:ARG:NH2	2.47	0.48
2:D:379:GLY:O	2:D:382:ALA:HB3	2.13	0.48
1:A:477:VAL:HG12	1:A:478:GLY:N	2.29	0.48
1:B:243:HIS:HB3	1:B:276:LEU:HD11	1.94	0.48
1:B:254:VAL:HB	1:B:289:THR:HG22	1.96	0.48
2:E:288:ALA:HB2	2:E:300:GLN:HG2	1.96	0.48
2:F:34:MET:HA	2:F:68:SER:OG	2.14	0.48
1:A:113:ASP:OD2	1:A:116:LYS:HB2	2.14	0.48
1:B:200:LYS:HB3	1:B:373:ILE:HG22	1.96	0.48
1:B:498:GLU:OE1	1:B:502:GLN:NE2	2.47	0.48
1:C:193:VAL:HG12	1:C:308:TYR:HB3	1.96	0.48
2:D:44:VAL:HA	2:D:54:VAL:HG12	1.94	0.48
1:B:567:LEU:HG	1:B:570:ILE:HD12	1.96	0.48
2:E:436:MET:SD	2:E:436:MET:N	2.71	0.48
2:E:442:LEU:HD12	2:E:442:LEU:HA	1.74	0.48
1:A:400:PRO:O	1:A:404:ASN:ND2	2.46	0.47
1:C:30:VAL:HG13	1:C:35:VAL:HG23	1.96	0.47
2:D:8:ILE:HD12	2:D:68:SER:HB2	1.95	0.47
1:A:513:THR:HG22	1:A:518:GLN:HG2	1.96	0.47
2:D:64:ASN:O	2:D:68:SER:OG	2.23	0.47
2:E:26:TYR:CE2	2:E:27:GLU:HG3	2.49	0.47
2:E:143:ARG:HH11	2:E:242:HIS:CE1	2.32	0.47
2:E:382:ALA:HB1	2:E:402:ALA:HB2	1.95	0.47
1:B:150:MET:HE3	1:B:320:MET:HG2	1.95	0.47
1:B:315:GLU:OE1	1:B:368:ARG:NH2	2.45	0.47
2:D:82:SER:O	2:D:85:MET:HG3	2.13	0.47
2:D:89:VAL:HG22	2:D:209:MET:HG3	1.97	0.47
2:D:278:TYR:HA	2:D:318:LEU:HD21	1.95	0.47
2:D:105:PRO:HG2	2:D:108:TYR:CZ	2.49	0.47
2:E:82:SER:CB	2:E:103:ILE:HD11	2.44	0.47
1:A:162:ILE:HD13	1:A:174:CYS:HB3	1.96	0.47
1:B:255:VAL:HG23	1:B:290:VAL:HB	1.97	0.47
1:B:492:VAL:O	1:B:496:ILE:HG13	2.15	0.47
1:C:2:GLN:OE1	1:C:21:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LYS:HG3	2:F:48:GLN:HB3	1.97	0.47
2:E:444:ARG:O	2:E:444:ARG:HG3	2.14	0.47
1:A:42:MET:HG2	2:E:65:LEU:HD13	1.95	0.47
1:A:340:GLU:OE2	2:D:279:THR:OG1	2.32	0.47
1:B:169:ILE:O	1:B:186:THR:OG1	2.32	0.47
1:B:206:ASP:HA	1:B:440:GLU:OE1	2.15	0.47
2:E:8:ILE:HD13	2:E:16:MET:SD	2.55	0.47
2:E:143:ARG:HD3	2:E:242:HIS:ND1	2.29	0.47
2:E:258:ARG:NH1	2:E:273:TYR:CE2	2.83	0.47
2:E:311:LYS:HD3	2:E:311:LYS:HA	1.62	0.47
2:E:401:TYR:HE1	2:E:437:LEU:HD11	1.77	0.47
1:B:261:GLU:OE1	1:B:330:SER:N	2.48	0.47
1:B:365:TYR:CD1	1:B:366:TYR:CD1	3.02	0.47
1:C:41:GLU:OE1	1:C:43:ARG:NH1	2.45	0.47
2:D:143:ARG:HH21	2:D:170:VAL:HG21	1.77	0.47
2:E:180:VAL:HA	2:E:208:VAL:O	2.15	0.47
2:E:281:LEU:HD13	2:E:319:THR:CG2	2.45	0.47
2:F:401:TYR:O	2:F:404:PHE:HB3	2.15	0.47
1:B:259:CYS:HB3	1:B:334:TRP:HB2	1.96	0.47
1:B:261:GLU:OE1	1:B:333:ARG:HG3	2.15	0.47
1:B:500:TYR:CE2	1:B:522:LEU:HD13	2.50	0.47
1:C:196:GLY:HA2	1:C:368:ARG:NH2	2.29	0.47
2:E:307:PRO:O	2:E:308:GLU:HB3	2.15	0.47
2:D:142:VAL:HG22	2:D:145:GLN:HB2	1.97	0.47
2:F:152:PRO:HD3	2:F:329:LEU:O	2.15	0.47
1:A:243:HIS:O	1:A:247:LYS:HG2	2.16	0.46
1:C:60:PRO:HD3	2:F:47:VAL:HG21	1.97	0.46
1:C:509:VAL:HG11	1:C:558:ARG:HA	1.97	0.46
2:E:315:ILE:HG13	2:E:316:PRO:CD	2.45	0.46
2:E:386:ALA:HA	2:E:389:LEU:CD2	2.45	0.46
2:E:404:PHE:HE1	2:E:433:LEU:O	1.98	0.46
2:F:161:ALA:HB2	2:F:303:ILE:HD12	1.97	0.46
1:A:244:GLN:NE2	1:A:505:ALA:HB1	2.31	0.46
1:A:467:GLU:OE2	1:A:497:ARG:NE	2.30	0.46
1:B:339:ARG:HD3	2:E:270:ARG:HH12	1.79	0.46
1:C:274:PRO:HD3	1:C:286:MET:HG3	1.96	0.46
2:D:152:PRO:HG2	2:D:155:ALA:HB2	1.97	0.46
2:E:44:VAL:HA	2:E:54:VAL:HG12	1.98	0.46
2:E:148:PRO:HG3	2:E:323:THR:HG21	1.96	0.46
2:E:338:ILE:HD13	2:E:341:PRO:HA	1.97	0.46
1:B:121:GLU:HB2	1:B:138:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:ALA:CB	2:D:314:PRO:HG3	2.41	0.46
2:E:258:ARG:HA	2:E:274:PRO:HG3	1.98	0.46
2:F:278:TYR:HB2	2:F:318:LEU:HD12	1.97	0.46
2:D:233:GLU:OE2	2:D:287:ARG:NE	2.37	0.46
2:F:157:LYS:HG3	2:F:158:SER:N	2.30	0.46
1:A:491:GLU:HG2	1:A:546:MET:CE	2.46	0.46
1:B:320:MET:HB2	1:B:322:TYR:CD2	2.50	0.46
1:B:380:ARG:CD	1:B:380:ARG:H	2.27	0.46
2:D:133:SER:HB3	2:D:421:ARG:HD2	1.98	0.46
2:D:138:LEU:HD13	2:D:138:LEU:H	1.80	0.46
2:F:285:PHE:CE2	2:F:319:THR:HG23	2.49	0.46
1:B:120:PHE:CZ	1:B:173:ILE:HD11	2.50	0.46
1:C:327:MET:HB3	1:C:387:ILE:HB	1.96	0.46
2:E:34:MET:CE	2:E:63:ILE:HG12	2.46	0.46
2:E:343:ASP:OD1	2:E:345:LEU:HD23	2.16	0.46
2:F:88:ARG:HA	2:F:98:ASP:OD2	2.15	0.46
1:C:168:THR:OG1	1:C:171:ASP:OD2	2.31	0.46
1:C:331:THR:OG1	1:C:390:VAL:HG12	2.16	0.46
1:B:497:ARG:HB3	1:B:501:LEU:HD12	1.98	0.46
1:B:522:LEU:O	1:B:526:LEU:HG	2.16	0.46
1:B:569:LYS:H	1:B:569:LYS:HD3	1.81	0.46
1:C:560:LYS:HG3	1:C:561:TYR:CD2	2.51	0.46
2:E:40:ARG:HD3	2:E:58:GLU:HB2	1.97	0.46
2:F:438:PRO:HB2	2:F:440:THR:HG22	1.98	0.46
1:B:391:SER:OG	1:B:391:SER:O	2.31	0.46
1:B:399:GLU:OE2	1:B:402:THR:HG23	2.16	0.46
1:C:159:VAL:HG12	1:C:176:ILE:CD1	2.46	0.46
2:D:160:LEU:N	2:D:417:PHE:HE2	2.13	0.46
2:E:149:VAL:HB	2:E:303:ILE:HG12	1.97	0.46
1:A:261:GLU:CG	1:A:266:MET:HE1	2.46	0.46
1:C:242:GLN:HG2	1:C:327:MET:HB2	1.98	0.46
1:C:356:ALA:HB1	2:D:259:GLU:HA	1.98	0.46
2:D:375:ALA:HB1	2:D:404:PHE:CE2	2.50	0.46
2:E:91:ASP:OD2	2:E:95:ARG:NH1	2.49	0.46
2:F:222:ILE:HD12	2:F:222:ILE:H	1.81	0.46
1:B:491:GLU:O	1:B:494:LYS:HG3	2.16	0.45
2:D:86:ILE:HA	2:D:208:VAL:CG2	2.46	0.45
2:E:116:ILE:HD11	2:E:291:ILE:HG12	1.99	0.45
2:F:85:MET:HB3	2:F:208:VAL:HG21	1.99	0.45
1:A:452:ASP:O	1:A:456:MET:HG3	2.16	0.45
1:B:380:ARG:H	1:B:380:ARG:HD3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ILE:O	1:C:315:GLU:HG3	2.17	0.45
2:D:57:PHE:CD1	2:D:219:ILE:HG21	2.51	0.45
2:E:137:HIS:CG	2:E:412:TYR:HH	2.35	0.45
2:F:315:ILE:HB	2:F:316:PRO:CD	2.45	0.45
1:A:75:LEU:HD13	1:A:316:TYR:HB2	1.98	0.45
1:A:444:TYR:O	1:A:448:ILE:HG22	2.15	0.45
1:B:34:GLY:O	1:B:108:GLN:NE2	2.50	0.45
1:B:528:PHE:HA	1:B:577:ILE:CD1	2.41	0.45
1:C:253:LEU:HD23	1:C:288:ARG:O	2.17	0.45
2:D:331:ARG:HB3	2:D:331:ARG:NH1	2.32	0.45
2:D:415:GLN:NE2	2:D:419:THR:O	2.50	0.45
2:D:425:GLU:O	2:D:428:ASP:N	2.49	0.45
2:E:255:GLU:HA	2:E:273:TYR:HE1	1.81	0.45
2:E:383:LYS:HA	2:E:386:ALA:HB3	1.98	0.45
2:F:201:THR:HG23	2:F:203:ALA:H	1.81	0.45
1:A:491:GLU:HG2	1:A:546:MET:HE2	1.99	0.45
2:D:338:ILE:HD11	2:D:413:VAL:HG11	1.97	0.45
2:E:44:VAL:HG22	2:E:54:VAL:HG12	1.98	0.45
2:F:75:HIS:ND1	2:F:78:GLN:OE1	2.49	0.45
1:A:329:ASP:HA	1:A:330:SER:HA	1.60	0.45
1:B:248:TRP:HA	1:B:248:TRP:CE3	2.51	0.45
1:C:240:VAL:O	1:C:244:GLN:NE2	2.46	0.45
1:C:560:LYS:C	1:C:560:LYS:HD3	2.37	0.45
2:D:382:ALA:HB1	2:D:401:TYR:HB3	1.95	0.45
2:E:197:ASP:O	2:E:201:THR:HG23	2.16	0.45
2:F:34:MET:SD	2:F:40:ARG:HD2	2.57	0.45
1:B:446:ASP:OD2	1:B:454:SER:OG	2.27	0.45
1:C:560:LYS:HG3	1:C:561:TYR:HD2	1.81	0.45
2:D:364:ASP:CG	2:D:427:LEU:HD13	2.37	0.45
2:E:146:LYS:CD	2:E:300:GLN:HG3	2.44	0.45
1:A:120:PHE:CE2	1:A:162:ILE:HD11	2.49	0.45
1:A:131:SER:N	1:A:134:ASP:OD2	2.30	0.45
1:B:71:LEU:O	1:B:193:VAL:HG12	2.16	0.45
2:D:364:ASP:OD2	2:D:427:LEU:HD13	2.17	0.45
2:E:60:THR:HG22	2:E:63:ILE:HD12	1.97	0.45
2:E:425:GLU:O	2:E:429:LEU:HG	2.17	0.45
2:F:222:ILE:HA	2:F:253:TYR:CE1	2.51	0.45
1:A:245:ILE:O	1:A:249:SER:OG	2.23	0.45
1:B:35:VAL:HG13	1:B:53:GLU:HB2	1.98	0.45
1:C:560:LYS:HD3	1:C:560:LYS:O	2.17	0.45
2:E:383:LYS:O	2:E:387:VAL:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.99	0.45
1:B:342:SER:HB2	1:B:355:PRO:HG3	1.99	0.45
2:D:416:GLY:O	2:D:419:THR:OG1	2.35	0.45
2:F:226:ARG:NH2	2:F:280:ASN:OD1	2.49	0.45
2:F:358:ALA:HB2	2:F:363:GLU:HB3	1.98	0.45
1:A:408:VAL:HA	2:E:187:THR:HG21	1.99	0.45
2:D:133:SER:HB2	2:D:426:THR:HG23	1.99	0.45
2:F:306:MET:HG3	2:F:316:PRO:CG	2.46	0.45
2:D:331:ARG:HB3	2:D:331:ARG:CZ	2.47	0.44
1:C:124:ILE:HB	1:C:136:ILE:HA	1.98	0.44
1:C:142:THR:HG21	1:C:287:GLU:O	2.17	0.44
1:C:206:ASP:OD1	1:C:371:ARG:NH1	2.50	0.44
1:C:390:VAL:CG2	1:C:402:THR:HG22	2.42	0.44
1:C:454:SER:O	1:C:457:VAL:HG22	2.17	0.44
1:B:124:ILE:HG22	1:B:162:ILE:HD11	1.99	0.44
1:B:549:THR:CG2	1:B:553:ARG:HG3	2.44	0.44
2:D:185:GLY:C	2:D:252:ASN:HD22	2.19	0.44
2:D:374:ALA:O	2:D:378:GLN:HB2	2.18	0.44
2:E:139:ASN:OD1	2:E:348:LEU:HA	2.17	0.44
2:F:434:LEU:HA	2:F:437:LEU:HD23	1.98	0.44
1:A:243:HIS:ND1	1:A:276:LEU:HD11	2.33	0.44
1:A:317:PHE:HA	1:A:320:MET:HG3	1.99	0.44
1:A:333:ARG:HA	1:A:333:ARG:HD2	1.89	0.44
2:F:88:ARG:NH2	2:F:101:PRO:HG2	2.31	0.44
1:C:146:GLN:H	1:C:146:GLN:HG2	1.53	0.44
1:C:413:TRP:HB3	1:C:428:ILE:HG12	2.00	0.44
1:C:419:LEU:HD12	1:C:419:LEU:HA	1.82	0.44
2:D:5:TYR:CD2	2:D:21:VAL:HG12	2.53	0.44
2:D:65:LEU:HD12	2:D:65:LEU:H	1.83	0.44
2:F:88:ARG:NH1	2:F:103:ILE:HG12	2.32	0.44
1:A:150:MET:CE	1:A:320:MET:HG2	2.47	0.44
1:B:307:ILE:HD11	1:B:334:TRP:CE2	2.52	0.44
2:E:255:GLU:HG2	2:E:273:TYR:OH	2.18	0.44
2:F:143:ARG:HD3	2:F:242:HIS:HD2	1.81	0.44
1:B:244:GLN:OE1	1:B:248:TRP:CD1	2.70	0.44
1:B:531:GLU:OE1	1:B:578:LYS:HG3	2.18	0.44
1:C:521:MET:HE3	1:C:556:ILE:HB	1.99	0.44
2:D:366:ALA:O	2:D:370:ASN:ND2	2.47	0.44
2:F:64:ASN:O	2:F:68:SER:HB2	2.18	0.44
1:A:230:VAL:O	1:A:389:ALA:HA	2.18	0.44
1:B:193:VAL:HG22	1:B:308:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:N	1:C:50:GLN:O	2.42	0.44
1:C:92:ASP:HA	2:F:119:ILE:CD1	2.48	0.44
1:A:88:GLN:HG2	1:A:111:ALA:HB1	2.00	0.44
2:E:371:GLN:CG	2:E:434:LEU:HD21	2.47	0.44
2:E:380:LYS:HD3	2:E:380:LYS:C	2.37	0.44
1:A:150:MET:HE1	1:A:320:MET:HG2	2.00	0.43
1:A:490:LEU:HA	1:A:490:LEU:HD22	1.77	0.43
1:B:176:ILE:HD13	1:B:178:THR:HG23	1.99	0.43
2:D:138:LEU:HD22	2:D:139:ASN:CG	2.39	0.43
2:E:135:ILE:HG13	2:E:327:ILE:CD1	2.48	0.43
2:E:439:ARG:HD3	2:E:439:ARG:N	2.33	0.43
1:B:6:ILE:HG22	1:B:60:PRO:HA	2.00	0.43
2:D:9:LYS:CG	2:D:19:GLU:HG3	2.48	0.43
2:D:129:GLN:OE1	2:D:423:ILE:N	2.43	0.43
2:D:173:SER:O	2:D:173:SER:OG	2.31	0.43
2:D:313:HIS:O	2:D:314:PRO:C	2.57	0.43
2:D:403:LYS:HG3	2:D:407:ARG:HD3	2.00	0.43
2:F:142:VAL:HG21	2:F:351:LEU:O	2.18	0.43
2:F:318:LEU:HD13	2:F:318:LEU:HA	1.87	0.43
1:A:36:ILE:HD12	1:A:36:ILE:HA	1.91	0.43
1:C:38:GLU:HB2	1:C:52:TYR:HE1	1.84	0.43
2:D:35:GLN:OE1	2:D:35:GLN:N	2.38	0.43
2:E:3:LYS:HD3	2:E:5:TYR:HE1	1.83	0.43
2:E:16:MET:CE	2:E:56:ILE:HD11	2.48	0.43
2:E:185:GLY:HA3	2:E:221:ARG:HD2	1.99	0.43
2:E:339:SER:HB3	2:E:417:PHE:CE2	2.52	0.43
2:E:389:LEU:HD12	2:E:392:SER:CB	2.36	0.43
2:F:242:HIS:ND1	2:F:296:GLY:HA2	2.33	0.43
1:B:140:ASP:OD1	1:B:146:GLN:HG2	2.17	0.43
1:B:257:VAL:HG23	1:B:328:ALA:HB2	2.01	0.43
1:C:42:MET:HG2	2:D:65:LEU:HD13	2.00	0.43
2:D:304:LEU:HD12	2:D:304:LEU:HA	1.69	0.43
2:F:147:LEU:HD23	2:F:147:LEU:HA	1.91	0.43
1:A:260:GLY:O	1:A:333:ARG:HG3	2.18	0.43
1:A:445:MET:HE3	1:A:515:ARG:NE	2.33	0.43
1:C:339:ARG:HB2	1:C:354:TYR:HD1	1.82	0.43
2:F:312:THR:HG22	2:F:312:THR:O	2.18	0.43
1:A:238:LYS:O	1:A:242:GLN:HG3	2.18	0.43
1:C:118:TRP:CH2	1:C:141:GLU:HG3	2.53	0.43
2:D:85:MET:O	2:D:88:ARG:HB2	2.18	0.43
2:E:7:THR:OG1	2:E:7:THR:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:ARG:HH11	2:E:242:HIS:HE1	1.65	0.43
2:F:14:PRO:HD2	2:F:15:LEU:HD12	2.00	0.43
1:A:267:THR:HG21	2:D:121:ARG:HB3	2.01	0.43
1:B:252:ASP:OD2	1:B:322:TYR:HA	2.19	0.43
2:E:148:PRO:HD2	2:E:326:GLN:HA	2.01	0.43
2:F:128:ILE:HG22	2:F:141:LEU:HB3	2.00	0.43
2:F:163:GLN:OE1	2:F:417:PHE:HA	2.18	0.43
2:F:356:THR:HG1	2:F:365:HIS:CE1	2.30	0.43
1:A:27:MET:O	1:A:67:THR:OG1	2.29	0.43
1:A:261:GLU:OE1	1:A:330:SER:N	2.52	0.43
1:C:565:GLU:O	1:C:569:LYS:HB2	2.18	0.43
2:D:414:ASN:OD1	2:D:414:ASN:O	2.37	0.43
2:F:7:THR:OG1	2:F:19:GLU:O	2.36	0.43
1:A:119:TRP:CZ3	1:A:165:GLY:HA2	2.54	0.43
1:C:30:VAL:HG23	1:C:64:VAL:CG2	2.48	0.43
1:C:248:TRP:HB3	1:C:512:PHE:CD1	2.54	0.43
2:D:138:LEU:HD13	2:D:138:LEU:N	2.34	0.43
2:E:308:GLU:O	2:E:309:ASP:HB2	2.19	0.43
2:F:157:LYS:HD3	2:F:305:THR:CG2	2.49	0.43
1:A:148:LYS:H	1:A:320:MET:HE1	1.84	0.43
1:A:194:ARG:NH2	1:A:304:GLU:OE2	2.47	0.43
1:B:120:PHE:HB2	1:B:139:VAL:HG22	2.01	0.43
1:B:191:TRP:CD1	1:B:197:ARG:HG3	2.54	0.43
1:B:453:TRP:CZ3	1:B:519:PHE:HA	2.53	0.43
1:C:84:PHE:HB3	1:C:88:GLN:HA	2.01	0.43
2:E:137:HIS:HD2	2:E:365:HIS:CD2	2.37	0.43
1:C:297:ASN:OD1	2:F:286:GLU:HB2	2.19	0.42
2:D:91:ASP:OD1	2:D:95:ARG:N	2.37	0.42
2:D:223:ALA:O	2:D:227:MET:HG2	2.19	0.42
2:E:119:ILE:O	2:E:292:ARG:NH1	2.51	0.42
2:E:322:ILE:HD12	2:E:323:THR:N	2.34	0.42
2:F:35:GLN:NE2	2:F:64:ASN:H	2.15	0.42
2:F:81:VAL:O	2:F:106:GLU:N	2.52	0.42
1:B:59:GLY:N	2:E:25:LYS:HG3	2.34	0.42
1:B:267:THR:HG21	2:E:121:ARG:O	2.19	0.42
1:C:517:LYS:HZ1	1:C:560:LYS:HB2	1.83	0.42
2:D:339:SER:H	2:D:414:ASN:HB2	1.82	0.42
2:E:29:LEU:HD11	2:E:77:LEU:HA	2.01	0.42
1:B:252:ASP:OD2	1:B:322:TYR:HD1	2.02	0.42
1:B:253:LEU:HD23	1:B:288:ARG:O	2.20	0.42
1:C:80:ILE:HG13	1:C:141:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:LEU:HD13	2:E:319:THR:HG23	2.01	0.42
2:F:394:LEU:CA	2:F:398:ASP:HB2	2.46	0.42
1:A:73:VAL:HG13	1:A:193:VAL:HG22	2.01	0.42
1:A:338:LEU:HD23	1:A:338:LEU:HA	1.83	0.42
1:B:9:VAL:HG11	1:B:58:ILE:O	2.19	0.42
1:B:225:GLY:O	1:B:370:GLY:HA2	2.19	0.42
1:C:169:ILE:CG2	1:C:188:MET:HB2	2.49	0.42
1:C:211:THR:HG22	1:C:213:GLN:HB2	2.00	0.42
1:C:577:ILE:O	1:C:581:ILE:HG12	2.19	0.42
2:F:88:ARG:HH11	2:F:103:ILE:HG12	1.85	0.42
1:A:208:PRO:HB3	1:A:441:VAL:HG22	2.01	0.42
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.88	0.42
1:B:455:ASP:N	1:B:455:ASP:OD1	2.51	0.42
1:B:486:ASP:HA	1:B:489:THR:OG1	2.19	0.42
1:C:262:ARG:H	1:C:262:ARG:HG3	1.56	0.42
1:C:553:ARG:O	1:C:556:ILE:HG12	2.19	0.42
2:D:427:LEU:HA	2:D:427:LEU:HD23	1.69	0.42
2:E:130:THR:O	2:E:167:GLN:HB2	2.20	0.42
2:F:149:VAL:HA	2:F:327:ILE:O	2.19	0.42
1:B:196:GLY:HA2	1:B:368:ARG:NH2	2.34	0.42
1:B:378:ASP:N	1:B:378:ASP:OD1	2.53	0.42
1:C:517:LYS:HE3	1:C:560:LYS:CE	2.50	0.42
2:E:144:GLY:HA2	2:E:298:VAL:O	2.20	0.42
2:E:166:ARG:NH2	2:E:418:TYR:HD1	2.17	0.42
2:F:111:ILE:HB	2:F:226:ARG:HB3	2.02	0.42
2:F:243:VAL:N	2:F:297:SER:O	2.52	0.42
2:F:383:LYS:HB2	2:F:383:LYS:HE2	1.88	0.42
1:C:514:SER:CB	1:C:560:LYS:NZ	2.83	0.42
2:F:79:LEU:HB2	2:F:227:MET:SD	2.60	0.42
1:A:378:ASP:OD1	1:A:378:ASP:N	2.53	0.42
1:B:118:TRP:CH2	1:B:141:GLU:HG3	2.55	0.42
1:B:217:ASP:OD1	1:B:217:ASP:N	2.53	0.42
1:C:189:GLN:NE2	1:C:197:ARG:HH12	2.17	0.42
2:D:147:LEU:O	2:D:302:PRO:HD2	2.19	0.42
2:E:60:THR:O	2:E:63:ILE:HG13	2.19	0.42
2:F:130:THR:OG1	2:F:132:ILE:HG12	2.20	0.42
1:A:2:GLN:OE1	1:A:21:GLU:N	2.52	0.42
2:D:109:LEU:HD23	2:D:109:LEU:HA	1.86	0.42
2:D:177:PHE:HE2	2:D:244:LEU:CB	2.20	0.42
2:D:430:GLY:O	2:D:434:LEU:HG	2.19	0.42
1:C:57:GLY:O	2:F:25:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:THR:OG1	4:C:602:ANP:O2B	2.38	0.42
1:C:391:SER:HB3	2:F:321:TYR:CZ	2.55	0.42
1:C:564:GLU:O	1:C:564:GLU:HG2	2.20	0.42
2:D:86:ILE:HA	2:D:208:VAL:HG22	2.01	0.42
2:D:361:THR:HG21	2:D:365:HIS:HD2	1.85	0.42
2:F:444:ARG:HD2	2:F:445:ILE:H	1.84	0.42
1:A:19:MET:HE1	1:A:49:ILE:HD11	2.01	0.41
1:A:73:VAL:HG11	1:A:309:THR:HG23	2.01	0.41
1:A:214:ARG:NH2	1:A:503:GLN:HG3	2.35	0.41
1:C:234:PHE:HB3	2:F:321:TYR:CE1	2.55	0.41
1:C:260:GLY:O	2:F:278:TYR:OH	2.31	0.41
1:C:467:GLU:OE1	1:C:497:ARG:NH1	2.50	0.41
2:D:26:TYR:CZ	2:D:27:GLU:HG3	2.55	0.41
2:D:318:LEU:O	2:D:322:ILE:HG13	2.20	0.41
2:E:175:ASP:OD2	2:E:295:LYS:NZ	2.44	0.41
2:E:195:MET:HE2	2:E:211:MET:HG3	2.02	0.41
2:F:90:PHE:HZ	2:F:103:ILE:HD11	1.84	0.41
2:F:112:ASN:C	2:F:287:ARG:HH12	2.23	0.41
1:B:351:ASP:OD1	2:F:258:ARG:NH1	2.53	0.41
1:B:550:VAL:HA	1:B:553:ARG:CZ	2.50	0.41
1:C:73:VAL:HG11	1:C:309:THR:HG23	2.01	0.41
1:C:225:GLY:O	1:C:370:GLY:HA2	2.19	0.41
2:D:28:GLU:O	2:D:44:VAL:HG23	2.20	0.41
2:E:138:LEU:CD1	2:E:344:VAL:HG11	2.50	0.41
2:E:236:ALA:HA	2:E:241:MET:O	2.20	0.41
2:F:141:LEU:HD23	2:F:142:VAL:N	2.34	0.41
2:F:232:ALA:HA	2:F:243:VAL:HG11	2.02	0.41
1:A:220:PHE:HA	1:A:435:SER:HB3	2.03	0.41
1:C:124:ILE:HD12	1:C:124:ILE:HA	1.95	0.41
1:C:500:TYR:CE1	1:C:522:LEU:HB2	2.54	0.41
2:D:151:GLY:O	2:D:305:THR:HA	2.21	0.41
2:F:83:GLU:H	2:F:83:GLU:HG2	1.68	0.41
2:F:327:ILE:HA	2:F:347:SER:OG	2.20	0.41
1:A:550:VAL:HG22	1:A:553:ARG:NH2	2.35	0.41
1:B:248:TRP:HZ2	1:B:511:THR:HG23	1.86	0.41
1:C:87:ILE:HG13	1:C:89:ARG:HG3	2.02	0.41
1:C:517:LYS:HZ3	1:C:560:LYS:HB2	1.85	0.41
2:D:362:ARG:HE	2:D:364:ASP:CG	2.24	0.41
2:E:362:ARG:NH2	2:E:364:ASP:OD2	2.47	0.41
2:E:372:LEU:HD21	2:E:408:PHE:HE2	1.85	0.41
1:B:119:TRP:HA	1:B:165:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:SER:HA	2:E:321:TYR:CE1	2.56	0.41
1:C:521:MET:O	1:C:524:VAL:HG22	2.20	0.41
2:E:385:LEU:HD23	2:E:385:LEU:HA	1.89	0.41
2:F:45:LEU:HD23	2:F:45:LEU:HA	1.88	0.41
2:F:226:ARG:CZ	2:F:284:LEU:HD21	2.50	0.41
1:A:231:PRO:HD2	1:A:413:TRP:O	2.20	0.41
1:A:351:ASP:OD1	2:E:258:ARG:CZ	2.67	0.41
1:C:36:ILE:HG23	1:C:52:TYR:HB2	2.03	0.41
1:C:234:PHE:HB3	2:F:321:TYR:HD1	1.83	0.41
1:C:245:ILE:CD1	1:C:387:ILE:HG13	2.46	0.41
2:D:339:SER:HB2	2:D:417:PHE:HD1	1.83	0.41
2:E:255:GLU:HA	2:E:273:TYR:CE1	2.55	0.41
2:E:271:ARG:NH2	2:E:271:ARG:HB2	2.35	0.41
2:E:383:LYS:O	2:E:383:LYS:HG3	2.20	0.41
2:E:404:PHE:CE1	2:E:433:LEU:O	2.73	0.41
2:F:93:LEU:CD2	2:F:220:GLU:HG2	2.51	0.41
1:A:549:THR:HA	1:A:552:VAL:HG12	2.02	0.41
1:B:285:LEU:O	1:B:289:THR:HG23	2.20	0.41
1:B:342:SER:CB	1:B:355:PRO:HG3	2.50	0.41
2:D:88:ARG:HD2	2:D:88:ARG:HA	1.82	0.41
2:D:339:SER:N	2:D:414:ASN:HB3	2.29	0.41
2:D:398:ASP:O	2:D:401:TYR:N	2.53	0.41
2:E:39:ILE:HD13	2:E:41:ARG:HH11	1.85	0.41
2:F:107:LYS:NZ	2:F:238:GLU:OE2	2.38	0.41
2:F:164:ILE:HD13	2:F:164:ILE:HA	1.92	0.41
1:A:351:ASP:N	2:E:258:ARG:NH2	2.68	0.41
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.88	0.41
1:B:144:ILE:HD13	1:B:144:ILE:HG21	1.87	0.41
1:B:364:GLU:O	1:B:368:ARG:HG3	2.21	0.41
1:B:499:ASP:OD2	1:B:557:SER:HA	2.20	0.41
2:D:3:LYS:HE2	2:D:3:LYS:HB2	1.87	0.41
2:D:4:GLU:OE2	2:D:71:ARG:NH2	2.54	0.41
2:D:84:ASP:HB2	2:D:103:ILE:HD12	2.02	0.41
2:F:141:LEU:HD23	2:F:142:VAL:H	1.86	0.41
1:A:89:ARG:HD2	1:A:94:PHE:CE2	2.55	0.41
1:A:497:ARG:O	1:A:502:GLN:HG3	2.20	0.41
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.84	0.41
1:A:560:LYS:HE2	1:A:561:TYR:CE1	2.55	0.41
1:B:45:ASP:OD2	1:B:45:ASP:N	2.41	0.41
1:C:308:TYR:HD1	1:C:308:TYR:HA	1.80	0.41
2:E:45:LEU:HD23	2:E:45:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:90:PHE:O	2:E:211:MET:N	2.53	0.41
2:E:319:THR:O	2:E:323:THR:HG23	2.20	0.41
2:E:376:TYR:CD1	2:E:408:PHE:CD1	3.09	0.41
2:E:407:ARG:NH2	2:E:436:MET:HE2	2.36	0.41
2:F:224:THR:HB	2:F:225:PRO:CD	2.50	0.41
2:F:309:ASP:O	2:F:311:LYS:N	2.54	0.41
1:A:406:LEU:HD22	1:A:434:TYR:OH	2.21	0.41
1:B:231:PRO:HB3	1:B:390:VAL:HG23	2.03	0.41
2:E:117:ASN:OD1	2:E:119:ILE:HG12	2.21	0.41
2:E:186:ILE:O	2:E:214:ALA:N	2.53	0.41
2:E:257:LEU:HD23	2:E:257:LEU:HA	1.96	0.41
1:A:218:THR:OG1	1:A:500:TYR:OH	2.08	0.40
1:A:239:THR:HG22	1:A:243:HIS:HE2	1.86	0.40
1:A:264:ASN:HB2	2:D:324:GLU:OE2	2.20	0.40
1:A:418:SER:O	1:A:422:LYS:HG3	2.21	0.40
1:A:560:LYS:HE2	1:A:561:TYR:HE1	1.85	0.40
1:B:487:ARG:O	1:B:487:ARG:HD3	2.21	0.40
1:C:211:THR:HG22	1:C:213:GLN:H	1.87	0.40
2:D:139:ASN:ND2	2:D:347:SER:C	2.75	0.40
2:D:151:GLY:O	2:D:306:MET:N	2.49	0.40
2:D:353:ASP:OD1	2:D:353:ASP:N	2.54	0.40
2:E:376:TYR:C	2:E:378:GLN:N	2.73	0.40
2:F:397:ILE:HG23	2:F:398:ASP:OD1	2.21	0.40
1:A:535:ALA:HA	1:A:538:LEU:HB2	2.03	0.40
2:D:225:PRO:O	2:D:229:LEU:HD12	2.21	0.40
2:E:34:MET:HE2	2:E:63:ILE:HG12	2.02	0.40
2:E:250:MET:O	2:E:253:TYR:N	2.54	0.40
2:E:444:ARG:HH21	2:E:446:LYS:HB3	1.86	0.40
1:A:182:LEU:H	1:A:182:LEU:HD23	1.86	0.40
1:A:215:VAL:HB	1:A:501:LEU:HD22	2.03	0.40
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.94	0.40
1:A:330:SER:HB3	1:A:333:ARG:HG2	2.02	0.40
1:B:173:ILE:HG22	1:B:186:THR:HA	2.04	0.40
1:C:274:PRO:HA	1:C:284:SER:HB2	2.03	0.40
1:C:338:LEU:HD12	1:C:338:LEU:HA	1.90	0.40
1:C:486:ASP:OD1	1:C:486:ASP:N	2.54	0.40
1:C:541:TYR:O	1:C:545:ILE:HG13	2.20	0.40
1:C:554:GLU:OE1	1:C:558:ARG:NH2	2.55	0.40
1:C:566:GLU:O	1:C:570:ILE:HG12	2.22	0.40
1:C:576:GLU:O	1:C:580:THR:OG1	2.31	0.40
2:D:427:LEU:O	2:D:431:TRP:CD1	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ARG:NH2	2:E:95:ARG:HE	2.18	0.40
2:F:80:GLY:HA2	2:F:108:TYR:HD1	1.86	0.40
2:F:129:GLN:OE1	2:F:423:ILE:N	2.46	0.40
2:F:248:GLU:OE1	2:F:248:GLU:HA	2.21	0.40
1:B:101:ASN:HB3	2:E:120:ALA:HB1	2.03	0.40
1:C:135:ILE:HD12	1:C:148:LYS:HB3	2.03	0.40
2:D:244:LEU:HD11	2:D:301:ILE:CD1	2.51	0.40
2:E:329:LEU:HA	2:E:341:PRO:O	2.21	0.40
2:F:139:ASN:HD22	2:F:347:SER:HB3	1.84	0.40
2:F:180:VAL:O	2:F:245:VAL:HA	2.21	0.40
1:A:88:GLN:HG2	1:A:111:ALA:CB	2.52	0.40
1:B:184:GLU:H	1:B:184:GLU:HG2	1.69	0.40
1:B:348:MET:HE3	2:F:265:ARG:HA	2.04	0.40
1:C:327:MET:HA	1:C:387:ILE:O	2.22	0.40
2:E:83:GLU:CG	2:E:239:LYS:HE2	2.51	0.40
2:E:146:LYS:CE	2:E:302:PRO:HG3	2.45	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:GLU:OE1	1:B:558:ARG:NH2[2_555]	2.14	0.06
1:A:547:GLU:OE1	2:E:446:LYS:NZ[2_555]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	584/596 (98%)	568 (97%)	14 (2%)	2 (0%)	41	75
1	B	584/596 (98%)	565 (97%)	16 (3%)	3 (0%)	29	66
1	C	582/596 (98%)	559 (96%)	20 (3%)	3 (0%)	29	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	430/458 (94%)	405 (94%)	22 (5%)	3 (1%)	22	60
2	E	447/458 (98%)	422 (94%)	24 (5%)	1 (0%)	47	80
2	F	443/458 (97%)	418 (94%)	22 (5%)	3 (1%)	22	60
All	All	3070/3162 (97%)	2937 (96%)	118 (4%)	15 (0%)	29	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	ILE
1	C	392	PRO
1	C	431	ILE
2	D	314	PRO
1	A	477	VAL
2	F	173	SER
1	B	260	GLY
2	D	388	VAL
2	D	148	PRO
2	F	388	VAL
1	C	479	ILE
1	A	395	GLY
1	B	397	ILE
2	F	148	PRO
2	E	390	GLY

### 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	502/509 (99%)	485 (97%)	17 (3%)	37	68
1	B	502/509 (99%)	476 (95%)	26 (5%)	23	55
1	C	500/509 (98%)	488 (98%)	12 (2%)	49	76
2	D	356/380 (94%)	342 (96%)	14 (4%)	32	64
2	E	372/380 (98%)	353 (95%)	19 (5%)	24	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	368/380 (97%)	352 (96%)	16 (4%)	29	61
All	All	2600/2667 (98%)	2496 (96%)	104 (4%)	31	63

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	43	ARG
1	A	45	ASP
1	A	65	ARG
1	A	94	PHE
1	A	153	ASN
1	A	174	CYS
1	A	188	MET
1	A	197	ARG
1	A	204	ASN
1	A	273	PHE
1	A	280	ASN
1	A	285	LEU
1	A	319	ASP
1	A	333	ARG
1	A	378	ASP
1	A	487	ARG
1	B	94	PHE
1	B	96	GLU
1	B	114	HIS
1	B	115	GLU
1	B	120	PHE
1	B	140	ASP
1	B	163	GLU
1	B	203	LEU
1	B	204	ASN
1	B	217	ASP
1	B	268	ASP
1	B	273	PHE
1	B	329	ASP
1	B	378	ASP
1	B	380	ARG
1	B	421	GLN
1	B	455	ASP
1	B	461	MET
1	B	470	LEU

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Mol	Chain	Res	Type
1	B	480	ASP
1	B	487	ARG
1	B	491	GLU
1	B	494	LYS
1	B	500	TYR
1	B	533	ARG
1	B	569	LYS
1	C	92	ASP
1	C	119	TRP
1	C	138	TYR
1	C	185	LEU
1	C	243	HIS
1	C	244	GLN
1	C	308	TYR
1	C	399	GLU
1	C	443	ARG
1	C	519	PHE
1	C	530	LYS
1	C	566	GLU
2	D	48	GLN
2	D	49	GLU
2	D	138	LEU
2	D	212	ASN
2	D	249	ASP
2	D	270	ARG
2	D	271	ARG
2	D	292	ARG
2	D	326	GLN
2	D	348	LEU
2	D	353	ASP
2	D	362	ARG
2	D	408	PHE
2	D	412	TYR
2	E	25	LYS
2	E	41	ARG
2	E	90	PHE
2	E	121	ARG
2	E	123	TYR
2	E	177	PHE
2	E	250	MET
2	E	271	ARG
2	E	278	TYR

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Mol	Chain	Res	Type
2	E	280	ASN
2	E	309	ASP
2	E	310	ASP
2	E	335	LYS
2	E	380	LYS
2	E	401	TYR
2	E	407	ARG
2	E	431	TRP
2	E	436	MET
2	E	439	ARG
2	F	33	ARG
2	F	41	ARG
2	F	85	MET
2	F	125	ASP
2	F	175	ASP
2	F	215	ASN
2	F	242	HIS
2	F	249	ASP
2	F	331	ARG
2	F	334	TYR
2	F	352	LYS
2	F	373	PHE
2	F	398	ASP
2	F	401	TYR
2	F	412	TYR
2	F	439	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	160	GLN
1	C	264	ASN
1	C	297	ASN
2	D	139	ASN
2	D	212	ASN
2	D	252	ASN
2	D	365	HIS
2	D	414	ASN
2	E	78	GLN
2	E	300	GLN
2	F	371	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	C	602	3	29,33,33	1.33	5 (17%)	31,52,52	1.57	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	C	602	3	-	6/14/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ANP	C4-N3	-4.37	1.29	1.35
4	C	602	ANP	PG-O1G	2.54	1.50	1.46
4	C	602	ANP	PG-N3B	2.35	1.69	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ANP	PB-O3A	-2.35	1.56	1.59
4	C	602	ANP	PB-O1B	2.33	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	ANP	C4-C5-N7	6.11	115.77	109.40
4	C	602	ANP	PA-O3A-PB	-4.06	118.31	132.62

There are no chirality outliers.

All (6) torsion outliers are listed below:

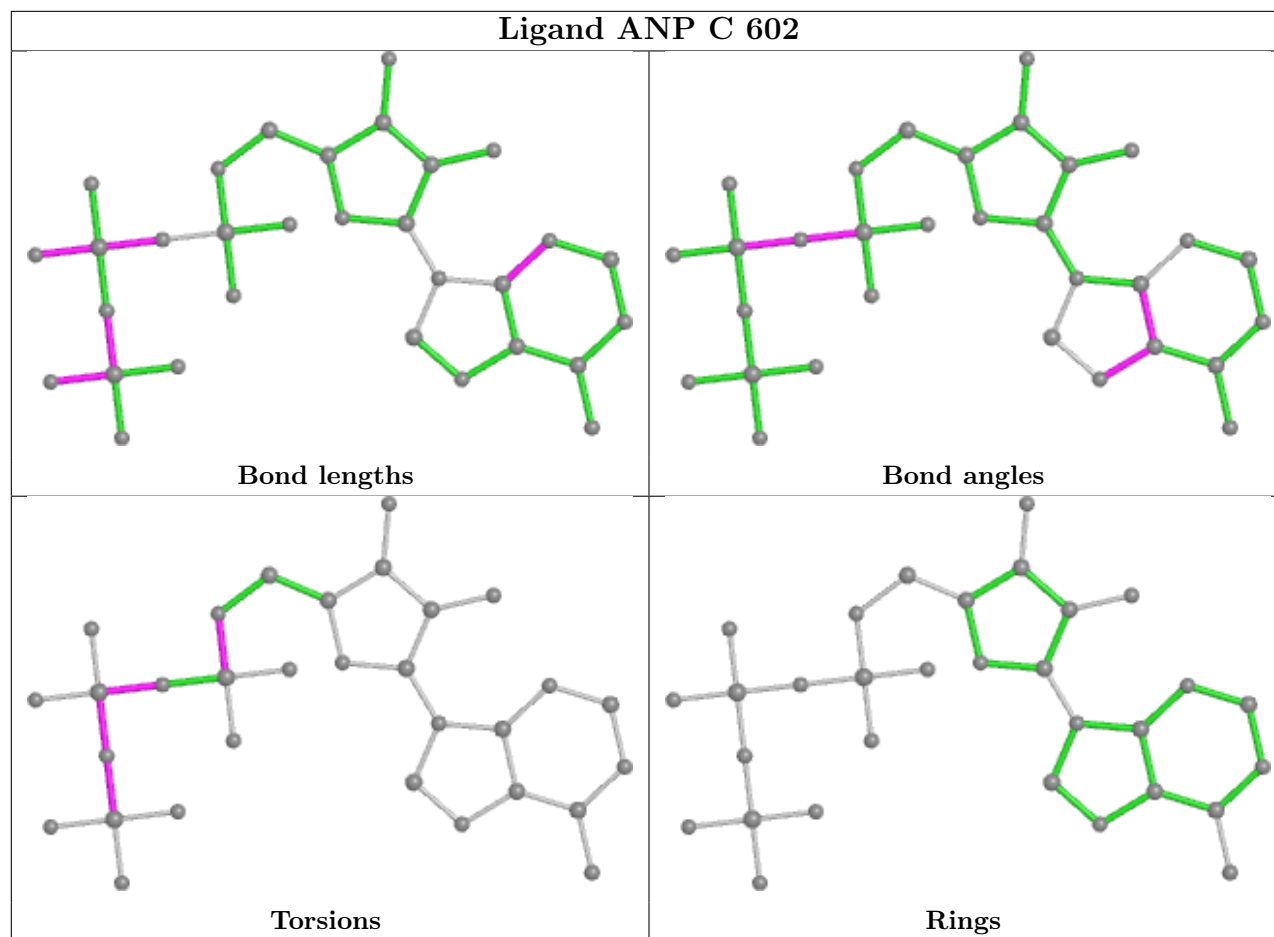
Mol	Chain	Res	Type	Atoms
4	C	602	ANP	PB-N3B-PG-O1G
4	C	602	ANP	PG-N3B-PB-O1B
4	C	602	ANP	PA-O3A-PB-O2B
4	C	602	ANP	C5'-O5'-PA-O1A
4	C	602	ANP	C5'-O5'-PA-O3A
4	C	602	ANP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	602	ANP	8	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

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	A	586/596 (98%)	-0.06	1 (0%) 95 94	50, 73, 117, 139	0
1	B	586/596 (98%)	0.11	16 (2%) 54 52	69, 107, 156, 174	0
1	C	584/596 (97%)	-0.02	9 (1%) 73 71	61, 83, 141, 167	0
2	D	432/458 (94%)	-0.01	13 (3%) 50 48	54, 85, 172, 196	0
2	E	449/458 (98%)	0.06	17 (3%) 40 39	57, 95, 162, 179	0
2	F	445/458 (97%)	-0.01	5 (1%) 80 77	63, 96, 142, 168	0
All	All	3082/3162 (97%)	0.01	61 (1%) 65 63	50, 90, 151, 196	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	GLY	4.8
1	C	561	TYR	4.5
1	B	539	GLY	3.7
2	E	319	THR	3.6
2	E	412	TYR	3.6
2	E	385	LEU	3.4
2	E	268	PRO	3.3
1	C	538	LEU	3.2
1	C	560	LYS	3.1
1	C	567	LEU	3.0
1	C	162	ILE	2.9
1	B	583	LEU	2.9
1	B	173	ILE	2.9
2	E	401	TYR	2.9
2	E	273	TYR	2.7
1	B	136	ILE	2.7
2	D	312	THR	2.7
2	D	413	VAL	2.7
2	E	321	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	313	HIS	2.6
2	F	104	LEU	2.6
2	E	310	ASP	2.5
2	D	376	TYR	2.5
2	E	388	VAL	2.5
1	B	123	THR	2.5
2	D	388	VAL	2.5
1	B	541	TYR	2.5
2	F	171	LEU	2.5
2	E	387	VAL	2.5
1	C	279	PRO	2.5
1	C	576	GLU	2.5
1	B	534	LYS	2.4
2	D	390	GLY	2.4
1	B	582	GLN	2.4
2	D	404	PHE	2.4
1	A	479	ILE	2.4
2	D	434	LEU	2.4
2	E	269	GLY	2.4
2	D	311	LYS	2.3
1	B	535	ALA	2.3
2	E	404	PHE	2.3
2	D	395	SER	2.3
2	F	309	ASP	2.2
1	B	570	ILE	2.2
2	E	274	PRO	2.2
2	D	393	ALA	2.2
1	B	531	GLU	2.2
2	E	381	GLN	2.2
1	B	479	ILE	2.2
1	C	253	LEU	2.2
1	B	519	PHE	2.1
2	E	397	ILE	2.1
1	B	185	LEU	2.1
2	F	434	LEU	2.1
2	D	389	LEU	2.1
2	E	272	GLY	2.1
1	C	562	ILE	2.1
2	E	80	GLY	2.1
2	F	444	ARG	2.0
2	D	401	TYR	2.0
1	B	53	GLU	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.

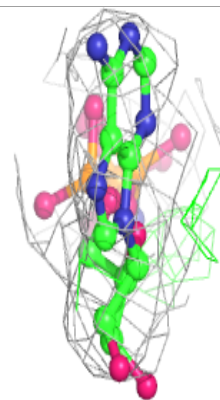
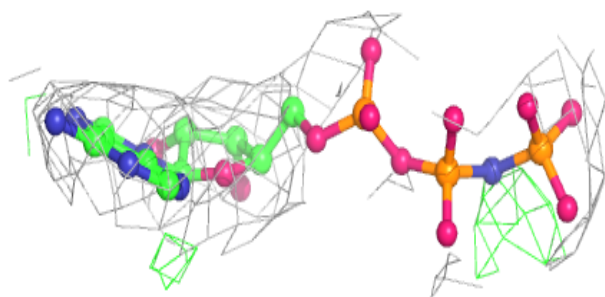
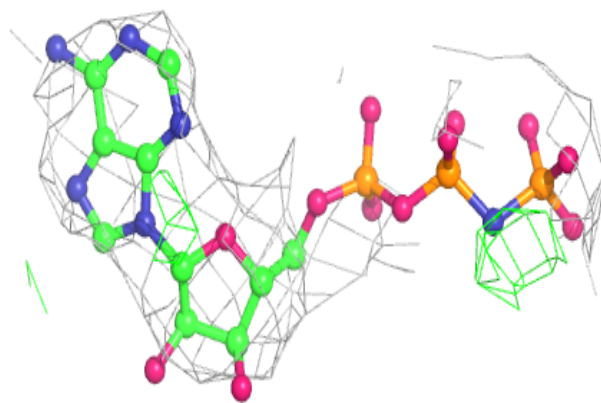
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ANP	C	602	31/31	0.94	0.34	76,90,103,112	0
3	MG	C	601	1/1	0.97	0.47	68,68,68,68	0

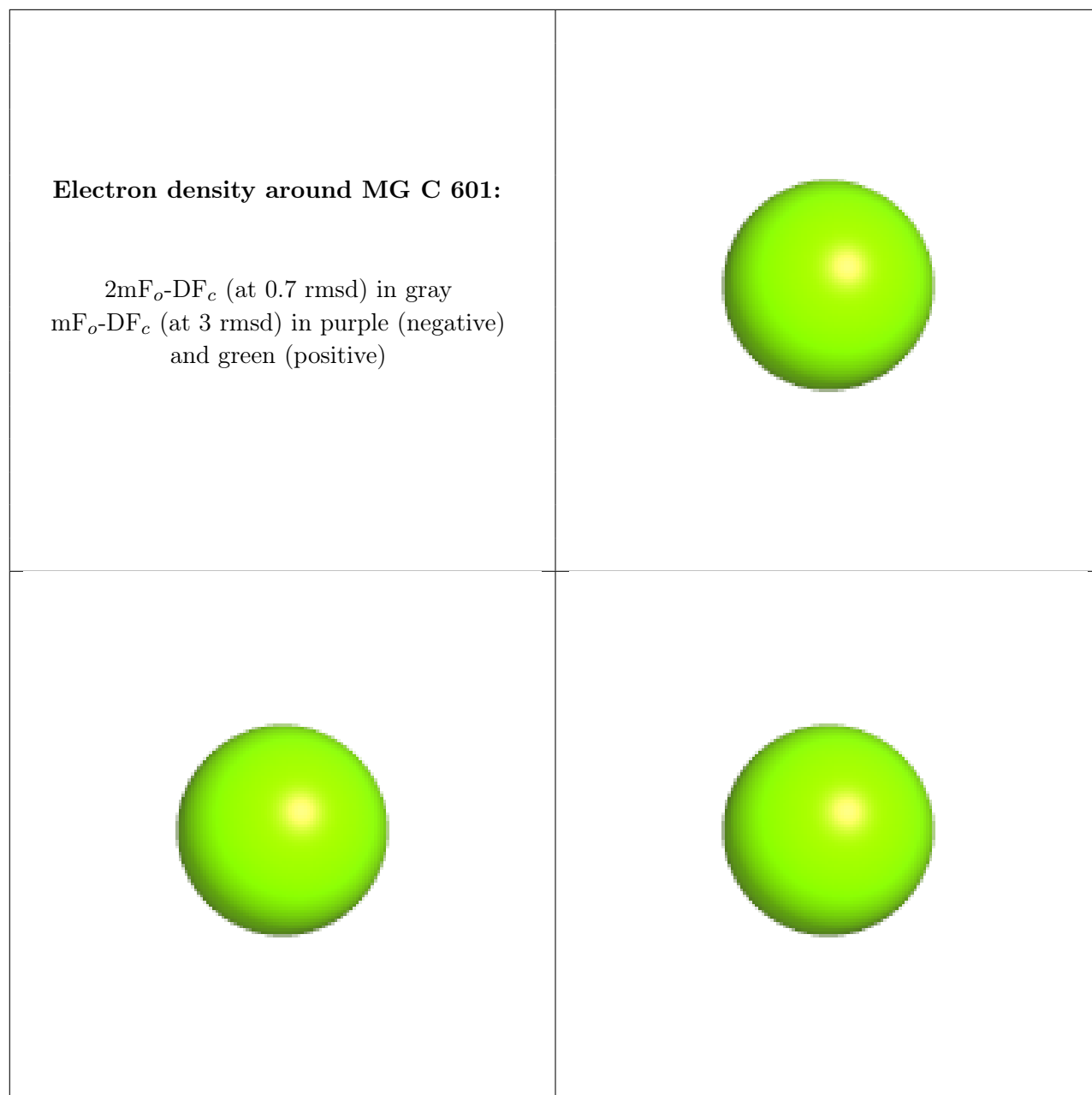
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around ANP C 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.