



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:35 am BST

PDB ID : 5JR7  
Title : Crystal structure of an ACRDYS heterodimer [RIa(92-365):C] of PKA  
Authors : Bruystens, J.G.H.; Wu, J.; Taylor, S.S.  
Deposited on : 2016-05-05  
Resolution : 3.56 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 : 2.11  
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) : 2.11

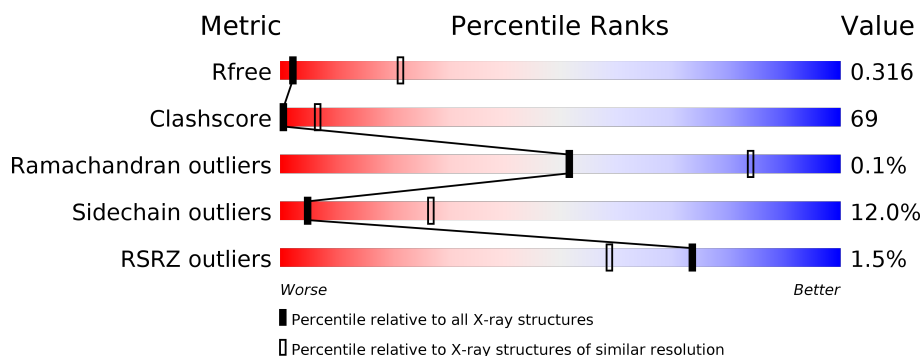
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.56 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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

Mol	Chain	Length	Quality of chain
1	A	350	<div> <div>42%</div> <div>48%</div> <div>6%</div> <div>.</div> </div>
1	C	350	<div>2%</div> <div>37%</div> <div>52%</div> <div>8%</div> <div>.</div>
2	B	275	<div>%</div> <div>37%</div> <div>53%</div> <div>6%</div> <div>.</div>
2	D	275	<div>3%</div> <div>32%</div> <div>52%</div> <div>13%</div> <div>.</div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	C	338	-	-	-	X
3	ADP	C	400	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9665 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.

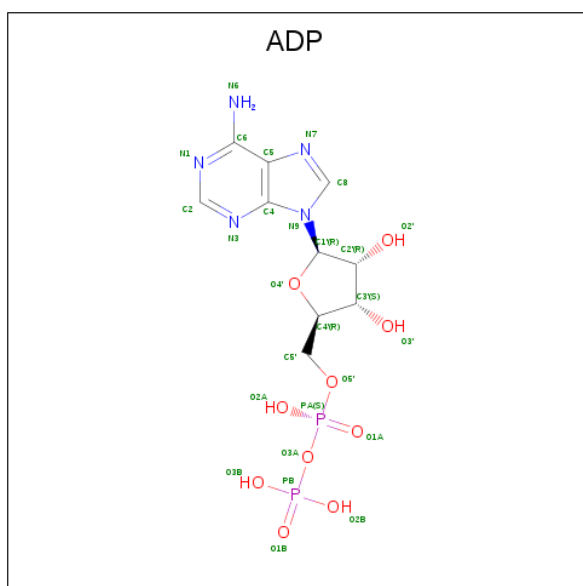
- Molecule 1 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	P	S	6	0	0
			2734	1773	451	499	3	8			
1	C	338	Total	C	N	O	P	S	0	0	0
			2729	1767	451	500	3	8			

- Molecule 2 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	267	Total	C	N	O	S	1	0	0
			2079	1321	354	397	7			
2	D	266	Total	C	N	O	S	1	0	0
			2069	1317	353	392	7			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

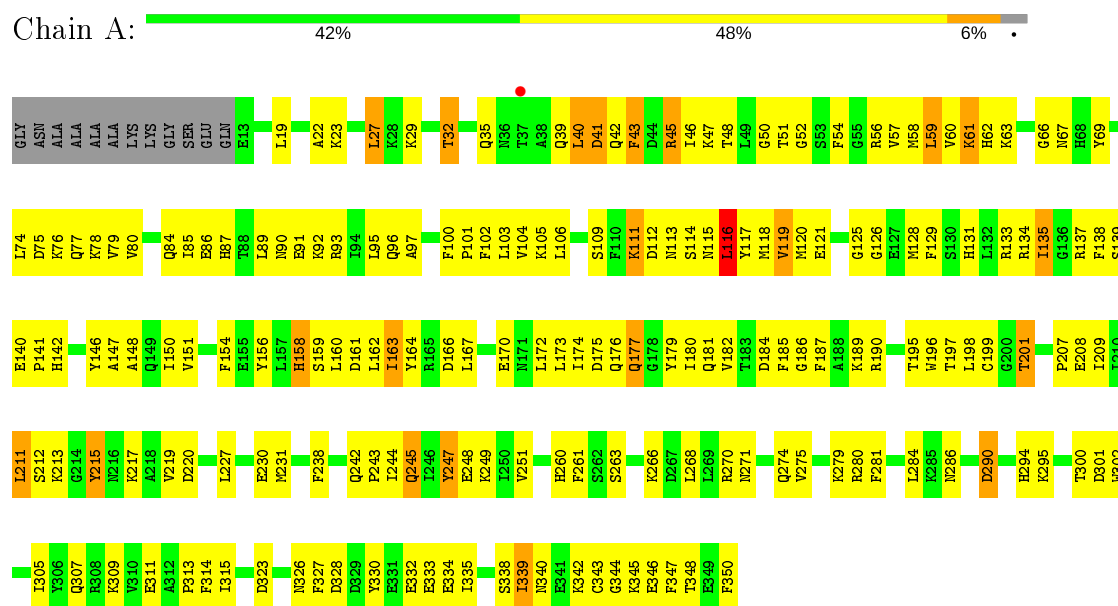


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

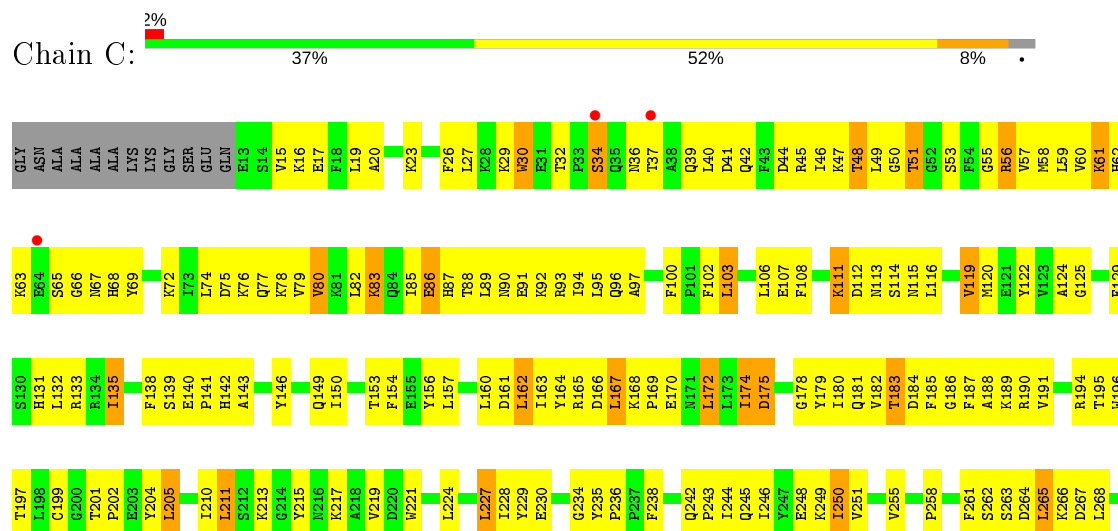
### 3 Residue-property plots

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 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: cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.15Å 66.79Å 87.93Å 101.76° 89.37° 105.27°	Depositor
Resolution (Å)	49.11 – 3.56 49.10 – 3.51	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.11-3.56) 96.1 (49.10-3.51)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, $R_{free}$	0.266 , 0.322 0.255 , 0.316	Depositor DCC
$R_{free}$ test set	785 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 99.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9665	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: TPO, ADP, SEP

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	0.48	1/2771 (0.0%)	0.92	5/3745 (0.1%)
1	C	0.41	1/2765 (0.0%)	0.76	3/3736 (0.1%)
2	B	0.51	1/2116 (0.0%)	0.94	4/2857 (0.1%)
2	D	0.57	4/2106 (0.2%)	0.92	5/2845 (0.2%)
All	All	0.49	7/9758 (0.1%)	0.88	17/13183 (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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	333	ARG	NE-CZ	12.59	1.49	1.33
2	D	333	ARG	NE-CZ	12.46	1.49	1.33
2	D	181	ASP	CB-CG	-9.06	1.32	1.51
2	D	188	TRP	CZ3-CH2	-7.05	1.28	1.40
1	A	111	LYS	CE-NZ	-7.00	1.31	1.49
1	C	30	TRP	CB-CG	-6.32	1.38	1.50
2	D	272	VAL	CB-CG1	-5.21	1.42	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	181	ASP	CB-CG-OD1	-23.64	97.02	118.30
2	D	181	ASP	CB-CG-OD2	18.74	135.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	LYS	CD-CE-NZ	-18.02	70.25	111.70
1	A	27	LEU	CB-CG-CD1	-17.41	81.41	111.00
1	C	227	LEU	CB-CG-CD1	-13.11	88.71	111.00
1	C	167	LEU	CB-CG-CD2	-10.21	93.65	111.00
2	B	333	ARG	CD-NE-CZ	-9.09	110.87	123.60
2	D	333	ARG	CD-NE-CZ	-7.72	112.80	123.60
1	A	116	LEU	CB-CG-CD1	-7.63	98.02	111.00
2	B	92	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	111	LYS	CB-CA-C	-6.55	97.29	110.40
2	B	126	LEU	CA-CB-CG	-6.12	101.22	115.30
2	D	258	ASP	CB-CG-OD1	-5.39	113.45	118.30
2	D	176	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	27	LEU	CB-CG-CD2	5.26	119.94	111.00
1	A	61	LYS	CD-CE-NZ	-5.13	99.89	111.70
2	B	95	ARG	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	189	ALA	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	2734	0	2640	372	0
1	C	2729	0	2630	366	0
2	B	2079	0	2030	264	0
2	D	2069	0	2023	351	0
3	A	27	0	12	4	0
3	C	27	0	12	1	0
All	All	9665	0	9347	1314	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 69.

All (1314) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HA	1:A:84:GLN:NE2	1.38	1.36
1:A:116:LEU:HD12	1:A:117:TYR:N	1.48	1.27
1:C:150:ILE:HG22	1:C:154:PHE:CE2	1.71	1.24
1:A:48:THR:HG21	1:A:330:TYR:HB2	1.20	1.16
1:A:175:ASP:HB3	1:A:181:GLN:NE2	1.60	1.15
2:D:181:ASP:OD1	2:D:188:TRP:CZ3	1.99	1.15
1:C:95:LEU:HB3	1:C:106:LEU:HD23	1.29	1.13
1:A:91:GLU:O	1:A:95:LEU:HD13	1.48	1.13
2:B:325:ILE:CD1	2:B:331:ARG:HD3	1.78	1.12
1:A:92:LYS:HD3	1:A:350:PHE:CE2	1.84	1.11
1:C:56:ARG:HD2	1:C:57:VAL:N	1.65	1.10
2:B:308:GLU:HG2	2:B:309:GLU:H	1.01	1.10
2:D:120:TYR:CE1	2:D:124:ALA:HB2	1.84	1.10
1:A:111:LYS:NZ	1:A:350:PHE:CD1	2.18	1.10
1:A:61:LYS:HZ1	1:A:66:GLY:HA2	1.04	1.08
1:A:48:THR:CG2	1:A:330:TYR:HB2	1.83	1.08
1:A:111:LYS:NZ	1:A:350:PHE:CG	2.22	1.08
1:C:56:ARG:HD2	1:C:57:VAL:H	0.97	1.07
2:B:325:ILE:HD13	2:B:331:ARG:HD3	1.18	1.07
1:C:167:LEU:HD21	1:C:227:LEU:HD11	1.36	1.07
1:C:50:GLY:H	1:C:56:ARG:NH1	1.52	1.06
2:D:154:VAL:HG23	2:D:221:LEU:HD11	1.33	1.05
1:C:100:PHE:HB3	1:C:103:LEU:HD13	1.34	1.05
2:D:172:PHE:HE1	2:D:198:PHE:N	1.55	1.05
1:C:95:LEU:HB3	1:C:106:LEU:CD2	1.86	1.04
1:A:46:ILE:HD11	1:A:59:LEU:HB3	1.38	1.04
1:C:30:TRP:HZ2	1:C:190:ARG:CZ	1.70	1.04
2:D:188:TRP:CH2	2:D:190:THR:C	2.31	1.04
1:C:30:TRP:HE1	1:C:190:ARG:NH1	1.55	1.03
2:D:181:ASP:OD1	2:D:188:TRP:CH2	2.12	1.03
1:A:46:ILE:HG12	1:A:59:LEU:HD22	1.39	1.03
2:B:151:MET:SD	2:B:224:ILE:HD11	1.98	1.02
1:C:150:ILE:HG22	1:C:154:PHE:HE2	0.85	1.02
1:C:89:LEU:HG	1:C:92:LYS:HZ1	1.22	1.01
2:D:154:VAL:O	2:D:221:LEU:HG	1.59	1.00
1:A:35:GLN:HE22	1:A:350:PHE:C	1.63	1.00
1:A:61:LYS:NZ	1:A:66:GLY:HA2	1.76	1.00
1:A:131:HIS:CD2	1:A:134:ARG:HH11	1.81	0.98
2:D:252:SER:OG	2:D:253:ILE:HD12	1.64	0.98
1:C:113:ASN:HB3	1:C:340:ASN:O	1.62	0.98
2:D:172:PHE:HD1	2:D:198:PHE:O	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:HIS:HD2	1:A:134:ARG:NH1	1.60	0.97
2:D:169:GLY:HA2	2:D:209:ARG:CZ	1.93	0.97
2:B:331:ARG:HG3	2:B:332:PRO:HD2	1.44	0.96
1:C:29:LYS:HE2	1:C:97:ALA:HA	1.45	0.96
2:D:151:MET:HE1	2:D:222:TRP:C	1.84	0.96
2:D:116:ILE:HD13	2:D:152:PHE:HB3	1.46	0.96
1:C:150:ILE:CG2	1:C:154:PHE:HE2	1.77	0.96
2:D:272:VAL:CG1	2:D:347:LYS:HE2	1.95	0.96
1:A:131:HIS:HD2	1:A:134:ARG:HH11	0.99	0.96
2:B:116:ILE:HD11	2:B:151:MET:O	1.66	0.95
2:D:257:LEU:HD11	2:D:262:ARG:CZ	1.96	0.95
2:D:144:ARG:O	2:D:147:ILE:HG13	1.66	0.95
1:C:50:GLY:H	1:C:56:ARG:HH12	1.10	0.95
1:A:215:TYR:HD1	1:A:219:VAL:HG11	1.28	0.95
1:C:169:PRO:HA	1:C:172:LEU:HD12	1.46	0.94
1:A:76:LYS:HD3	1:A:342:LYS:O	1.67	0.94
1:C:164:TYR:CE2	1:C:166:ASP:O	2.21	0.94
1:C:157:LEU:O	1:C:162:LEU:HD12	1.65	0.94
1:A:242:GLN:HE22	1:A:245:GLN:HB2	1.32	0.93
2:D:188:TRP:CH2	2:D:190:THR:O	2.22	0.93
2:D:175:ILE:HD13	2:D:192:VAL:HG21	1.49	0.92
1:C:30:TRP:HZ2	1:C:190:ARG:NE	1.66	0.92
1:A:48:THR:HG21	1:A:330:TYR:CB	1.98	0.92
2:D:257:LEU:CD1	2:D:262:ARG:HG3	2.00	0.92
2:D:171:ASN:CB	2:D:173:TYR:HE1	1.83	0.92
1:C:129:PHE:HE1	1:C:133:ARG:CZ	1.82	0.92
1:C:89:LEU:HG	1:C:92:LYS:NZ	1.85	0.92
1:A:116:LEU:HD12	1:A:117:TYR:H	1.17	0.91
2:B:308:GLU:HG2	2:B:309:GLU:N	1.81	0.91
2:B:104:THR:HG23	2:B:107:ASP:OD2	1.69	0.91
1:C:30:TRP:CZ2	1:C:190:ARG:CZ	2.53	0.91
2:B:148:PHE:HA	2:B:151:MET:HE2	1.53	0.91
1:A:79:VAL:CA	1:A:84:GLN:NE2	2.33	0.91
1:A:92:LYS:HD3	1:A:350:PHE:CD2	2.06	0.91
1:C:243:PRO:HA	1:C:246:ILE:HD12	1.51	0.91
1:C:56:ARG:NH1	1:C:57:VAL:O	2.04	0.91
1:C:80:VAL:HA	1:C:85:ILE:HD11	1.51	0.91
2:B:191:SER:HB2	2:B:216:LYS:NZ	1.86	0.91
1:A:95:LEU:HD11	1:A:185:PHE:HB2	1.51	0.90
2:B:259:LYS:HG2	2:B:262:ARG:HH21	1.35	0.90
1:A:79:VAL:HA	1:A:84:GLN:HE22	1.10	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HB2	1:A:162:LEU:HD12	1.53	0.89
2:D:172:PHE:CZ	2:D:197:SER:HB2	2.07	0.89
1:A:43:PHE:O	1:A:45:ARG:NH1	2.05	0.89
1:A:175:ASP:CB	1:A:181:GLN:NE2	2.35	0.88
1:A:160:LEU:HB2	1:A:162:LEU:CD1	2.03	0.88
1:C:44:ASP:HB2	1:C:63:LYS:HE3	1.54	0.88
1:A:40:LEU:HD12	1:A:45:ARG:HH21	1.38	0.88
1:C:106:LEU:O	1:C:106:LEU:HD12	1.74	0.88
2:D:154:VAL:HB	2:D:221:LEU:HD21	1.54	0.88
1:A:46:ILE:HD12	1:A:47:LYS:N	1.89	0.87
2:D:290:PHE:CD1	2:D:291:PHE:N	2.42	0.87
1:A:111:LYS:CE	1:A:350:PHE:CD1	2.58	0.87
2:B:301:LEU:HB2	2:B:336:THR:HG23	1.56	0.87
1:C:87:HIS:O	1:C:90:ASN:HB3	1.74	0.86
1:A:131:HIS:HA	1:A:134:ARG:HE	1.39	0.86
2:D:350:ARG:HG3	2:D:351:PRO:HD3	1.57	0.86
2:B:107:ASP:HB3	2:B:231:ARG:HH22	1.38	0.86
1:C:90:ASN:HD21	1:C:189:LYS:HA	1.39	0.86
1:C:167:LEU:CD2	1:C:227:LEU:HD11	2.06	0.85
2:D:257:LEU:HD12	2:D:257:LEU:C	1.97	0.85
2:D:172:PHE:CD1	2:D:198:PHE:O	2.28	0.85
2:B:331:ARG:CG	2:B:332:PRO:HD2	2.05	0.85
2:B:188:TRP:CH2	2:B:190:THR:HA	2.11	0.85
2:D:257:LEU:O	2:D:257:LEU:HD12	1.77	0.84
1:A:131:HIS:O	1:A:135:ILE:HD13	1.77	0.84
1:A:163:ILE:HD12	1:A:164:TYR:H	1.42	0.84
1:A:115:ASN:HB2	1:A:117:TYR:OH	1.77	0.84
2:B:188:TRP:CZ2	2:B:190:THR:HA	2.13	0.84
2:D:224:ILE:HG13	2:D:225:ASP:N	1.91	0.84
1:A:74:LEU:HB2	1:A:116:LEU:HB3	1.57	0.84
1:C:90:ASN:OD1	1:C:94:ILE:HD13	1.78	0.84
2:D:177:GLN:HB2	2:D:220:LYS:H	1.42	0.83
1:A:146:TYR:HD1	1:A:180:ILE:HD11	1.44	0.83
1:A:315:ILE:HD12	1:A:315:ILE:O	1.78	0.83
1:A:175:ASP:CB	1:A:181:GLN:HE22	1.91	0.83
2:B:308:GLU:CG	2:B:309:GLU:H	1.89	0.83
1:C:87:HIS:O	1:C:90:ASN:N	2.11	0.83
2:D:111:TYR:CD1	2:D:231:ARG:HD2	2.14	0.83
2:B:251:VAL:HG11	2:B:254:LEU:HD12	1.60	0.83
1:A:116:LEU:C	1:A:116:LEU:HD12	1.79	0.83
1:C:164:TYR:HE2	1:C:166:ASP:O	1.62	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:NZ	1:A:350:PHE:CD2	2.44	0.83
1:C:61:LYS:HZ1	1:C:68:HIS:CE1	1.97	0.83
1:A:111:LYS:HE2	1:A:350:PHE:CD1	2.13	0.82
1:C:108:PHE:HB2	1:C:119:VAL:HG13	1.59	0.82
1:C:129:PHE:CE1	1:C:133:ARG:CZ	2.61	0.82
1:C:61:LYS:NZ	1:C:68:HIS:CG	2.47	0.82
1:C:68:HIS:CE1	1:C:321:PRO:HB2	2.14	0.82
1:C:96:GLN:N	1:C:106:LEU:HD21	1.93	0.82
2:D:172:PHE:HE1	2:D:198:PHE:H	0.84	0.82
2:D:202:ALA:O	2:D:226:ARG:HD3	1.79	0.82
2:D:275:GLU:OE1	2:D:275:GLU:N	2.13	0.82
2:B:276:ASP:HB2	2:B:341:GLY:HA2	1.60	0.82
1:C:30:TRP:NE1	1:C:190:ARG:NH1	2.27	0.82
2:B:177:GLN:O	2:B:219:VAL:HG23	1.80	0.81
1:A:48:THR:HA	1:A:58:MET:HG2	1.62	0.81
1:A:61:LYS:HE2	1:A:66:GLY:C	1.99	0.81
1:C:166:ASP:HB2	1:C:187:PHE:HD2	1.46	0.81
1:A:131:HIS:HA	1:A:134:ARG:NE	1.96	0.81
1:C:48:THR:C	1:C:56:ARG:NH2	2.34	0.81
1:A:111:LYS:CE	1:A:350:PHE:CG	2.64	0.81
1:C:50:GLY:N	1:C:56:ARG:NH2	2.28	0.81
1:C:56:ARG:HH11	1:C:57:VAL:H	1.26	0.81
2:B:259:LYS:HG2	2:B:262:ARG:NH2	1.94	0.80
1:A:133:ARG:NH2	2:B:95:ARG:HH22	1.79	0.80
1:A:328:ASP:OD2	2:B:92:ARG:NH2	2.13	0.80
1:A:334:GLU:CB	2:D:260:TRP:CZ2	2.64	0.80
1:C:204:TYR:CE2	1:C:227:LEU:HD23	2.17	0.80
2:B:171:ASN:ND2	2:B:173:TYR:CE1	2.50	0.80
1:A:27:LEU:N	1:A:27:LEU:HD12	1.95	0.80
1:C:90:ASN:HA	1:C:93:ARG:HG2	1.61	0.80
1:A:242:GLN:NE2	1:A:245:GLN:HB2	1.97	0.79
1:A:195:THR:HG22	1:A:197:TPO:O2P	1.81	0.79
1:C:50:GLY:H	1:C:56:ARG:CZ	1.96	0.79
2:D:151:MET:CE	2:D:152:PHE:O	2.30	0.79
1:A:85:ILE:HD12	1:A:86:GLU:H	1.48	0.79
1:C:80:VAL:HG12	1:C:85:ILE:HD11	1.64	0.79
2:B:191:SER:HB2	2:B:216:LYS:HZ1	1.48	0.79
2:B:236:SER:HA	2:B:239:ARG:NH1	1.98	0.79
2:D:272:VAL:CG1	2:D:347:LYS:CE	2.61	0.78
2:D:294:LEU:HD11	2:D:346:VAL:HG13	1.64	0.78
1:C:90:ASN:ND2	1:C:188:ALA:O	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:HD23	1:C:93:ARG:HD3	1.64	0.78
2:B:184:VAL:HG22	2:B:189:ALA:HB2	1.66	0.78
1:C:174:ILE:HD13	1:C:178:GLY:HA2	1.65	0.78
2:D:300:VAL:O	2:D:301:LEU:HD23	1.83	0.78
1:A:61:LYS:HD2	1:A:67:ASN:O	1.84	0.78
1:C:150:ILE:O	1:C:154:PHE:HD2	1.67	0.78
1:C:319:LYS:O	1:C:323:ASP:HB2	1.83	0.78
1:C:174:ILE:CD1	1:C:178:GLY:HA2	2.13	0.78
2:B:293:ILE:HD13	2:B:318:PRO:HA	1.66	0.78
1:C:161:ASP:HA	1:C:217:LYS:HE2	1.66	0.78
2:B:293:ILE:HD11	2:B:320:ASP:H	1.48	0.78
1:A:40:LEU:HA	1:A:43:PHE:CE1	2.18	0.78
1:A:92:LYS:HG3	1:A:93:ARG:N	1.99	0.78
1:C:95:LEU:CB	1:C:106:LEU:HD23	2.12	0.78
1:C:50:GLY:N	1:C:56:ARG:HH22	1.80	0.78
2:D:171:ASN:CB	2:D:173:TYR:CE1	2.67	0.78
2:D:257:LEU:HD13	2:D:262:ARG:HG3	1.65	0.78
1:C:122:TYR:CE2	1:C:124:ALA:HB2	2.20	0.77
1:C:55:GLY:HA3	1:C:74:LEU:HD23	1.65	0.77
1:A:142:HIS:CE1	1:A:146:TYR:HE2	2.01	0.77
1:A:35:GLN:NE2	1:A:350:PHE:C	2.37	0.77
1:A:46:ILE:HD12	1:A:47:LYS:H	1.48	0.77
1:C:30:TRP:CZ2	1:C:190:ARG:NE	2.51	0.77
2:D:291:PHE:HD2	2:D:347:LYS:HZ2	1.32	0.77
1:A:332:GLU:OE1	1:A:332:GLU:HA	1.85	0.77
1:C:167:LEU:HD21	1:C:227:LEU:CD1	2.12	0.77
2:B:219:VAL:HG22	2:B:220:LYS:N	1.99	0.76
1:A:112:ASP:OD1	1:A:117:TYR:OH	2.03	0.76
2:B:187:GLU:HB3	1:C:37:THR:HG21	1.68	0.76
2:D:257:LEU:HD11	2:D:262:ARG:HG3	1.67	0.76
1:A:77:GLN:NE2	1:A:342:LYS:HD2	1.99	0.76
2:B:244:TYR:O	2:B:248:LEU:HD13	1.86	0.76
2:D:171:ASN:HB2	2:D:173:TYR:CE1	2.20	0.76
1:C:80:VAL:CG1	1:C:85:ILE:HD11	2.15	0.76
1:A:46:ILE:CD1	1:A:59:LEU:HD13	2.15	0.76
1:C:48:THR:HA	1:C:58:MET:HG3	1.66	0.76
2:D:177:GLN:CG	2:D:220:LYS:HG2	2.16	0.76
1:A:146:TYR:CD1	1:A:180:ILE:HD11	2.22	0.75
1:C:51:THR:HG23	1:C:56:ARG:HD3	1.68	0.75
1:A:23:LYS:O	1:A:27:LEU:CD1	2.35	0.75
2:D:116:ILE:CD1	2:D:152:PHE:HB3	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:MET:HG2	2:D:215:ALA:HA	1.67	0.75
1:C:107:GLU:O	1:C:108:PHE:CG	2.39	0.75
2:B:180:MET:HG2	2:B:215:ALA:HA	1.68	0.75
1:A:138:PHE:HD2	1:A:231:MET:HE2	1.51	0.75
1:C:68:HIS:NE2	1:C:322:GLY:N	2.35	0.75
1:A:76:LYS:CD	1:A:342:LYS:O	2.33	0.74
2:B:350:ARG:O	2:B:354:GLU:HG3	1.87	0.74
1:C:133:ARG:HH22	2:D:95:ARG:HH22	1.32	0.74
1:A:61:LYS:CD	1:A:67:ASN:O	2.34	0.74
2:D:147:ILE:HD12	2:D:148:PHE:N	2.01	0.74
2:D:346:VAL:C	2:D:347:LYS:HD3	2.07	0.74
1:A:77:GLN:HE22	1:A:342:LYS:NZ	1.84	0.74
1:A:244:ILE:HD11	2:B:201:LEU:HB2	1.70	0.74
2:D:171:ASN:HB3	2:D:173:TYR:HE1	1.50	0.74
1:A:215:TYR:CD1	1:A:219:VAL:HG11	2.19	0.74
1:A:244:ILE:HG22	1:A:248:GLU:OE1	1.87	0.74
1:A:268:LEU:HD13	1:A:294:HIS:CD2	2.21	0.74
2:D:181:ASP:C	2:D:181:ASP:OD1	2.19	0.74
1:C:132:LEU:HD13	1:C:138:PHE:CE2	2.22	0.74
1:C:50:GLY:O	1:C:56:ARG:NH1	2.21	0.74
1:A:48:THR:HA	1:A:58:MET:CG	2.17	0.74
2:B:288:ASP:OD2	2:B:289:GLU:OE1	2.06	0.74
2:D:151:MET:HE3	2:D:152:PHE:O	1.88	0.74
1:A:243:PRO:HB2	2:B:201:LEU:HD13	1.69	0.73
1:C:48:THR:OG1	1:C:56:ARG:NH2	2.21	0.73
1:A:42:GLN:C	1:A:63:LYS:HE2	2.07	0.73
1:A:46:ILE:HD12	1:A:47:LYS:HB2	1.70	0.73
1:C:16:LYS:O	1:C:19:LEU:HG	1.88	0.73
2:B:259:LYS:CG	2:B:262:ARG:NH2	2.51	0.73
2:D:290:PHE:HD1	2:D:291:PHE:H	1.33	0.73
1:A:100:PHE:CD2	1:A:101:PRO:HD2	2.23	0.73
2:B:144:ARG:O	2:B:147:ILE:HG13	1.89	0.73
2:B:182:VAL:HG13	2:B:189:ALA:HB3	1.71	0.73
2:B:352:ARG:HA	2:B:355:ARG:CZ	2.19	0.73
2:D:151:MET:CE	2:D:222:TRP:C	2.56	0.73
2:D:93:ARG:O	2:D:93:ARG:HG3	1.87	0.73
1:A:245:GLN:HA	1:A:248:GLU:OE2	1.88	0.73
1:A:45:ARG:HH11	1:A:45:ARG:HG3	1.52	0.73
1:A:46:ILE:HG13	1:A:59:LEU:O	1.89	0.73
2:B:249:SER:O	2:B:255:GLU:OE2	2.06	0.73
2:B:240:LYS:O	2:B:243:MET:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:CG	2:B:92:ARG:NH2	2.41	0.73
1:C:48:THR:HG22	1:C:332:GLU:HG2	1.71	0.73
2:D:173:TYR:HA	2:D:222:TRP:O	1.88	0.73
1:A:266:LYS:O	1:A:270:ARG:HG3	1.89	0.73
1:C:297:PHE:O	1:C:300:THR:HG22	1.88	0.72
2:D:116:ILE:HD13	2:D:152:PHE:CB	2.16	0.72
1:A:116:LEU:CD1	1:A:117:TYR:H	2.00	0.72
2:D:288:ASP:HA	2:D:350:ARG:NH1	2.04	0.72
2:B:240:LYS:HA	2:B:243:MET:HG2	1.69	0.72
2:D:151:MET:CE	2:D:222:TRP:HB3	2.19	0.72
2:B:224:ILE:N	2:B:224:ILE:HD12	2.04	0.72
1:C:166:ASP:HB2	1:C:187:PHE:CD2	2.25	0.72
1:A:245:GLN:HA	1:A:248:GLU:CD	2.10	0.72
2:B:293:ILE:HD11	2:B:317:GLY:O	1.89	0.72
1:A:109:SER:OG	1:A:350:PHE:HE1	1.73	0.72
2:D:154:VAL:CG2	2:D:221:LEU:HD11	2.17	0.72
1:C:184:ASP:HB2	3:C:400:ADP:O1A	1.90	0.72
2:D:175:ILE:HD13	2:D:192:VAL:CG2	2.20	0.71
2:D:188:TRP:HH2	2:D:190:THR:O	1.73	0.71
1:C:201:THR:HG21	2:D:95:ARG:CD	2.20	0.71
1:A:46:ILE:HD11	1:A:59:LEU:HD13	1.72	0.71
2:D:182:VAL:O	2:D:188:TRP:CZ3	2.43	0.71
2:D:156:PHE:HE1	2:D:221:LEU:CD2	2.02	0.71
2:D:239:ARG:HB3	2:D:239:ARG:CZ	2.19	0.71
1:A:111:LYS:HZ2	1:A:116:LEU:CD1	2.01	0.71
2:B:245:GLU:OE2	2:B:262:ARG:HD2	1.90	0.71
2:B:356:VAL:HG23	2:B:357:LEU:H	1.55	0.71
2:D:182:VAL:O	2:D:188:TRP:CE3	2.44	0.71
1:C:61:LYS:NZ	1:C:68:HIS:CE1	2.58	0.71
1:C:90:ASN:ND2	1:C:189:LYS:HA	2.06	0.71
2:D:181:ASP:OD1	2:D:182:VAL:N	2.23	0.71
1:A:100:PHE:HB3	1:A:103:LEU:HD13	1.70	0.71
1:A:163:ILE:HD12	1:A:164:TYR:N	2.05	0.71
1:A:27:LEU:HD12	1:A:27:LEU:H	1.55	0.71
2:B:236:SER:O	2:B:239:ARG:HG3	1.90	0.71
1:C:154:PHE:HZ	1:C:167:LEU:CD1	2.04	0.71
2:B:261:GLU:O	2:B:265:VAL:HG12	1.91	0.71
2:D:272:VAL:HG13	2:D:347:LYS:HE2	1.71	0.71
1:C:169:PRO:HD3	1:C:227:LEU:CD2	2.20	0.70
1:C:102:PHE:C	1:C:103:LEU:HD12	2.10	0.70
2:D:273:GLN:NE2	2:D:274:PHE:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TYR:N	1:A:247:TYR:HD2	1.89	0.70
1:A:197:TPO:O	1:A:215:TYR:OH	2.10	0.70
1:A:148:ALA:HB1	1:A:302:TRP:HZ3	1.57	0.70
1:A:244:ILE:CD1	2:B:201:LEU:HB2	2.21	0.70
1:C:29:LYS:HE2	1:C:97:ALA:CA	2.21	0.70
2:B:245:GLU:OE1	2:B:262:ARG:HB3	1.92	0.70
1:C:174:ILE:HD12	1:C:175:ASP:N	2.07	0.70
1:C:45:ARG:NH1	1:C:335:ILE:HG22	2.06	0.70
1:A:32:THR:O	1:A:32:THR:HG23	1.92	0.70
1:C:51:THR:CG2	1:C:56:ARG:HD3	2.21	0.70
2:D:167:ASP:O	2:D:208:PRO:HA	1.92	0.70
1:A:92:LYS:NZ	1:A:350:PHE:HA	2.07	0.69
1:A:175:ASP:CG	1:A:181:GLN:HE22	1.95	0.69
1:A:208:GLU:HA	1:A:211:LEU:HG	1.74	0.69
2:B:258:ASP:O	2:B:262:ARG:HG3	1.92	0.69
2:B:275:GLU:OE1	2:B:276:ASP:O	2.10	0.69
1:C:264:ASP:OD1	1:C:295:LYS:HE3	1.92	0.69
2:B:182:VAL:HG12	2:B:190:THR:H	1.57	0.69
1:C:45:ARG:HB2	1:C:58:MET:HE2	1.75	0.69
2:D:274:PHE:HD2	2:D:278:GLN:OE1	1.75	0.69
1:C:51:THR:HG23	1:C:56:ARG:NE	2.07	0.69
1:C:60:VAL:O	1:C:61:LYS:HD3	1.92	0.69
1:A:76:LYS:HD3	1:A:343:CYS:HB2	1.74	0.69
1:C:51:THR:HG23	1:C:56:ARG:CD	2.22	0.69
1:C:202:PRO:HA	1:C:205:LEU:HD22	1.73	0.69
2:D:156:PHE:CE1	2:D:221:LEU:HD23	2.27	0.69
1:A:104:VAL:HA	1:A:121:GLU:OE2	1.92	0.69
2:D:156:PHE:HE1	2:D:221:LEU:HD23	1.58	0.69
1:A:111:LYS:HZ2	1:A:116:LEU:CD2	2.05	0.68
1:C:258:PRO:HD2	1:C:261:PHE:CD1	2.27	0.68
2:D:249:SER:HA	2:D:262:ARG:NH1	2.08	0.68
2:D:288:ASP:OD2	2:D:289:GLU:HG3	1.92	0.68
1:A:166:ASP:HB3	1:A:187:PHE:HD2	1.57	0.68
1:A:39:GLN:O	1:A:42:GLN:OE1	2.11	0.68
1:A:129:PHE:HE1	1:A:133:ARG:NE	1.91	0.68
2:B:130:ILE:C	2:B:130:ILE:HD12	2.14	0.68
2:D:346:VAL:O	2:D:347:LYS:HD3	1.93	0.68
1:A:40:LEU:HA	1:A:43:PHE:HE1	1.57	0.68
1:C:263:SER:HA	1:C:266:LYS:HE3	1.76	0.68
1:C:204:TYR:CE2	1:C:227:LEU:CD2	2.76	0.68
1:C:297:PHE:HD2	1:C:300:THR:HG21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HD11	1:A:138:PHE:CE1	2.29	0.67
2:B:243:MET:HE3	2:B:247:PHE:CE2	2.29	0.67
1:A:247:TYR:N	1:A:247:TYR:CD2	2.61	0.67
1:C:204:TYR:HE2	1:C:227:LEU:HD23	1.59	0.67
1:C:243:PRO:O	1:C:246:ILE:N	2.28	0.67
1:A:133:ARG:HH21	2:B:95:ARG:HH22	1.42	0.67
1:A:85:ILE:HD12	1:A:86:GLU:N	2.09	0.67
2:D:316:LEU:HD23	2:D:320:ASP:HB3	1.75	0.67
1:C:87:HIS:O	1:C:90:ASN:CB	2.42	0.67
2:D:94:ARG:HG2	2:D:94:ARG:HH11	1.60	0.67
1:C:29:LYS:HE2	1:C:96:GLN:O	1.94	0.67
2:B:116:ILE:HG12	2:B:118:LYS:NZ	2.10	0.67
2:B:223:GLY:C	2:B:224:ILE:HD12	2.14	0.67
1:A:115:ASN:HB2	1:A:117:TYR:CZ	2.30	0.67
1:A:69:TYR:HB3	1:A:119:VAL:HG23	1.75	0.67
1:A:92:LYS:HE2	1:A:350:PHE:CD2	2.30	0.67
2:B:325:ILE:CD1	2:B:331:ARG:CD	2.67	0.67
2:D:151:MET:HE2	2:D:152:PHE:O	1.94	0.67
2:D:302:GLN:OE1	2:D:313:VAL:HG11	1.95	0.67
2:B:245:GLU:OE1	2:B:262:ARG:CB	2.42	0.67
1:C:23:LYS:O	1:C:27:LEU:HG	1.95	0.66
1:A:129:PHE:HE1	1:A:133:ARG:CZ	2.08	0.66
1:C:68:HIS:O	1:C:69:TYR:CD2	2.48	0.66
2:D:301:LEU:CD2	2:D:312:GLU:HA	2.26	0.66
2:B:308:GLU:OE1	2:B:308:GLU:N	2.28	0.66
1:A:334:GLU:CB	2:D:260:TRP:HZ2	2.08	0.66
1:C:61:LYS:NZ	1:C:68:HIS:ND1	2.44	0.66
2:D:175:ILE:CD1	2:D:192:VAL:HG21	2.25	0.66
1:A:247:TYR:H	1:A:247:TYR:HD2	1.41	0.66
2:B:236:SER:O	2:B:239:ARG:CG	2.44	0.66
1:C:107:GLU:O	1:C:108:PHE:CD2	2.49	0.66
1:C:133:ARG:HD3	1:C:133:ARG:N	2.10	0.66
1:C:50:GLY:N	1:C:56:ARG:CZ	2.58	0.66
1:C:56:ARG:HH11	1:C:57:VAL:N	1.93	0.66
1:A:57:VAL:HG21	3:A:400:ADP:C8	2.30	0.66
2:B:171:ASN:OD1	2:B:172:PHE:N	2.28	0.66
1:C:169:PRO:CA	1:C:172:LEU:HD12	2.22	0.66
1:C:29:LYS:CE	1:C:96:GLN:O	2.44	0.66
2:D:273:GLN:HE21	2:D:274:PHE:N	1.94	0.66
1:A:109:SER:OG	1:A:350:PHE:CE1	2.49	0.66
1:C:61:LYS:NZ	1:C:68:HIS:CD2	2.63	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:GLY:N	2:D:320:ASP:OD2	2.29	0.66
2:B:311:VAL:CG2	2:B:312:GLU:N	2.59	0.66
2:D:257:LEU:CD1	2:D:257:LEU:C	2.64	0.66
2:D:287:GLY:HA3	2:D:333:ARG:HE	1.60	0.66
1:A:201:THR:HG21	2:B:95:ARG:CD	2.26	0.65
1:C:265:LEU:HD13	1:C:296:TRP:CZ2	2.30	0.65
1:A:113:ASN:ND2	1:A:338:SEP:O	2.29	0.65
1:A:46:ILE:CD1	1:A:47:LYS:H	2.09	0.65
2:B:132:LYS:O	2:B:132:LYS:HG2	1.97	0.65
1:A:75:ASP:HB3	1:A:78:LYS:HG2	1.77	0.65
2:B:251:VAL:CG1	2:B:254:LEU:HD12	2.25	0.65
2:B:118:LYS:HZ3	2:B:149:ASP:HA	1.61	0.65
2:B:185:ASN:HB2	1:C:34:SER:HB2	1.78	0.65
2:B:188:TRP:HE3	2:B:188:TRP:O	1.80	0.65
1:A:105:LYS:H	1:A:121:GLU:CD	2.00	0.65
1:A:242:GLN:NE2	1:A:245:GLN:CB	2.59	0.65
2:D:151:MET:HE2	2:D:222:TRP:HB3	1.77	0.65
2:D:257:LEU:HD11	2:D:262:ARG:NE	2.12	0.65
1:A:243:PRO:O	1:A:247:TYR:CD2	2.49	0.64
1:A:128:MET:CE	1:A:172:LEU:HD13	2.27	0.64
1:C:204:TYR:HE2	1:C:227:LEU:CD2	2.10	0.64
1:A:59:LEU:HD23	1:A:60:VAL:N	2.12	0.64
2:D:169:GLY:HA2	2:D:209:ARG:NE	2.13	0.64
1:A:32:THR:O	1:A:32:THR:CG2	2.45	0.64
1:A:46:ILE:HD11	1:A:59:LEU:CB	2.22	0.64
2:B:166:GLY:HA2	2:B:208:PRO:HB3	1.79	0.64
2:D:251:VAL:HG11	2:D:254:LEU:HG	1.79	0.64
1:A:92:LYS:CD	1:A:350:PHE:CD2	2.79	0.64
1:A:148:ALA:HB1	1:A:302:TRP:CZ3	2.32	0.64
1:C:30:TRP:HE1	1:C:190:ARG:HH12	1.43	0.64
1:A:23:LYS:HE3	1:A:27:LEU:HD11	1.80	0.64
1:C:250:ILE:HG22	1:C:251:VAL:N	2.12	0.64
1:A:111:LYS:CE	1:A:350:PHE:HB3	2.28	0.64
2:B:305:SER:O	2:B:308:GLU:OE1	2.16	0.64
2:D:249:SER:HA	2:D:262:ARG:CZ	2.28	0.64
1:A:106:LEU:HD11	1:A:118:MET:HG3	1.79	0.64
1:A:92:LYS:HD3	1:A:350:PHE:CZ	2.34	0.64
2:B:166:GLY:O	2:B:208:PRO:HB3	1.97	0.64
1:A:102:PHE:HE1	1:A:179:TYR:HD1	1.46	0.63
1:A:46:ILE:CG1	1:A:59:LEU:HD22	2.21	0.63
1:A:79:VAL:HA	1:A:84:GLN:CD	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:CD	1:C:57:VAL:H	1.91	0.63
1:A:77:GLN:NE2	1:A:342:LYS:CD	2.61	0.63
2:B:264:THR:O	2:B:267:ASP:OD1	2.15	0.63
1:C:132:LEU:HD13	1:C:138:PHE:HE2	1.63	0.63
2:D:182:VAL:N	2:D:188:TRP:HZ3	1.96	0.63
1:A:242:GLN:HE22	1:A:245:GLN:CB	2.10	0.63
2:B:308:GLU:HB2	2:B:309:GLU:OE1	1.98	0.63
2:D:272:VAL:HG11	2:D:347:LYS:CE	2.28	0.63
1:A:328:ASP:CG	2:B:92:ARG:HH22	2.00	0.63
1:C:266:LYS:O	1:C:267:ASP:C	2.37	0.63
2:D:345:CYS:HB2	2:D:347:LYS:NZ	2.13	0.63
1:A:131:HIS:CD2	1:A:134:ARG:NH1	2.50	0.63
2:B:283:GLN:HG2	2:B:335:ALA:HA	1.79	0.63
1:C:140:GLU:O	1:C:143:ALA:N	2.32	0.63
1:C:297:PHE:CD2	1:C:300:THR:HG21	2.34	0.63
2:D:275:GLU:OE1	2:D:278:GLN:OE1	2.16	0.63
1:A:111:LYS:NZ	1:A:116:LEU:HD11	2.13	0.63
2:B:293:ILE:CD1	2:B:317:GLY:O	2.47	0.63
1:A:244:ILE:O	1:A:248:GLU:HG3	1.99	0.63
2:D:151:MET:CE	2:D:223:GLY:N	2.62	0.63
2:D:216:LYS:HG3	2:D:217:THR:HG23	1.81	0.63
2:B:164:GLN:HB3	2:B:167:ASP:OD2	1.98	0.63
2:B:356:VAL:HG23	2:B:357:LEU:N	2.14	0.63
1:C:238:PHE:HD1	1:C:249:LYS:HG3	1.63	0.63
1:A:195:THR:CG2	1:A:197:TPO:O2P	2.47	0.62
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.14	0.62
1:C:133:ARG:NH2	2:D:95:ARG:HH22	1.97	0.62
2:B:330:ASN:OD1	2:B:330:ASN:N	2.30	0.62
1:C:62:HIS:HB2	1:C:69:TYR:HE1	1.65	0.62
1:A:174:ILE:N	1:A:174:ILE:HD13	2.14	0.62
2:D:221:LEU:HD12	2:D:222:TRP:N	2.13	0.62
2:D:294:LEU:CD1	2:D:346:VAL:HG13	2.30	0.62
2:D:188:TRP:HH2	2:D:190:THR:C	2.00	0.62
1:A:189:LYS:HZ3	1:A:195:THR:CG2	2.13	0.62
1:C:168:LYS:HA	1:C:227:LEU:HD21	1.81	0.62
2:D:281:VAL:HG11	2:D:333:ARG:CZ	2.28	0.62
1:C:163:ILE:HG12	1:C:165:ARG:HG3	1.81	0.62
2:D:120:TYR:CZ	2:D:124:ALA:HB2	2.32	0.62
1:A:40:LEU:CD1	1:A:45:ARG:HH21	2.11	0.62
2:B:229:TYR:O	2:B:233:LEU:HD11	2.00	0.62
2:B:298:ALA:HB2	2:B:343:LEU:HD21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:PHE:CD2	2:D:327:LEU:HD11	2.34	0.62
2:B:305:SER:O	2:B:308:GLU:OE2	2.17	0.62
2:D:329:MET:SD	2:D:331:ARG:NE	2.73	0.62
1:A:189:LYS:NZ	1:A:195:THR:HG21	2.15	0.61
2:B:293:ILE:HD11	2:B:320:ASP:N	2.14	0.61
2:D:113:ARG:HG2	2:D:114:LYS:N	2.15	0.61
2:D:126:LEU:HB3	2:D:148:PHE:CE2	2.35	0.61
2:D:182:VAL:H	2:D:188:TRP:HZ3	1.47	0.61
1:A:125:GLY:O	1:A:131:HIS:CE1	2.53	0.61
1:A:41:ASP:N	1:A:41:ASP:OD1	2.31	0.61
2:B:116:ILE:HG12	2:B:118:LYS:HZ2	1.64	0.61
1:C:55:GLY:HA3	1:C:74:LEU:CD2	2.29	0.61
1:A:50:GLY:HA3	3:A:400:ADP:H4'	1.82	0.61
1:A:77:GLN:NE2	1:A:342:LYS:NZ	2.48	0.61
2:B:245:GLU:OE2	2:B:262:ARG:CD	2.48	0.61
2:B:281:VAL:HG22	2:B:337:VAL:CG1	2.31	0.61
1:A:301:ASP:O	1:A:305:ILE:HG12	2.00	0.61
2:B:251:VAL:HG11	2:B:254:LEU:CD1	2.30	0.61
2:D:172:PHE:CE1	2:D:197:SER:HB2	2.35	0.61
1:A:142:HIS:CE1	1:A:146:TYR:CE2	2.87	0.61
2:D:348:LEU:CD2	2:D:352:ARG:HD3	2.31	0.61
2:D:260:TRP:CD1	2:D:261:GLU:HG3	2.36	0.61
1:C:221:TRP:O	1:C:272:LEU:HD23	2.01	0.61
2:D:151:MET:HE3	2:D:223:GLY:N	2.15	0.61
2:D:221:LEU:HD12	2:D:221:LEU:C	2.20	0.61
1:A:106:LEU:CD1	1:A:118:MET:HG3	2.30	0.61
1:C:114:SER:HB2	1:C:337:VAL:HG13	1.83	0.61
1:C:49:LEU:N	1:C:56:ARG:HH22	1.99	0.61
2:B:297:SER:O	2:B:343:LEU:HD11	2.01	0.61
1:C:170:GLU:OE2	2:D:95:ARG:NH1	2.33	0.61
1:C:201:THR:HG21	2:D:95:ARG:HD3	1.81	0.61
1:A:111:LYS:HD3	1:A:116:LEU:HD13	1.83	0.60
1:C:48:THR:OG1	1:C:56:ARG:CZ	2.48	0.60
2:D:259:LYS:HG3	2:D:260:TRP:N	2.15	0.60
1:C:154:PHE:CZ	1:C:167:LEU:CD1	2.84	0.60
1:C:62:HIS:ND1	1:C:65:SER:OG	2.25	0.60
2:B:293:ILE:HD13	2:B:318:PRO:CA	2.31	0.60
1:A:139:SEP:OG	1:A:141:PRO:HD2	2.01	0.60
1:A:46:ILE:C	1:A:47:LYS:HD2	2.21	0.60
1:C:103:LEU:N	1:C:103:LEU:HD12	2.16	0.60
2:D:234:MET:O	2:D:238:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLN:HG2	1:A:279:LYS:HB2	1.82	0.60
2:D:116:ILE:HD13	2:D:152:PHE:CA	2.31	0.60
2:D:177:GLN:O	2:D:219:VAL:HG12	2.01	0.60
2:B:115:VAL:HG13	2:B:149:ASP:CG	2.22	0.60
2:B:293:ILE:CD1	2:B:319:SER:N	2.64	0.60
1:C:238:PHE:CD1	1:C:249:LYS:HG3	2.36	0.60
2:D:180:MET:HB2	2:D:192:VAL:HG13	1.83	0.60
2:D:290:PHE:O	2:D:291:PHE:CD1	2.55	0.60
1:A:111:LYS:HE2	1:A:350:PHE:HB3	1.84	0.60
1:A:40:LEU:O	1:A:45:ARG:NH2	2.29	0.60
1:C:114:SER:HB2	1:C:337:VAL:HA	1.82	0.60
1:C:48:THR:OG1	1:C:56:ARG:NE	2.35	0.60
2:D:169:GLY:CA	2:D:209:ARG:CZ	2.77	0.60
2:D:176:ASP:OD1	2:D:220:LYS:HG3	2.02	0.60
2:B:143:GLU:O	2:B:146:ASP:HB2	2.01	0.60
2:B:219:VAL:CG2	2:B:220:LYS:N	2.64	0.60
2:D:173:TYR:O	2:D:198:PHE:CE2	2.54	0.60
1:C:265:LEU:CD1	1:C:296:TRP:CZ2	2.85	0.60
2:D:356:VAL:O	2:D:357:LEU:HD22	2.02	0.60
1:A:79:VAL:CA	1:A:84:GLN:HE22	2.00	0.59
2:B:118:LYS:NZ	2:B:149:ASP:O	2.35	0.59
1:A:147:ALA:O	1:A:151:VAL:HG23	2.02	0.59
1:A:23:LYS:CE	1:A:27:LEU:HD11	2.32	0.59
1:A:338:SEP:O1P	1:A:339:ILE:HG12	2.02	0.59
1:A:138:PHE:CD2	1:A:231:MET:HE2	2.33	0.59
1:A:271:ASN:HB3	1:A:281:PHE:CD2	2.36	0.59
1:A:23:LYS:O	1:A:27:LEU:HD12	2.01	0.59
2:D:244:TYR:O	2:D:248:LEU:HD13	2.02	0.59
1:A:92:LYS:CG	1:A:93:ARG:N	2.64	0.59
1:C:108:PHE:HB2	1:C:119:VAL:CG1	2.30	0.59
1:C:80:VAL:HA	1:C:85:ILE:CD1	2.29	0.59
2:D:152:PHE:O	2:D:222:TRP:HE3	1.84	0.59
1:A:111:LYS:NZ	1:A:350:PHE:CE1	2.54	0.59
1:C:48:THR:C	1:C:56:ARG:HH22	2.05	0.59
2:B:166:GLY:C	2:B:208:PRO:HB3	2.22	0.59
2:B:151:MET:CG	2:B:224:ILE:HD11	2.33	0.59
1:C:49:LEU:C	1:C:56:ARG:HH22	2.06	0.59
1:C:80:VAL:CA	1:C:85:ILE:HD11	2.31	0.59
1:C:328:ASP:HB2	1:C:330:TYR:OH	2.03	0.59
2:D:120:TYR:O	2:D:123:MET:N	2.36	0.59
2:D:136:PHE:N	2:D:136:PHE:CD2	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:GLU:N	2:D:217:THR:OG1	2.34	0.59
2:B:244:TYR:CD1	2:B:269:LEU:HD12	2.38	0.59
2:B:283:GLN:HG3	2:B:336:THR:N	2.18	0.59
1:C:100:PHE:HB3	1:C:103:LEU:CD1	2.22	0.59
1:C:195:THR:C	1:C:196:TRP:CD1	2.77	0.59
1:C:50:GLY:N	1:C:56:ARG:HH12	1.92	0.59
2:D:172:PHE:C	2:D:173:TYR:CD1	2.76	0.59
2:B:151:MET:HG2	2:B:222:TRP:HB3	1.83	0.58
2:D:350:ARG:CG	2:D:351:PRO:HD3	2.33	0.58
2:D:182:VAL:N	2:D:188:TRP:CZ3	2.71	0.58
2:B:185:ASN:HB2	1:C:34:SER:CB	2.34	0.58
1:C:201:THR:CG2	2:D:95:ARG:HD3	2.33	0.58
2:D:290:PHE:CE1	2:D:291:PHE:O	2.57	0.58
1:C:180:ILE:CG2	1:C:181:GLN:N	2.66	0.58
1:C:91:GLU:HG3	1:C:186:GLY:HA2	1.85	0.58
2:D:172:PHE:CE1	2:D:198:PHE:N	2.48	0.58
1:A:61:LYS:CE	1:A:66:GLY:HA2	2.33	0.58
1:C:50:GLY:O	1:C:56:ARG:CZ	2.51	0.58
2:D:172:PHE:HZ	2:D:197:SER:HB2	1.64	0.58
2:D:321:TYR:HE1	2:D:324:GLU:CD	2.06	0.58
1:A:261:PHE:O	1:A:266:LYS:HE2	2.02	0.58
1:A:40:LEU:HD12	1:A:45:ARG:NH2	2.14	0.58
2:B:179:GLU:HB2	2:B:216:LYS:HG2	1.85	0.58
1:C:169:PRO:HD3	1:C:227:LEU:HD22	1.84	0.58
2:D:158:ALA:CB	2:D:216:LYS:O	2.51	0.58
2:D:170:ASP:HB3	2:D:171:ASN:OD1	2.03	0.58
2:D:181:ASP:CG	2:D:188:TRP:CH2	2.77	0.58
2:B:276:ASP:HB2	2:B:341:GLY:CA	2.32	0.58
2:D:221:LEU:HD12	2:D:222:TRP:CA	2.33	0.58
2:D:291:PHE:HD2	2:D:347:LYS:NZ	2.01	0.58
1:A:189:LYS:NZ	1:A:195:THR:CG2	2.67	0.58
1:A:211:LEU:HD12	1:A:212:SER:N	2.17	0.58
1:C:68:HIS:CD2	1:C:322:GLY:N	2.71	0.58
1:C:75:ASP:O	1:C:79:VAL:HG23	2.04	0.58
2:D:171:ASN:HB3	2:D:173:TYR:CE1	2.33	0.58
2:D:345:CYS:HB2	2:D:347:LYS:CE	2.34	0.58
1:A:102:PHE:CE1	1:A:179:TYR:HD1	2.21	0.58
2:D:176:ASP:OD1	2:D:220:LYS:CG	2.52	0.58
1:A:102:PHE:C	1:A:103:LEU:HD12	2.24	0.57
1:A:339:ILE:HD13	1:A:339:ILE:N	2.19	0.57
2:B:151:MET:SD	2:B:224:ILE:CD1	2.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:CA	1:C:106:LEU:HD21	2.34	0.57
2:D:224:ILE:CG1	2:D:225:ASP:N	2.67	0.57
2:B:236:SER:HA	2:B:239:ARG:CZ	2.34	0.57
2:B:185:ASN:CB	1:C:34:SER:HB2	2.33	0.57
1:A:195:THR:HG22	1:A:196:TRP:N	2.18	0.57
2:D:174:VAL:HA	2:D:197:SER:HB3	1.86	0.57
1:A:208:GLU:O	1:A:211:LEU:HD12	2.03	0.57
2:B:281:VAL:HG22	2:B:337:VAL:HG12	1.86	0.57
1:C:89:LEU:O	1:C:92:LYS:HG3	2.05	0.57
2:D:156:PHE:HB2	2:D:219:VAL:HG23	1.86	0.57
1:A:79:VAL:HG22	1:A:84:GLN:HE21	1.69	0.57
1:C:224:LEU:O	1:C:228:ILE:HG13	2.05	0.57
2:D:151:MET:HE1	2:D:222:TRP:HB3	1.86	0.57
2:D:260:TRP:CD1	2:D:261:GLU:CG	2.87	0.57
2:B:152:PHE:CZ	2:B:171:ASN:ND2	2.73	0.57
1:C:187:PHE:CD1	1:C:199:CYS:HB2	2.39	0.57
2:D:345:CYS:HB2	2:D:347:LYS:HE2	1.87	0.57
1:C:42:GLN:OE1	1:C:42:GLN:N	2.38	0.57
2:D:329:MET:SD	2:D:331:ARG:CZ	2.93	0.57
2:B:283:GLN:HG3	2:B:336:THR:H	1.69	0.57
1:C:150:ILE:CG2	1:C:154:PHE:CE2	2.64	0.57
1:C:211:LEU:CD1	1:C:213:LYS:HD2	2.35	0.57
1:C:80:VAL:HG12	1:C:85:ILE:CD1	2.32	0.57
1:C:77:GLN:O	1:C:80:VAL:HG23	2.04	0.57
2:D:251:VAL:HA	2:D:321:TYR:HE2	1.69	0.57
2:D:151:MET:SD	2:D:224:ILE:HG22	2.45	0.57
2:D:254:LEU:O	2:D:257:LEU:HG	2.04	0.57
1:A:173:LEU:O	1:A:181:GLN:OE1	2.22	0.57
1:C:165:ARG:HD2	1:C:199:CYS:SG	2.44	0.57
2:D:257:LEU:HD13	2:D:258:ASP:O	2.05	0.57
1:A:131:HIS:HA	1:A:134:ARG:HG2	1.87	0.56
1:A:43:PHE:N	1:A:63:LYS:HE2	2.20	0.56
1:C:133:ARG:NH2	1:C:230:GLU:OE1	2.37	0.56
1:C:49:LEU:N	1:C:56:ARG:NH2	2.53	0.56
2:B:233:LEU:HD12	2:B:233:LEU:H	1.70	0.56
2:B:275:GLU:OE2	2:B:276:ASP:HB3	2.05	0.56
1:A:134:ARG:NH1	1:A:314:PHE:CZ	2.72	0.56
2:B:233:LEU:HD12	2:B:233:LEU:N	2.20	0.56
2:B:275:GLU:CD	2:B:276:ASP:N	2.59	0.56
1:C:16:LYS:CG	1:C:17:GLU:H	2.18	0.56
1:C:195:THR:OG1	1:C:196:TRP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:ASP:CG	2:D:341:GLY:H	2.09	0.56
2:B:251:VAL:CB	2:B:254:LEU:HD12	2.34	0.56
1:C:131:HIS:O	1:C:135:ILE:HD13	2.06	0.56
1:A:134:ARG:HH12	1:A:314:PHE:HZ	1.49	0.56
2:D:257:LEU:HD21	2:D:262:ARG:NH1	2.21	0.56
1:A:201:THR:HG21	2:B:95:ARG:HD2	1.87	0.56
1:A:47:LYS:O	1:A:58:MET:HG2	2.05	0.56
2:B:310:PHE:CE1	2:B:336:THR:HG21	2.39	0.56
1:C:47:LYS:O	1:C:58:MET:HG2	2.05	0.56
2:D:130:ILE:HA	2:D:133:ASN:OD1	2.06	0.56
2:D:116:ILE:HD13	2:D:152:PHE:HA	1.87	0.56
1:A:111:LYS:CE	1:A:350:PHE:CB	2.84	0.56
1:A:131:HIS:O	1:A:134:ARG:HG2	2.05	0.56
1:A:58:MET:SD	1:A:332:GLU:OE2	2.64	0.56
1:A:111:LYS:NZ	1:A:116:LEU:HD21	2.21	0.56
1:A:126:GLY:HA2	1:A:327:PHE:CE1	2.41	0.56
1:A:195:THR:HG22	1:A:196:TRP:H	1.71	0.56
2:B:147:ILE:HD11	2:B:148:PHE:CE2	2.41	0.56
2:B:245:GLU:OE2	2:B:262:ARG:NE	2.39	0.56
2:B:295:GLU:HG3	2:B:344:LYS:HE2	1.88	0.56
1:C:26:PHE:HD1	1:C:97:ALA:O	1.88	0.56
2:D:171:ASN:ND2	2:D:224:ILE:O	2.35	0.56
2:D:282:VAL:HB	2:D:285:GLU:CG	2.35	0.56
2:D:272:VAL:HG12	2:D:347:LYS:HG2	1.87	0.56
1:A:125:GLY:O	1:A:131:HIS:HE1	1.89	0.56
1:A:150:ILE:HG22	1:A:154:PHE:CE2	2.40	0.56
2:B:267:ASP:OD1	2:B:268:ALA:N	2.39	0.56
2:B:107:ASP:N	2:B:107:ASP:OD2	2.39	0.55
2:B:305:SER:O	2:B:308:GLU:CD	2.45	0.55
1:C:311:GLU:H	1:C:311:GLU:CD	2.09	0.55
2:D:182:VAL:CG1	2:D:211:ALA:HB1	2.36	0.55
2:B:179:GLU:HB3	2:B:216:LYS:HE3	1.89	0.55
1:C:174:ILE:HD12	1:C:175:ASP:O	2.05	0.55
2:D:176:ASP:C	2:D:176:ASP:OD1	2.44	0.55
1:A:142:HIS:ND1	1:A:146:TYR:HE2	2.04	0.55
2:B:351:PRO:O	2:B:355:ARG:HG3	2.06	0.55
2:D:173:TYR:HB3	2:D:221:LEU:HD13	1.87	0.55
2:D:151:MET:SD	2:D:223:GLY:O	2.64	0.55
1:A:46:ILE:HD13	1:A:59:LEU:HD13	1.87	0.55
1:C:238:PHE:CD2	1:C:250:ILE:HG13	2.42	0.55
2:D:292:ILE:O	2:D:345:CYS:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:GLY:CA	2:B:208:PRO:HB3	2.37	0.55
2:D:251:VAL:HA	2:D:321:TYR:CE2	2.42	0.55
1:A:89:LEU:O	1:A:93:ARG:HG3	2.06	0.55
1:A:91:GLU:HG3	1:A:185:PHE:HB2	1.88	0.55
2:B:188:TRP:CE3	2:B:188:TRP:O	2.59	0.55
2:B:257:LEU:HG	2:B:261:GLU:HB2	1.89	0.55
1:C:287:GLY:O	1:C:290:ASP:OD2	2.25	0.55
1:A:100:PHE:CG	1:A:101:PRO:HD2	2.41	0.54
1:A:95:LEU:CD1	1:A:185:PHE:HB2	2.28	0.54
1:A:77:GLN:CD	1:A:342:LYS:HD2	2.28	0.54
2:B:325:ILE:HD11	2:B:331:ARG:HD3	1.82	0.54
1:C:243:PRO:HA	1:C:246:ILE:CD1	2.30	0.54
2:D:317:GLY:O	2:D:320:ASP:OD2	2.24	0.54
1:C:170:GLU:OE2	2:D:95:ARG:HG2	2.07	0.54
2:B:173:TYR:HB2	2:B:198:PHE:CZ	2.42	0.54
1:C:289:ASN:OD1	1:C:292:LYS:HE3	2.08	0.54
1:C:154:PHE:HZ	1:C:167:LEU:HD13	1.72	0.54
2:D:183:TYR:HE1	2:D:214:LYS:HZ1	1.53	0.54
1:A:268:LEU:HB2	1:A:294:HIS:NE2	2.23	0.54
2:B:152:PHE:HZ	2:B:171:ASN:ND2	2.04	0.54
1:C:75:ASP:OD1	1:C:75:ASP:C	2.46	0.54
1:A:103:LEU:N	1:A:103:LEU:HD12	2.23	0.54
2:B:230:ARG:O	2:B:233:LEU:CD1	2.56	0.54
1:C:40:LEU:CD2	1:C:112:ASP:OD2	2.56	0.54
1:C:91:GLU:HG2	1:C:185:PHE:C	2.28	0.54
1:A:77:GLN:HE22	1:A:342:LYS:HZ3	1.52	0.54
2:B:182:VAL:HG23	2:B:213:VAL:HG22	1.88	0.54
1:C:258:PRO:HD2	1:C:261:PHE:CE1	2.43	0.54
1:A:111:LYS:NZ	1:A:350:PHE:CE2	2.76	0.54
2:B:353:PHE:O	2:B:356:VAL:HG23	2.08	0.54
2:D:154:VAL:O	2:D:221:LEU:CG	2.45	0.54
1:A:189:LYS:NZ	1:A:197:TPO:O1P	2.40	0.54
1:A:40:LEU:O	1:A:43:PHE:CE1	2.60	0.54
1:C:268:LEU:HB2	1:C:294:HIS:CE1	2.43	0.54
2:D:149:ASP:C	2:D:151:MET:H	2.11	0.54
2:D:188:TRP:CZ3	2:D:190:THR:O	2.60	0.54
2:D:255:GLU:HA	2:D:255:GLU:OE1	2.07	0.54
1:A:166:ASP:HB3	1:A:187:PHE:CD2	2.42	0.54
2:D:288:ASP:HB2	2:D:350:ARG:HG2	1.90	0.54
1:A:173:LEU:C	1:A:174:ILE:HD13	2.28	0.53
1:C:153:THR:O	1:C:156:TYR:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ILE:O	1:C:188:ALA:HA	2.08	0.53
1:C:245:GLN:O	1:C:249:LYS:HB2	2.07	0.53
2:D:172:PHE:O	2:D:173:TYR:HD1	1.90	0.53
2:D:188:TRP:CZ2	2:D:190:THR:C	2.82	0.53
1:A:307:GLN:NE2	1:A:309:LYS:CD	2.71	0.53
1:C:75:ASP:HB3	1:C:78:LYS:HE2	1.90	0.53
2:D:158:ALA:HB1	2:D:216:LYS:O	2.09	0.53
1:C:234:GLY:C	1:C:235:TYR:HD1	2.11	0.53
2:D:258:ASP:OD2	2:D:260:TRP:CZ2	2.61	0.53
2:D:345:CYS:CB	2:D:347:LYS:NZ	2.71	0.53
1:A:103:LEU:N	1:A:103:LEU:CD1	2.71	0.53
1:A:328:ASP:OD1	2:B:92:ARG:NH2	2.41	0.53
1:A:84:GLN:OE1	1:A:84:GLN:N	2.41	0.53
2:B:116:ILE:CG1	2:B:118:LYS:HZ2	2.22	0.53
1:C:154:PHE:CZ	1:C:167:LEU:HD13	2.43	0.53
2:D:273:GLN:NE2	2:D:274:PHE:N	2.56	0.53
1:A:133:ARG:NH2	2:B:95:ARG:NH2	2.53	0.53
1:A:75:ASP:HB3	1:A:78:LYS:HZ3	1.73	0.53
2:B:238:LEU:C	2:B:238:LEU:HD23	2.28	0.53
2:B:325:ILE:CD1	2:B:331:ARG:HH21	2.20	0.53
2:D:135:LEU:HB2	2:D:136:PHE:CE2	2.44	0.53
2:D:250:LYS:O	2:D:250:LYS:HG2	2.08	0.53
1:A:61:LYS:HE2	1:A:66:GLY:O	2.09	0.53
1:A:86:GLU:O	1:A:89:LEU:HG	2.08	0.53
1:C:92:LYS:HD2	1:C:93:ARG:N	2.24	0.53
2:B:93:ARG:HA	2:B:93:ARG:NE	2.24	0.53
2:D:183:TYR:HD2	2:D:188:TRP:N	2.07	0.53
2:D:261:GLU:O	2:D:265:VAL:HG12	2.09	0.53
2:D:272:VAL:HG11	2:D:347:LYS:HE3	1.91	0.53
1:A:131:HIS:CA	1:A:134:ARG:HE	2.18	0.52
1:A:215:TYR:CD2	1:A:215:TYR:N	2.77	0.52
1:A:133:ARG:HH21	2:B:95:ARG:NH2	2.07	0.52
2:B:104:THR:HG23	2:B:107:ASP:CG	2.29	0.52
1:C:86:GLU:H	1:C:86:GLU:CD	2.12	0.52
2:B:330:ASN:HA	2:B:350:ARG:HH22	1.74	0.52
1:C:150:ILE:O	1:C:154:PHE:CD2	2.55	0.52
1:C:174:ILE:CD1	1:C:175:ASP:O	2.58	0.52
2:D:173:TYR:O	2:D:198:PHE:HE2	1.92	0.52
2:D:257:LEU:HD11	2:D:262:ARG:CG	2.39	0.52
2:D:290:PHE:O	2:D:291:PHE:CG	2.63	0.52
2:D:349:ASP:OD2	2:D:351:PRO:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:HD3	1:A:116:LEU:CD1	2.38	0.52
1:A:343:CYS:C	1:A:346:GLU:OE1	2.47	0.52
1:A:61:LYS:HD3	1:A:67:ASN:O	2.08	0.52
1:A:79:VAL:HG11	1:A:347:PHE:HZ	1.74	0.52
1:A:208:GLU:O	1:A:211:LEU:CD1	2.57	0.52
2:B:300:VAL:HG23	2:B:314:GLY:N	2.25	0.52
1:C:68:HIS:NE2	1:C:321:PRO:HB2	2.24	0.52
1:A:238:PHE:HD1	1:A:249:LYS:HD2	1.74	0.52
2:B:188:TRP:CE3	2:B:188:TRP:C	2.83	0.52
2:B:337:VAL:HG22	2:B:338:VAL:N	2.25	0.52
1:C:103:LEU:N	1:C:103:LEU:CD1	2.72	0.52
1:C:86:GLU:CD	2:D:102:VAL:HG21	2.29	0.52
2:D:136:PHE:O	2:D:139:LEU:HG	2.09	0.52
2:D:272:VAL:CG1	2:D:347:LYS:HG2	2.40	0.52
1:C:154:PHE:HZ	1:C:167:LEU:HD11	1.75	0.52
1:C:89:LEU:O	1:C:92:LYS:NZ	2.35	0.52
1:A:156:TYR:O	1:A:159:SER:OG	2.21	0.52
1:C:139:SEP:O	1:C:142:HIS:HB3	2.10	0.52
1:C:224:LEU:HG	1:C:228:ILE:HD11	1.92	0.52
1:C:68:HIS:CD2	1:C:322:GLY:H	2.27	0.52
2:D:272:VAL:HG11	2:D:347:LYS:CG	2.39	0.52
1:A:46:ILE:CD1	1:A:47:LYS:N	2.68	0.52
1:A:75:ASP:HB3	1:A:78:LYS:NZ	2.24	0.52
2:B:147:ILE:HD11	2:B:148:PHE:CD2	2.44	0.52
1:C:23:LYS:HG3	1:C:27:LEU:HD11	1.92	0.52
2:D:154:VAL:HB	2:D:221:LEU:CD2	2.32	0.52
1:A:201:THR:HG21	2:B:95:ARG:HD3	1.91	0.52
1:C:129:PHE:HE1	1:C:133:ARG:NH2	2.08	0.52
1:C:174:ILE:HD13	1:C:178:GLY:CA	2.39	0.52
2:D:135:LEU:C	2:D:136:PHE:CD2	2.83	0.52
2:D:162:VAL:HG12	2:D:163:ILE:HG12	1.91	0.52
2:D:293:ILE:HG22	2:D:318:PRO:HA	1.92	0.52
2:D:98:ILE:HG13	2:D:98:ILE:O	2.10	0.52
1:A:201:THR:CG2	2:B:95:ARG:HD3	2.40	0.51
1:A:29:LYS:HD2	1:A:97:ALA:O	2.10	0.51
2:B:240:LYS:HA	2:B:243:MET:CG	2.39	0.51
1:C:56:ARG:CD	1:C:57:VAL:N	2.57	0.51
1:C:90:ASN:CG	1:C:94:ILE:HD13	2.31	0.51
2:D:181:ASP:CG	2:D:188:TRP:CZ3	2.81	0.51
2:D:262:ARG:O	2:D:265:VAL:HG13	2.10	0.51
2:D:245:GLU:HA	2:D:248:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:O	1:A:270:ARG:CG	2.55	0.51
1:A:56:ARG:HH22	1:A:333:GLU:CB	2.24	0.51
1:A:85:ILE:CD1	1:A:86:GLU:H	2.22	0.51
2:D:258:ASP:CG	2:D:260:TRP:CZ2	2.83	0.51
2:D:288:ASP:HB3	2:D:350:ARG:CZ	2.40	0.51
1:A:29:LYS:HD3	1:A:97:ALA:HA	1.92	0.51
1:C:61:LYS:HZ1	1:C:68:HIS:CD2	2.27	0.51
2:D:149:ASP:C	2:D:151:MET:N	2.64	0.51
1:A:211:LEU:CD1	1:A:213:LYS:H	2.24	0.51
2:D:113:ARG:NH1	2:D:149:ASP:OD2	2.36	0.51
1:A:197:TPO:O2P	1:A:197:TPO:N	2.43	0.51
1:A:294:HIS:ND1	1:A:295:LYS:N	2.59	0.51
1:A:92:LYS:CE	1:A:350:PHE:CD2	2.94	0.51
1:A:46:ILE:HD12	1:A:47:LYS:CB	2.39	0.51
1:A:79:VAL:O	1:A:84:GLN:OE1	2.29	0.51
2:B:236:SER:HA	2:B:239:ARG:HG2	1.92	0.51
1:C:315:ILE:O	1:C:315:ILE:HD12	2.10	0.51
2:D:113:ARG:NH1	2:D:149:ASP:CB	2.74	0.51
1:A:111:LYS:NZ	1:A:116:LEU:CD2	2.74	0.51
1:A:131:HIS:O	1:A:135:ILE:CD1	2.56	0.51
2:D:182:VAL:HG23	2:D:190:THR:O	2.11	0.51
1:A:243:PRO:O	1:A:247:TYR:CE2	2.64	0.51
2:B:130:ILE:C	2:B:130:ILE:CD1	2.79	0.51
2:B:295:GLU:HG3	2:B:344:LYS:CE	2.41	0.51
2:D:116:ILE:HD12	2:D:151:MET:O	2.11	0.51
2:D:233:LEU:N	2:D:233:LEU:CD1	2.74	0.51
1:A:48:THR:O	1:A:48:THR:HG23	2.09	0.51
1:C:146:TYR:O	1:C:150:ILE:HG12	2.11	0.51
2:D:182:VAL:O	2:D:188:TRP:HZ3	1.93	0.51
2:D:252:SER:OG	2:D:253:ILE:N	2.44	0.51
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.94	0.51
2:D:183:TYR:HD2	2:D:187:GLU:C	2.14	0.51
2:D:282:VAL:HB	2:D:285:GLU:HG3	1.92	0.51
2:B:179:GLU:HB3	2:B:216:LYS:CD	2.41	0.50
2:B:191:SER:HB2	2:B:216:LYS:HZ3	1.69	0.50
1:C:124:ALA:O	1:C:327:PHE:HE2	1.95	0.50
1:C:92:LYS:HG3	1:C:93:ARG:H	1.75	0.50
2:D:153:PRO:HG3	2:D:222:TRP:CZ3	2.46	0.50
2:D:258:ASP:HB2	2:D:261:GLU:HG3	1.94	0.50
2:D:353:PHE:CD2	2:D:353:PHE:C	2.85	0.50
1:A:46:ILE:CG1	1:A:47:LYS:H	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:NZ	1:A:66:GLY:CA	2.64	0.50
2:B:151:MET:HA	2:B:224:ILE:HG13	1.93	0.50
2:B:300:VAL:HG22	2:B:314:GLY:O	2.11	0.50
2:B:330:ASN:HA	2:B:350:ARG:NH2	2.25	0.50
2:D:133:ASN:ND2	2:D:200:GLU:OE1	2.43	0.50
2:D:295:GLU:HB2	2:D:344:LYS:HB2	1.92	0.50
1:A:102:PHE:HE1	1:A:179:TYR:CD1	2.28	0.50
2:B:93:ARG:HB2	2:B:93:ARG:CZ	2.42	0.50
2:D:113:ARG:CG	2:D:114:LYS:N	2.74	0.50
2:D:136:PHE:HD2	2:D:136:PHE:N	2.07	0.50
2:B:179:GLU:HB3	2:B:216:LYS:CE	2.41	0.50
1:C:264:ASP:O	1:C:267:ASP:N	2.44	0.50
2:B:161:THR:HA	2:B:214:LYS:HG2	1.93	0.50
2:B:179:GLU:HB3	2:B:216:LYS:HD2	1.94	0.50
1:A:184:ASP:HB2	3:A:400:ADP:O1A	2.11	0.50
1:A:47:LYS:N	1:A:58:MET:CE	2.74	0.50
1:A:189:LYS:HZ3	1:A:195:THR:HG23	1.76	0.50
1:C:86:GLU:OE2	1:C:87:HIS:CD2	2.65	0.50
1:A:140:GLU:HB2	1:A:141:PRO:HD3	1.93	0.50
1:A:247:TYR:O	1:A:251:VAL:HG23	2.12	0.50
1:C:30:TRP:CZ2	1:C:190:ARG:CD	2.95	0.50
1:C:89:LEU:HD11	1:C:349:GLU:CG	2.41	0.50
2:D:112:VAL:HG12	2:D:113:ARG:O	2.12	0.50
1:A:111:LYS:NZ	1:A:350:PHE:CZ	2.80	0.50
1:A:135:ILE:CD1	1:A:138:PHE:HE1	2.25	0.50
1:A:161:ASP:HA	1:A:217:LYS:HE2	1.94	0.50
1:A:274:GLN:HG2	1:A:279:LYS:CB	2.42	0.50
2:B:171:ASN:OD1	2:B:172:PHE:O	2.29	0.50
2:B:245:GLU:OE1	2:B:262:ARG:HB2	2.11	0.49
2:B:281:VAL:CG2	2:B:337:VAL:HG12	2.42	0.49
2:B:311:VAL:HG23	2:B:312:GLU:H	1.77	0.49
2:B:353:PHE:O	2:B:356:VAL:CG2	2.60	0.49
2:B:151:MET:HG3	2:B:224:ILE:HD11	1.93	0.49
1:C:90:ASN:HD21	1:C:189:LYS:CA	2.19	0.49
2:B:181:ASP:OD1	2:B:214:LYS:HB2	2.11	0.49
2:B:311:VAL:HG22	2:B:312:GLU:N	2.26	0.49
2:D:126:LEU:HD13	2:D:148:PHE:CD2	2.47	0.49
2:B:148:PHE:HD2	2:B:151:MET:CE	2.26	0.49
1:C:183:THR:OG1	1:C:184:ASP:N	2.45	0.49
1:C:195:THR:OG1	1:C:197:TPO:O2P	2.29	0.49
1:A:175:ASP:CG	1:A:181:GLN:NE2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:ILE:HD12	2:B:331:ARG:HH21	1.77	0.49
2:D:173:TYR:CA	2:D:222:TRP:O	2.60	0.49
2:D:183:TYR:CD2	2:D:188:TRP:HA	2.47	0.49
1:A:334:GLU:CB	2:D:260:TRP:CH2	2.96	0.49
2:B:201:LEU:HD21	2:B:205:TYR:CZ	2.48	0.49
1:C:215:TYR:CD1	1:C:219:VAL:HG11	2.48	0.49
1:C:235:TYR:CD1	1:C:235:TYR:N	2.81	0.49
1:C:87:HIS:O	1:C:88:THR:C	2.50	0.49
2:D:162:VAL:HG21	2:D:180:MET:SD	2.53	0.49
1:A:176:GLN:NE2	1:A:177:GLN:OE1	2.38	0.49
1:A:39:GLN:HG3	1:A:40:LEU:N	2.28	0.49
1:A:46:ILE:HD11	1:A:59:LEU:CD1	2.39	0.49
1:C:201:THR:O	1:C:205:LEU:HD13	2.12	0.49
1:C:90:ASN:C	1:C:90:ASN:OD1	2.51	0.49
1:C:194:ARG:HE	2:D:241:ARG:NH2	2.10	0.49
2:B:173:TYR:HA	2:B:222:TRP:O	2.13	0.49
2:B:180:MET:N	2:B:216:LYS:HE3	2.27	0.49
2:B:243:MET:CE	2:B:244:TYR:HD2	2.26	0.48
1:C:115:ASN:ND2	1:C:337:VAL:HG22	2.28	0.48
1:A:111:LYS:NZ	1:A:116:LEU:CD1	2.71	0.48
2:B:190:THR:OG1	2:B:191:SER:N	2.46	0.48
2:B:161:THR:CA	2:B:214:LYS:HG2	2.43	0.48
2:B:153:PRO:HB3	2:B:222:TRP:CZ3	2.48	0.48
1:C:163:ILE:HD11	1:C:219:VAL:CG2	2.43	0.48
1:C:23:LYS:HD2	1:C:160:LEU:HD23	1.94	0.48
1:C:48:THR:O	1:C:56:ARG:NH2	2.46	0.48
1:C:60:VAL:O	1:C:61:LYS:CD	2.62	0.48
2:D:136:PHE:HA	2:D:139:LEU:CD1	2.43	0.48
2:D:282:VAL:HB	2:D:285:GLU:HG2	1.96	0.48
1:A:148:ALA:CB	1:A:302:TRP:HZ3	2.24	0.48
2:D:180:MET:HB2	2:D:192:VAL:CG1	2.42	0.48
2:D:176:ASP:OD2	2:D:220:LYS:HE2	2.14	0.48
1:C:285:LYS:HD3	2:D:357:LEU:HD13	1.96	0.48
1:A:135:ILE:CD1	1:A:138:PHE:CE1	2.96	0.48
1:A:43:PHE:C	1:A:63:LYS:NZ	2.67	0.48
2:B:180:MET:SD	2:B:213:VAL:HG12	2.53	0.48
2:B:275:GLU:CD	2:B:275:GLU:C	2.72	0.48
1:C:115:ASN:HD22	1:C:337:VAL:HG22	1.78	0.48
1:C:204:TYR:CZ	1:C:227:LEU:HD23	2.48	0.48
1:A:105:LYS:N	1:A:121:GLU:OE1	2.47	0.48
1:A:109:SER:HG	1:A:350:PHE:HE1	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LYS:HB3	1:C:116:LEU:HD23	1.95	0.48
2:D:104:THR:O	2:D:105:GLU:C	2.51	0.48
2:D:151:MET:HE1	2:D:222:TRP:CA	2.44	0.48
1:A:172:LEU:HD11	1:A:227:LEU:HD11	1.95	0.48
2:D:105:GLU:O	2:D:107:ASP:N	2.47	0.48
2:D:272:VAL:HG22	2:D:273:GLN:N	2.29	0.48
2:D:281:VAL:CG1	2:D:333:ARG:CZ	2.92	0.48
1:A:105:LYS:O	1:A:121:GLU:OE1	2.31	0.48
1:C:185:PHE:N	1:C:185:PHE:CD2	2.81	0.48
1:A:105:LYS:N	1:A:121:GLU:OE2	2.39	0.48
2:B:172:PHE:CD1	2:B:198:PHE:O	2.66	0.48
2:B:230:ARG:O	2:B:233:LEU:HD12	2.14	0.48
2:B:236:SER:HB2	2:B:239:ARG:NH2	2.29	0.48
1:A:111:LYS:HZ2	1:A:116:LEU:CG	2.26	0.48
1:A:345:LYS:O	1:A:348:THR:HG23	2.13	0.48
1:C:135:ILE:HD11	1:C:138:PHE:CE2	2.49	0.48
1:C:93:ARG:HG3	1:C:94:ILE:HD12	1.96	0.48
2:D:280:ILE:HB	2:D:337:VAL:CG2	2.44	0.48
2:D:283:GLN:HE22	2:D:303:ARG:N	2.12	0.48
2:D:321:TYR:C	2:D:321:TYR:CD1	2.86	0.48
2:D:94:ARG:HG2	2:D:94:ARG:NH1	2.28	0.48
1:A:48:THR:CG2	1:A:330:TYR:CB	2.72	0.47
2:B:293:ILE:O	2:B:293:ILE:HD12	2.13	0.47
1:C:30:TRP:CZ2	1:C:190:ARG:HD3	2.48	0.47
1:C:329:ASP:C	1:C:330:TYR:CD2	2.88	0.47
1:C:55:GLY:CA	1:C:74:LEU:HD23	2.40	0.47
2:D:269:LEU:HD23	2:D:348:LEU:HG	1.96	0.47
1:A:198:LEU:HD12	1:A:209:ILE:HG22	1.96	0.47
1:A:142:HIS:HE1	1:A:146:TYR:CE2	2.33	0.47
1:C:90:ASN:O	1:C:91:GLU:C	2.53	0.47
2:D:151:MET:CE	2:D:222:TRP:CA	2.92	0.47
2:D:111:TYR:HD1	2:D:231:ARG:NH2	2.12	0.47
1:A:172:LEU:CD1	1:A:227:LEU:HD11	2.43	0.47
1:A:51:THR:HG22	1:A:52:GLY:N	2.30	0.47
2:B:172:PHE:CE1	2:B:200:GLU:HG3	2.50	0.47
2:B:297:SER:N	2:B:343:LEU:HD11	2.30	0.47
1:C:234:GLY:C	1:C:235:TYR:CD1	2.88	0.47
1:A:104:VAL:HG13	1:A:182:VAL:O	2.14	0.47
2:B:308:GLU:HG3	2:B:309:GLU:OE2	2.14	0.47
1:C:46:ILE:N	1:C:58:MET:CE	2.78	0.47
2:D:272:VAL:CG1	2:D:347:LYS:CG	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:GLU:HA	1:C:235:TYR:O	2.15	0.47
1:C:244:ILE:O	1:C:248:GLU:HG2	2.14	0.47
2:D:163:ILE:HD11	2:D:198:PHE:HE1	1.79	0.47
2:D:260:TRP:CD1	2:D:261:GLU:HG2	2.49	0.47
2:D:93:ARG:CG	2:D:93:ARG:O	2.60	0.47
1:A:39:GLN:HG3	1:A:40:LEU:H	1.79	0.47
1:A:92:LYS:HG3	1:A:93:ARG:H	1.77	0.47
1:C:235:TYR:HB2	1:C:236:PRO:HD2	1.95	0.47
1:C:242:GLN:O	1:C:243:PRO:C	2.52	0.47
1:C:271:ASN:HB3	1:C:281:PHE:CD2	2.49	0.47
2:D:221:LEU:CD1	2:D:223:GLY:N	2.78	0.47
1:A:311:GLU:O	1:A:311:GLU:HG2	2.14	0.47
2:B:274:PHE:CG	2:B:280:ILE:HD11	2.50	0.47
1:C:265:LEU:CD1	1:C:296:TRP:CE2	2.98	0.47
2:D:115:VAL:HG22	2:D:149:ASP:HB3	1.96	0.47
2:D:173:TYR:CD1	2:D:223:GLY:HA2	2.50	0.47
2:D:301:LEU:HD23	2:D:312:GLU:HA	1.96	0.47
2:D:357:LEU:HA	2:D:357:LEU:HD13	1.73	0.47
1:A:131:HIS:HA	1:A:134:ARG:CD	2.45	0.47
1:A:271:ASN:HB3	1:A:281:PHE:CE2	2.49	0.47
2:B:236:SER:O	2:B:239:ARG:HG2	2.14	0.47
1:C:65:SER:OG	1:C:67:ASN:OD1	2.33	0.47
1:C:26:PHE:CE1	1:C:97:ALA:HB1	2.50	0.47
1:A:129:PHE:CE1	1:A:133:ARG:NE	2.79	0.47
1:A:91:GLU:HG3	1:A:95:LEU:HD11	1.96	0.47
2:B:253:ILE:HD12	2:B:253:ILE:N	2.29	0.47
1:C:48:THR:CG2	1:C:332:GLU:HG2	2.42	0.47
1:C:119:VAL:O	1:C:119:VAL:HG22	2.13	0.47
1:C:91:GLU:CG	1:C:186:GLY:HA2	2.45	0.47
2:D:294:LEU:HG	2:D:345:CYS:HA	1.97	0.47
1:A:164:TYR:CD2	1:A:164:TYR:C	2.87	0.46
1:A:48:THR:O	1:A:48:THR:CG2	2.62	0.46
1:A:59:LEU:HD23	1:A:59:LEU:C	2.35	0.46
1:A:92:LYS:CG	1:A:93:ARG:H	2.28	0.46
2:B:141:ASP:OD1	2:B:144:ARG:NH2	2.48	0.46
2:B:352:ARG:HA	2:B:355:ARG:NH2	2.30	0.46
2:D:172:PHE:C	2:D:173:TYR:HD1	2.18	0.46
2:D:176:ASP:OD1	2:D:220:LYS:O	2.33	0.46
2:D:300:VAL:C	2:D:301:LEU:HD23	2.36	0.46
1:A:77:GLN:HE22	1:A:342:LYS:HZ2	1.62	0.46
2:B:202:ALA:O	2:B:226:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD23	1:C:112:ASP:OD2	2.15	0.46
1:C:167:LEU:CD2	1:C:227:LEU:CD1	2.83	0.46
1:C:16:LYS:HA	1:C:19:LEU:HD23	1.98	0.46
1:C:179:TYR:CZ	1:C:308:ARG:HA	2.50	0.46
1:C:185:PHE:O	1:C:188:ALA:N	2.40	0.46
1:C:61:LYS:HD2	1:C:67:ASN:O	2.15	0.46
2:D:220:LYS:HG3	2:D:220:LYS:O	2.14	0.46
2:D:244:TYR:CZ	2:D:346:VAL:HG11	2.50	0.46
2:D:321:TYR:CE1	2:D:324:GLU:CG	2.99	0.46
2:B:156:PHE:HD1	2:B:160:GLU:OE2	1.98	0.46
2:B:353:PHE:CD2	2:B:353:PHE:C	2.88	0.46
1:C:307:GLN:HG3	1:C:307:GLN:O	2.15	0.46
1:C:32:THR:O	1:C:32:THR:HG23	2.16	0.46
2:D:238:LEU:HA	2:D:238:LEU:HD23	1.68	0.46
2:D:282:VAL:O	2:D:285:GLU:HB2	2.15	0.46
1:A:46:ILE:C	1:A:58:MET:HE3	2.36	0.46
2:B:261:GLU:O	2:B:265:VAL:CG1	2.61	0.46
2:B:275:GLU:C	2:B:275:GLU:OE1	2.53	0.46
1:C:41:ASP:HB2	1:C:42:GLN:OE1	2.15	0.46
1:C:46:ILE:HG21	1:C:59:LEU:HD23	1.98	0.46
1:A:43:PHE:C	1:A:63:LYS:HZ1	2.18	0.46
2:B:219:VAL:HG22	2:B:220:LYS:H	1.79	0.46
1:C:189:LYS:HE2	1:C:191:VAL:HG22	1.98	0.46
1:A:128:MET:HE1	1:A:172:LEU:HD13	1.96	0.46
1:C:174:ILE:C	1:C:174:ILE:HD12	2.36	0.46
2:D:151:MET:CE	2:D:222:TRP:CB	2.93	0.46
2:B:308:GLU:CG	2:B:309:GLU:OE2	2.64	0.46
2:D:350:ARG:HG3	2:D:351:PRO:CD	2.38	0.46
2:D:94:ARG:HG2	2:D:94:ARG:O	2.16	0.46
1:C:111:LYS:O	1:C:112:ASP:OD1	2.34	0.46
1:C:140:GLU:O	1:C:141:PRO:C	2.52	0.46
2:D:140:ASP:OD2	2:D:140:ASP:C	2.53	0.46
1:A:47:LYS:N	1:A:58:MET:HE3	2.31	0.46
2:B:157:ILE:HG12	2:B:160:GLU:OE1	2.16	0.46
1:C:23:LYS:HE3	1:C:160:LEU:HA	1.98	0.46
1:C:80:VAL:CG1	1:C:85:ILE:CD1	2.89	0.46
2:D:330:ASN:OD1	2:D:330:ASN:N	2.44	0.46
1:C:30:TRP:CE2	1:C:190:ARG:NH1	2.83	0.45
1:C:300:THR:O	1:C:300:THR:HG23	2.16	0.45
2:D:188:TRP:CH2	2:D:190:THR:CA	3.00	0.45
1:A:103:LEU:HA	1:A:182:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:HE2	1:A:350:PHE:CG	2.40	0.45
2:B:185:ASN:HD22	2:B:185:ASN:N	2.14	0.45
2:B:337:VAL:CG2	2:B:338:VAL:N	2.79	0.45
1:C:138:PHE:O	1:C:139:SEP:C	2.62	0.45
1:C:196:TRP:O	1:C:197:TPO:C	2.64	0.45
2:D:126:LEU:HD23	2:D:174:VAL:HG11	1.98	0.45
1:A:116:LEU:HD13	1:A:116:LEU:HA	1.09	0.45
2:B:147:ILE:CD1	2:B:148:PHE:CD2	2.99	0.45
2:B:243:MET:C	2:B:243:MET:HE2	2.37	0.45
1:C:267:ASP:OD2	1:C:294:HIS:NE2	2.36	0.45
2:D:188:TRP:CE3	2:D:189:ALA:N	2.84	0.45
2:D:321:TYR:CE1	2:D:324:GLU:HG2	2.51	0.45
1:A:111:LYS:HE2	1:A:350:PHE:CB	2.47	0.45
1:A:54:PHE:O	1:A:78:LYS:HE2	2.16	0.45
1:A:96:GLN:HB3	1:A:106:LEU:HD23	1.98	0.45
2:B:104:THR:OG1	2:B:105:GLU:N	2.50	0.45
1:C:264:ASP:O	1:C:265:LEU:C	2.55	0.45
2:D:247:PHE:N	2:D:247:PHE:CD1	2.84	0.45
1:A:211:LEU:HD12	1:A:211:LEU:C	2.37	0.45
2:B:333:ARG:HD2	2:B:333:ARG:HA	1.72	0.45
1:C:67:ASN:CB	1:C:69:TYR:OH	2.64	0.45
1:C:91:GLU:OE2	1:C:185:PHE:N	2.49	0.45
2:B:116:ILE:HG12	2:B:149:ASP:O	2.17	0.45
2:B:248:LEU:HD21	2:B:265:VAL:HG22	1.97	0.45
1:C:125:GLY:HA3	1:C:174:ILE:O	2.17	0.45
1:C:23:LYS:HG3	1:C:27:LEU:CD1	2.46	0.45
2:D:136:PHE:C	2:D:138:HIS:N	2.65	0.45
2:D:302:GLN:O	2:D:310:PHE:HA	2.17	0.45
2:D:95:ARG:O	2:D:95:ARG:HG3	2.16	0.45
1:A:160:LEU:HB2	1:A:162:LEU:HD11	1.95	0.45
1:A:189:LYS:HZ2	1:A:195:THR:HG21	1.80	0.45
1:A:344:GLY:O	1:A:348:THR:HG22	2.16	0.45
1:A:326:ASN:H	1:A:326:ASN:HD22	1.65	0.45
2:B:179:GLU:C	2:B:216:LYS:HE3	2.37	0.45
2:B:246:GLU:O	2:B:249:SER:OG	2.28	0.45
1:A:170:GLU:OE2	2:B:95:ARG:HG2	2.17	0.45
1:A:111:LYS:CD	1:A:116:LEU:HD13	2.47	0.45
2:B:305:SER:N	2:B:308:GLU:OE2	2.50	0.45
1:C:107:GLU:N	1:C:119:VAL:O	2.45	0.45
1:C:140:GLU:HB2	1:C:141:PRO:HD3	1.99	0.44
1:C:182:VAL:CG1	1:C:183:THR:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:HIS:CE1	1:C:321:PRO:CB	2.94	0.44
2:D:148:PHE:O	2:D:151:MET:HB3	2.16	0.44
2:D:111:TYR:HD1	2:D:231:ARG:HD2	1.72	0.44
2:D:258:ASP:OD2	2:D:260:TRP:CE2	2.70	0.44
1:A:59:LEU:CD2	1:A:59:LEU:C	2.86	0.44
2:B:281:VAL:H	2:B:337:VAL:HG13	1.81	0.44
1:C:194:ARG:HG3	2:D:241:ARG:NH1	2.32	0.44
2:D:136:PHE:O	2:D:138:HIS:N	2.50	0.44
2:D:201:LEU:O	2:D:201:LEU:HG	2.17	0.44
1:A:211:LEU:CD1	1:A:211:LEU:C	2.86	0.44
1:A:195:THR:O	1:A:215:TYR:CD2	2.71	0.44
1:A:75:ASP:HB3	1:A:78:LYS:CG	2.44	0.44
2:B:116:ILE:CG1	2:B:118:LYS:NZ	2.78	0.44
2:B:348:LEU:HD23	2:B:352:ARG:HD3	1.99	0.44
1:C:16:LYS:CG	1:C:17:GLU:N	2.78	0.44
1:A:129:PHE:CE1	1:A:133:ARG:HG3	2.53	0.44
1:A:307:GLN:HE21	1:A:309:LYS:CD	2.31	0.44
2:B:182:VAL:HG22	2:B:211:ALA:HB1	2.00	0.44
2:B:269:LEU:HB3	2:B:346:VAL:HB	1.99	0.44
1:C:62:HIS:O	1:C:66:GLY:N	2.50	0.44
1:C:91:GLU:O	1:C:95:LEU:HB2	2.18	0.44
2:D:105:GLU:N	2:D:105:GLU:OE1	2.36	0.44
2:D:151:MET:HE1	2:D:222:TRP:O	2.13	0.44
2:D:248:LEU:H	2:D:248:LEU:HD13	1.82	0.44
2:D:285:GLU:O	2:D:333:ARG:HG2	2.16	0.44
2:D:295:GLU:O	2:D:343:LEU:HD12	2.17	0.44
2:B:182:VAL:HG12	2:B:190:THR:N	2.29	0.44
2:B:248:LEU:CD2	2:B:265:VAL:HG22	2.47	0.44
2:B:298:ALA:HB3	2:B:316:LEU:HB2	1.99	0.44
1:C:19:LEU:HG	1:C:20:ALA:H	1.81	0.44
2:D:173:TYR:N	2:D:173:TYR:CD1	2.83	0.44
2:D:176:ASP:OD2	2:D:222:TRP:NE1	2.50	0.44
1:A:133:ARG:NH2	1:A:230:GLU:OE1	2.35	0.44
1:A:280:ARG:O	1:A:284:LEU:HD13	2.18	0.44
1:A:77:GLN:NE2	1:A:342:LYS:CE	2.81	0.44
2:D:174:VAL:HG22	2:D:197:SER:HB3	1.98	0.44
2:D:316:LEU:HB3	2:D:320:ASP:HB2	2.00	0.44
2:B:173:TYR:HD2	2:B:198:PHE:CE1	2.36	0.44
2:B:287:GLY:HA3	2:B:333:ARG:CZ	2.48	0.44
1:C:169:PRO:HA	1:C:172:LEU:CD1	2.33	0.44
2:D:116:ILE:HB	2:D:118:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:PHE:CE1	2:D:223:GLY:O	2.71	0.44
1:A:195:THR:CG2	1:A:196:TRP:N	2.81	0.44
1:A:23:LYS:O	1:A:27:LEU:HD13	2.15	0.44
1:A:92:LYS:HZ3	1:A:350:PHE:HA	1.81	0.44
2:B:259:LYS:HG3	2:B:262:ARG:NH2	2.30	0.44
1:C:48:THR:CA	1:C:58:MET:HG3	2.41	0.44
1:C:88:THR:OG1	1:C:89:LEU:N	2.51	0.44
1:A:62:HIS:HB2	1:A:69:TYR:HE1	1.82	0.44
2:B:251:VAL:HG21	2:B:254:LEU:HD12	2.00	0.44
2:B:275:GLU:HA	2:B:342:PRO:HA	1.99	0.44
2:D:136:PHE:HA	2:D:139:LEU:HG	2.00	0.44
2:D:155:SER:OG	2:D:220:LYS:HA	2.18	0.44
1:A:23:LYS:NZ	1:A:190:ARG:HH12	2.16	0.43
1:C:165:ARG:HH21	1:C:189:LYS:HB2	1.82	0.43
1:C:230:GLU:HG3	1:C:235:TYR:HA	1.99	0.43
2:D:350:ARG:O	2:D:353:PHE:HB3	2.18	0.43
1:A:315:ILE:CD1	1:A:315:ILE:O	2.60	0.43
1:C:262:SER:O	1:C:266:LYS:HE2	2.18	0.43
2:D:151:MET:HE1	2:D:222:TRP:CB	2.46	0.43
1:A:131:HIS:CA	1:A:134:ARG:HG2	2.48	0.43
1:A:79:VAL:HG22	1:A:84:GLN:NE2	2.32	0.43
1:C:89:LEU:CD2	1:C:93:ARG:HD3	2.42	0.43
2:D:188:TRP:CZ2	2:D:191:SER:HB3	2.53	0.43
1:C:327:PHE:N	1:C:327:PHE:CD2	2.86	0.43
2:D:147:ILE:C	2:D:149:ASP:N	2.71	0.43
2:D:166:GLY:O	2:D:208:PRO:HB3	2.17	0.43
1:A:48:THR:HA	1:A:58:MET:HG3	1.96	0.43
2:B:153:PRO:HA	2:B:221:LEU:O	2.19	0.43
1:C:180:ILE:HD13	1:C:180:ILE:HA	1.88	0.43
2:D:111:TYR:CE2	2:D:113:ARG:HA	2.53	0.43
2:D:309:GLU:C	2:D:310:PHE:HD1	2.21	0.43
2:B:164:GLN:O	2:B:167:ASP:HB2	2.18	0.43
2:B:254:LEU:O	2:B:257:LEU:HB2	2.19	0.43
2:D:204:ILE:H	2:D:204:ILE:HG12	1.60	0.43
1:A:75:ASP:H	1:A:78:LYS:NZ	2.17	0.43
1:C:245:GLN:O	1:C:249:LYS:CB	2.66	0.43
1:C:92:LYS:CG	1:C:93:ARG:N	2.82	0.43
1:A:46:ILE:HD12	1:A:47:LYS:CA	2.48	0.43
2:B:305:SER:C	2:B:308:GLU:OE1	2.57	0.43
1:C:211:LEU:HD13	1:C:213:LYS:HD2	2.00	0.43
1:A:148:ALA:CB	1:A:302:TRP:CZ3	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HE2	1:A:66:GLY:CA	2.49	0.43
2:B:171:ASN:H	2:B:209:ARG:NH1	2.17	0.43
1:A:244:ILE:HD12	2:B:201:LEU:HB2	2.01	0.43
1:C:47:LYS:O	1:C:58:MET:CG	2.67	0.43
2:D:179:GLU:HA	2:D:192:VAL:O	2.18	0.43
2:D:240:LYS:O	2:D:244:TYR:CG	2.71	0.43
1:C:261:PHE:HB3	1:C:266:LYS:HG3	2.01	0.43
2:D:246:GLU:O	2:D:249:SER:OG	2.21	0.43
2:D:283:GLN:HG3	2:D:336:THR:N	2.34	0.43
2:D:354:GLU:HA	2:D:357:LEU:C	2.39	0.43
2:B:225:ASP:OD1	2:B:227:ASP:HB3	2.19	0.42
2:B:233:LEU:O	2:B:237:THR:HG23	2.19	0.42
1:C:265:LEU:HD12	1:C:296:TRP:CE2	2.53	0.42
2:D:165:GLN:HB3	2:D:212:THR:OG1	2.18	0.42
2:D:259:LYS:CG	2:D:260:TRP:N	2.82	0.42
2:D:322:PHE:CE1	2:D:337:VAL:HG11	2.53	0.42
1:A:137:ARG:NH2	1:A:260:HIS:CD2	2.86	0.42
1:A:57:VAL:HG11	3:A:400:ADP:C8	2.54	0.42
1:A:95:LEU:HD11	1:A:185:PHE:CB	2.36	0.42
2:B:148:PHE:HD2	2:B:151:MET:HE2	1.83	0.42
1:C:292:LYS:HA	1:C:302:TRP:CZ2	2.53	0.42
2:D:113:ARG:CG	2:D:114:LYS:H	2.32	0.42
2:D:272:VAL:HG12	2:D:347:LYS:HE2	1.91	0.42
1:A:131:HIS:HA	1:A:134:ARG:CG	2.49	0.42
1:A:111:LYS:HE3	1:A:350:PHE:HB3	2.01	0.42
1:C:96:GLN:HB2	1:C:106:LEU:HD11	2.01	0.42
1:C:51:THR:HG22	1:C:56:ARG:HD3	1.98	0.42
1:C:96:GLN:N	1:C:106:LEU:CD2	2.75	0.42
2:D:135:LEU:HB2	2:D:136:PHE:HE2	1.83	0.42
2:D:241:ARG:HH21	2:D:267:ASP:CG	2.23	0.42
1:A:215:TYR:HD2	1:A:215:TYR:N	2.18	0.42
1:A:335:ILE:HG23	1:A:335:ILE:O	2.19	0.42
2:B:167:ASP:O	2:B:209:ARG:HG2	2.19	0.42
1:C:230:GLU:HG3	1:C:235:TYR:CA	2.50	0.42
1:C:329:ASP:C	1:C:330:TYR:CG	2.93	0.42
1:C:349:GLU:N	1:C:349:GLU:OE1	2.49	0.42
2:D:183:TYR:CD2	2:D:188:TRP:N	2.87	0.42
2:D:262:ARG:HG2	2:D:262:ARG:HH11	1.85	0.42
1:A:40:LEU:CA	1:A:43:PHE:HE1	2.30	0.42
1:C:185:PHE:O	1:C:186:GLY:C	2.57	0.42
1:C:185:PHE:O	1:C:187:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:GLN:O	2:D:311:VAL:HG12	2.19	0.42
2:D:288:ASP:CA	2:D:350:ARG:NH1	2.80	0.42
1:A:117:TYR:N	1:A:117:TYR:CD1	2.86	0.42
2:B:323:GLY:O	2:B:326:ALA:HB3	2.19	0.42
1:C:56:ARG:HH11	1:C:57:VAL:CA	2.33	0.42
1:C:75:ASP:OD1	1:C:77:GLN:N	2.53	0.42
2:D:272:VAL:CG2	2:D:273:GLN:N	2.82	0.42
1:A:286:ASN:HB2	1:A:290:ASP:OD1	2.19	0.42
1:C:195:THR:C	1:C:196:TRP:CG	2.92	0.42
1:C:94:ILE:HD12	1:C:94:ILE:N	2.34	0.42
2:D:147:ILE:O	2:D:151:MET:HB2	2.19	0.42
2:D:344:LYS:C	2:D:345:CYS:SG	2.98	0.42
2:B:229:TYR:O	2:B:233:LEU:CD1	2.66	0.42
2:B:258:ASP:HA	2:B:262:ARG:HH12	1.83	0.42
2:B:301:LEU:HA	2:B:311:VAL:O	2.19	0.42
2:B:321:TYR:N	2:B:321:TYR:CD2	2.88	0.42
1:C:91:GLU:HG2	1:C:185:PHE:HB2	2.02	0.42
1:C:76:LYS:O	1:C:80:VAL:HG22	2.20	0.42
2:B:248:LEU:N	2:B:248:LEU:CD1	2.82	0.42
1:C:179:TYR:CE1	1:C:308:ARG:HA	2.55	0.42
1:C:287:GLY:O	1:C:290:ASP:CG	2.57	0.42
2:D:113:ARG:HG2	2:D:114:LYS:H	1.83	0.42
2:D:236:SER:O	2:D:240:LYS:NZ	2.35	0.42
2:D:283:GLN:NE2	2:D:302:GLN:HA	2.35	0.42
2:D:301:LEU:HD22	2:D:312:GLU:HA	2.00	0.42
1:C:175:ASP:OD2	1:C:178:GLY:N	2.53	0.42
1:C:228:ILE:HG13	1:C:228:ILE:H	1.62	0.42
1:C:264:ASP:O	1:C:266:LYS:N	2.52	0.42
1:C:50:GLY:N	1:C:56:ARG:NH1	2.37	0.42
1:A:187:PHE:CZ	2:B:99:SER:OG	2.72	0.41
1:A:19:LEU:O	1:A:22:ALA:HB3	2.21	0.41
1:A:43:PHE:N	1:A:43:PHE:CD1	2.87	0.41
2:B:133:ASN:HB3	2:B:136:PHE:CD2	2.55	0.41
2:B:182:VAL:CG1	2:B:189:ALA:HB3	2.46	0.41
1:A:116:LEU:HD21	1:A:350:PHE:CE2	2.55	0.41
1:A:185:PHE:CD2	1:A:185:PHE:N	2.89	0.41
1:C:164:TYR:CE2	1:C:166:ASP:C	2.91	0.41
1:C:50:GLY:C	1:C:56:ARG:CZ	2.88	0.41
2:D:167:ASP:O	2:D:209:ARG:HG2	2.19	0.41
1:A:113:ASN:HB2	1:A:340:ASN:O	2.20	0.41
1:A:195:THR:CG2	1:A:196:TRP:H	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:N	1:A:58:MET:HE2	2.35	0.41
1:C:196:TRP:N	1:C:196:TRP:CD1	2.88	0.41
1:C:82:LEU:O	1:C:83:LYS:HD3	2.20	0.41
2:D:316:LEU:HB3	2:D:320:ASP:CB	2.50	0.41
2:D:336:THR:CG2	2:D:337:VAL:N	2.83	0.41
2:B:236:SER:CA	2:B:239:ARG:NH1	2.78	0.41
1:C:180:ILE:HG22	1:C:181:GLN:N	2.34	0.41
1:C:75:ASP:OD1	1:C:76:LYS:N	2.54	0.41
1:C:89:LEU:HD11	1:C:349:GLU:HG2	2.01	0.41
1:A:142:HIS:CE1	1:A:313:PRO:HG2	2.56	0.41
1:A:160:LEU:CB	1:A:162:LEU:HD12	2.38	0.41
2:B:300:VAL:HG22	2:B:314:GLY:C	2.41	0.41
2:B:329:MET:O	2:B:350:ARG:NH2	2.53	0.41
1:C:146:TYR:HA	1:C:149:GLN:NE2	2.36	0.41
1:C:165:ARG:NH2	1:C:189:LYS:HB2	2.34	0.41
1:C:16:LYS:HA	1:C:19:LEU:CD2	2.50	0.41
1:C:49:LEU:CA	1:C:56:ARG:HH22	2.33	0.41
2:D:183:TYR:HE1	2:D:214:LYS:NZ	2.16	0.41
1:A:167:LEU:HG	1:A:227:LEU:HD13	2.02	0.41
1:C:79:VAL:HG13	1:C:88:THR:HG21	2.01	0.41
2:D:111:TYR:HD1	2:D:231:ARG:HH21	1.69	0.41
1:A:80:VAL:H	1:A:80:VAL:HG22	1.68	0.41
1:A:86:GLU:O	1:A:90:ASN:ND2	2.53	0.41
1:C:210:ILE:HD13	1:C:250:ILE:HG21	2.02	0.41
1:C:204:TYR:OH	1:C:227:LEU:HD23	2.21	0.41
2:D:152:PHE:O	2:D:222:TRP:CE3	2.70	0.41
1:A:129:PHE:CE1	1:A:133:ARG:CZ	2.97	0.41
2:B:185:ASN:HB3	1:C:96:GLN:HG2	2.03	0.41
2:B:161:THR:HA	2:B:214:LYS:HA	2.03	0.41
2:B:350:ARG:HG3	2:B:351:PRO:HD3	2.03	0.41
1:C:91:GLU:HG2	1:C:185:PHE:CB	2.51	0.41
1:A:189:LYS:HZ3	1:A:195:THR:HG21	1.81	0.41
1:A:154:PHE:CD1	1:A:220:ASP:OD2	2.74	0.41
2:B:325:ILE:HD11	2:B:331:ARG:CD	2.46	0.41
1:C:129:PHE:CE1	1:C:133:ARG:NE	2.88	0.41
1:C:167:LEU:O	1:C:168:LYS:HB3	2.20	0.41
1:C:102:PHE:HE1	1:C:179:TYR:HB3	1.86	0.41
1:C:65:SER:O	1:C:67:ASN:ND2	2.54	0.41
2:D:173:TYR:HB3	2:D:222:TRP:C	2.41	0.41
2:D:294:LEU:HD11	2:D:346:VAL:CG1	2.42	0.41
1:A:146:TYR:O	1:A:150:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:OD2	1:A:175:ASP:C	2.60	0.41
1:A:207:PRO:HG2	1:A:275:VAL:HG22	2.03	0.41
2:B:126:LEU:HD23	2:B:126:LEU:HA	1.74	0.41
1:A:170:GLU:OE2	2:B:95:ARG:NH1	2.54	0.41
1:C:132:LEU:HA	1:C:138:PHE:HE2	1.86	0.41
1:C:150:ILE:HD12	1:C:150:ILE:HG23	1.60	0.41
1:C:19:LEU:HG	1:C:20:ALA:N	2.35	0.41
1:C:39:GLN:HB2	1:C:42:GLN:HE22	1.86	0.41
1:C:89:LEU:CG	1:C:92:LYS:NZ	2.71	0.41
2:D:118:LYS:NZ	2:D:151:MET:O	2.26	0.41
2:D:237:THR:O	2:D:238:LEU:C	2.58	0.41
2:D:294:LEU:HD11	2:D:346:VAL:HG22	2.02	0.41
1:C:245:GLN:HA	1:C:248:GLU:HG2	2.03	0.41
1:C:261:PHE:HA	1:C:261:PHE:HD2	1.70	0.41
1:C:36:ASN:CG	1:C:36:ASN:O	2.58	0.41
2:D:247:PHE:HD1	2:D:247:PHE:N	2.19	0.41
2:D:275:GLU:OE2	2:D:278:GLN:HB2	2.21	0.41
1:C:330:TYR:N	1:C:330:TYR:CD2	2.88	0.40
2:D:135:LEU:C	2:D:136:PHE:HD2	2.23	0.40
1:A:175:ASP:OD1	1:A:181:GLN:NE2	2.54	0.40
2:B:219:VAL:CG2	2:B:220:LYS:H	2.31	0.40
1:C:132:LEU:HD21	1:C:230:GLU:HG2	2.02	0.40
2:B:270:GLU:HA	2:B:271:PRO:HD3	1.89	0.40
1:C:349:GLU:H	1:C:349:GLU:CD	2.24	0.40
1:C:44:ASP:O	1:C:46:ILE:HG12	2.21	0.40
1:A:87:HIS:HB3	1:A:186:GLY:O	2.22	0.40
2:B:243:MET:HG3	2:B:244:TYR:N	2.36	0.40
2:B:291:PHE:CD2	2:B:322:PHE:CE2	3.09	0.40
2:B:303:ARG:C	2:B:308:GLU:OE2	2.60	0.40
2:B:340:ARG:HD3	2:B:340:ARG:HA	1.71	0.40
1:C:133:ARG:HH22	2:D:95:ARG:NH2	2.08	0.40
1:C:68:HIS:NE2	1:C:321:PRO:CB	2.85	0.40
1:C:82:LEU:O	1:C:83:LYS:CD	2.70	0.40
2:D:258:ASP:CB	2:D:260:TRP:CE2	3.05	0.40
2:D:272:VAL:HG11	2:D:347:LYS:HG3	2.03	0.40
1:A:76:LYS:HB2	1:A:114:SER:O	2.21	0.40
2:B:172:PHE:HD1	2:B:198:PHE:O	2.04	0.40
1:C:265:LEU:HD13	1:C:296:TRP:CE2	2.56	0.40
1:C:61:LYS:HD3	1:C:61:LYS:HA	1.74	0.40
2:D:176:ASP:OD1	2:D:220:LYS:HG2	2.21	0.40
2:D:198:PHE:CD2	2:D:198:PHE:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:ASN:O	2:D:202:ALA:HB3	2.21	0.40
2:D:253:ILE:HD12	2:D:253:ILE:H	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	333/350 (95%)	323 (97%)	10 (3%)	0	100	100
1	C	333/350 (95%)	296 (89%)	36 (11%)	1 (0%)	41	74
2	B	265/275 (96%)	255 (96%)	10 (4%)	0	100	100
2	D	264/275 (96%)	234 (89%)	30 (11%)	0	100	100
All	All	1195/1250 (96%)	1108 (93%)	86 (7%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	TYR

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	278/302 (92%)	254 (91%)	24 (9%)	10	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	277/302 (92%)	240 (87%)	37 (13%)	4	23
2	B	212/230 (92%)	192 (91%)	20 (9%)	8	37
2	D	210/230 (91%)	174 (83%)	36 (17%)	2	13
All	All	977/1064 (92%)	860 (88%)	117 (12%)	5	27

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	40	LEU
1	A	41	ASP
1	A	43	PHE
1	A	45	ARG
1	A	59	LEU
1	A	116	LEU
1	A	119	VAL
1	A	120	MET
1	A	135	ILE
1	A	158	HIS
1	A	163	ILE
1	A	177	GLN
1	A	199	CYS
1	A	201	THR
1	A	211	LEU
1	A	215	TYR
1	A	245	GLN
1	A	247	TYR
1	A	263	SER
1	A	290	ASP
1	A	300	THR
1	A	323	ASP
1	A	339	ILE
2	B	102	VAL
2	B	104	THR
2	B	154	VAL
2	B	161	THR
2	B	182	VAL
2	B	194	GLU
2	B	197	SER
2	B	233	LEU
2	B	236	SER

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Mol	Chain	Res	Type
2	B	243	MET
2	B	265	VAL
2	B	282	VAL
2	B	293	ILE
2	B	309	GLU
2	B	311	VAL
2	B	328	LEU
2	B	330	ASN
2	B	333	ARG
2	B	336	THR
2	B	348	LEU
1	C	15	VAL
1	C	34	SER
1	C	48	THR
1	C	51	THR
1	C	53	SER
1	C	56	ARG
1	C	72	LYS
1	C	80	VAL
1	C	83	LYS
1	C	86	GLU
1	C	103	LEU
1	C	111	LYS
1	C	119	VAL
1	C	120	MET
1	C	135	ILE
1	C	162	LEU
1	C	172	LEU
1	C	174	ILE
1	C	175	ASP
1	C	183	THR
1	C	205	LEU
1	C	211	LEU
1	C	250	ILE
1	C	255	VAL
1	C	265	LEU
1	C	272	LEU
1	C	273	LEU
1	C	284	LEU
1	C	286	ASN
1	C	288	VAL
1	C	295	LYS

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Mol	Chain	Res	Type
1	C	303	ILE
1	C	310	VAL
1	C	311	GLU
1	C	324	THR
1	C	340	ASN
1	C	348	THR
2	D	93	ARG
2	D	94	ARG
2	D	104	THR
2	D	136	PHE
2	D	152	PHE
2	D	154	VAL
2	D	161	THR
2	D	173	TYR
2	D	182	VAL
2	D	192	VAL
2	D	204	ILE
2	D	207	THR
2	D	209	ARG
2	D	213	VAL
2	D	219	VAL
2	D	224	ILE
2	D	233	LEU
2	D	237	THR
2	D	239	ARG
2	D	242	LYS
2	D	248	LEU
2	D	250	LYS
2	D	255	GLU
2	D	257	LEU
2	D	264	THR
2	D	265	VAL
2	D	290	PHE
2	D	300	VAL
2	D	319	SER
2	D	321	TYR
2	D	324	GLU
2	D	330	ASN
2	D	345	CYS
2	D	348	LEU
2	D	356	VAL
2	D	357	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	77	GLN
1	A	131	HIS
1	A	158	HIS
1	A	181	GLN
1	A	307	GLN
1	A	326	ASN
1	C	87	HIS
2	D	273	GLN
2	D	283	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	SEP	C	139	1	8,9,10	1.62	1 (12%)	8,12,14	1.56	2 (25%)
1	SEP	A	338	1	8,9,10	1.54	1 (12%)	8,12,14	1.74	2 (25%)
1	SEP	C	338	1	8,9,10	1.55	1 (12%)	8,12,14	1.77	2 (25%)
1	TPO	C	197	1	8,10,11	1.53	1 (12%)	10,14,16	2.17	1 (10%)
1	SEP	A	139	1	8,9,10	1.54	1 (12%)	8,12,14	2.29	2 (25%)
1	TPO	A	197	1	8,10,11	1.52	1 (12%)	10,14,16	2.12	1 (10%)

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
1	SEP	C	139	1	-	0/5/8/10	-
1	SEP	A	338	1	-	5/5/8/10	-
1	SEP	C	338	1	-	5/5/8/10	-
1	TPO	C	197	1	-	0/9/11/13	-
1	SEP	A	139	1	-	4/5/8/10	-
1	TPO	A	197	1	-	0/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	SEP	P-O1P	3.52	1.61	1.50
1	C	338	SEP	P-O1P	3.39	1.61	1.50
1	A	197	TPO	P-O1P	3.37	1.61	1.50
1	A	139	SEP	P-O1P	3.37	1.61	1.50
1	C	197	TPO	P-O1P	3.33	1.61	1.50
1	A	338	SEP	P-O1P	3.32	1.61	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	TPO	P-OG1-CB	-6.41	103.86	123.21
1	A	197	TPO	P-OG1-CB	-6.25	104.32	123.21
1	A	139	SEP	P-OG-CB	-4.93	104.72	118.30
1	A	139	SEP	OG-CB-CA	3.88	111.92	108.14
1	C	338	SEP	OG-CB-CA	3.75	111.80	108.14
1	A	338	SEP	P-OG-CB	-3.58	108.44	118.30
1	C	139	SEP	P-OG-CB	-3.08	109.80	118.30
1	A	338	SEP	OG-CB-CA	2.77	110.84	108.14
1	C	338	SEP	P-OG-CB	-2.69	110.89	118.30
1	C	139	SEP	OG-CB-CA	2.58	110.65	108.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	CB-OG-P-O2P
1	A	338	SEP	CB-OG-P-O3P
1	C	338	SEP	N-CA-CB-OG
1	C	338	SEP	CB-OG-P-O2P
1	C	338	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
1	A	139	SEP	N-CA-CB-OG
1	A	139	SEP	CB-OG-P-O1P
1	A	139	SEP	CB-OG-P-O2P
1	A	139	SEP	CB-OG-P-O3P
1	A	338	SEP	CB-OG-P-O1P
1	C	338	SEP	CB-OG-P-O1P
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	N-CA-CB-OG
1	C	338	SEP	CA-CB-OG-P

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	139	SEP	2	0
1	A	338	SEP	2	0
1	C	197	TPO	2	0
1	A	139	SEP	1	0
1	A	197	TPO	5	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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
3	ADP	A	400	-	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
3	ADP	C	400	-	24,29,29	0.99	1 (4%)	29,45,45	1.31	4 (13%)

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
3	ADP	A	400	-	-	3/12/32/32	0/3/3/3
3	ADP	C	400	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ADP	C5-C4	2.53	1.47	1.40
3	C	400	ADP	C5-C4	2.53	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	ADP	C3'-C2'-C1'	3.19	105.78	100.98
3	A	400	ADP	N3-C2-N1	-3.09	123.85	128.68
3	C	400	ADP	N3-C2-N1	-3.08	123.87	128.68
3	C	400	ADP	C3'-C2'-C1'	2.98	105.46	100.98
3	A	400	ADP	C4-C5-N7	-2.71	106.57	109.40
3	C	400	ADP	C4-C5-N7	-2.54	106.75	109.40
3	C	400	ADP	PA-O3A-PB	-2.41	124.56	132.83
3	A	400	ADP	PA-O3A-PB	-2.19	125.29	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

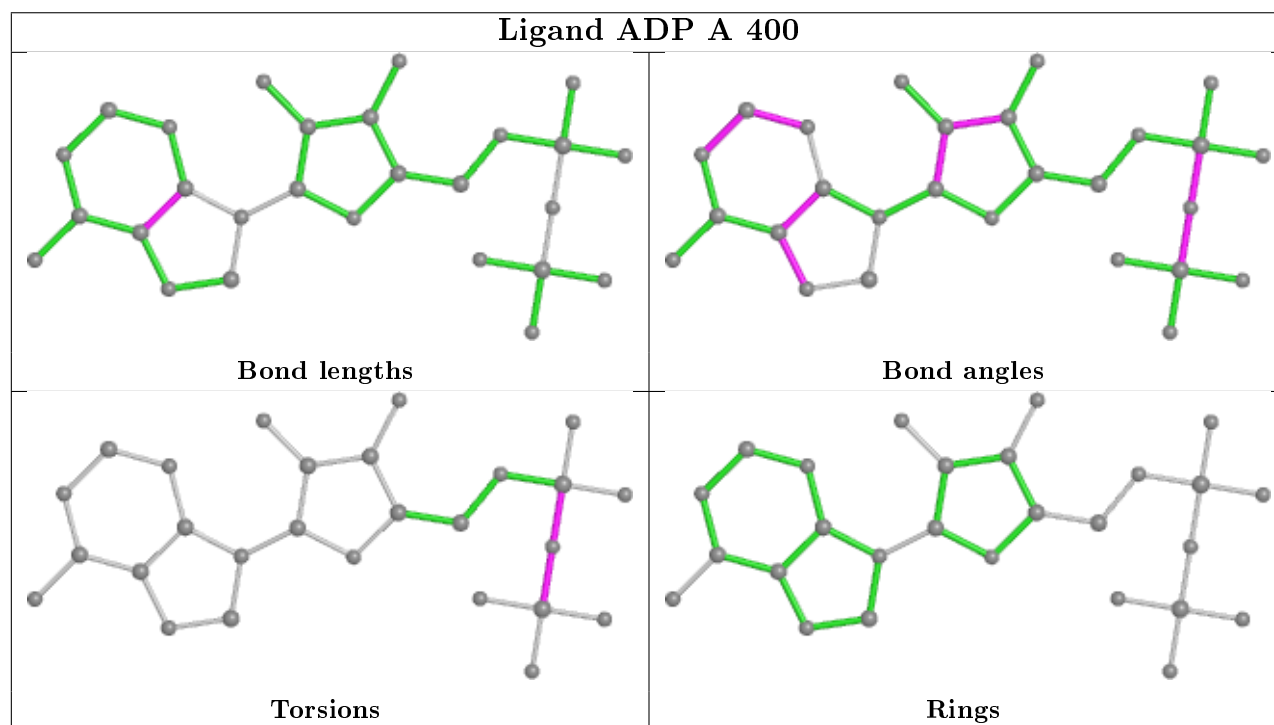
Mol	Chain	Res	Type	Atoms
3	C	400	ADP	PA-O3A-PB-O2B
3	C	400	ADP	PA-O3A-PB-O3B
3	C	400	ADP	C5'-O5'-PA-O2A
3	A	400	ADP	PA-O3A-PB-O3B
3	C	400	ADP	C5'-O5'-PA-O3A
3	C	400	ADP	C5'-O5'-PA-O1A
3	A	400	ADP	PB-O3A-PA-O1A
3	A	400	ADP	PA-O3A-PB-O2B
3	C	400	ADP	PB-O3A-PA-O1A

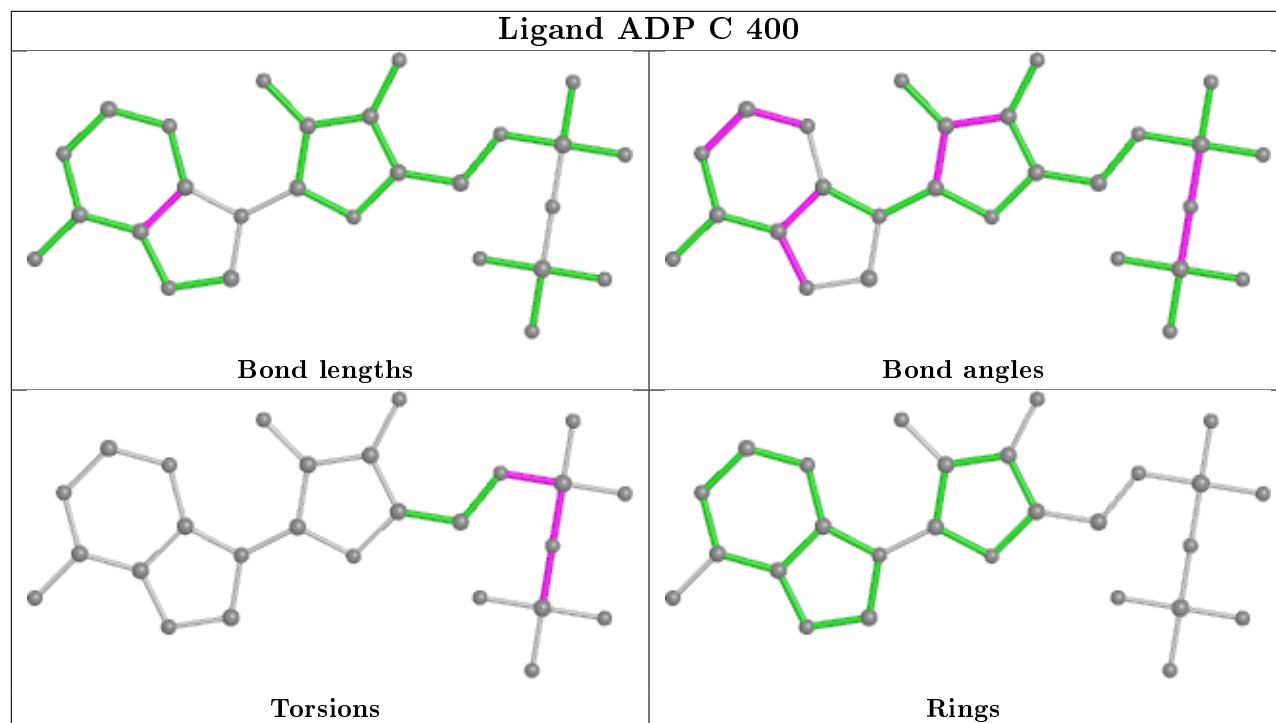
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	ADP	4	0
3	C	400	ADP	1	0

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





## 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	335/350 (95%)	-0.23	1 (0%) 94 88	33, 84, 183, 220	1 (0%)
1	C	335/350 (95%)	-0.11	6 (1%) 68 52	29, 101, 194, 292	0
2	B	267/275 (97%)	-0.02	4 (1%) 73 59	54, 100, 185, 222	1 (0%)
2	D	266/275 (96%)	0.08	7 (2%) 56 39	51, 119, 214, 254	2 (0%)
All	All	1203/1250 (96%)	-0.08	18 (1%) 73 59	29, 100, 196, 292	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	161	THR	7.7
1	C	64	GLU	3.9
1	C	34	SER	3.9
2	B	196	GLY	3.8
2	D	158	ALA	3.8
1	C	343	CYS	3.7
2	D	157	ILE	3.4
2	D	160	GLU	3.2
2	D	103	TYR	3.2
2	B	92	ARG	3.0
1	C	37	THR	2.8
2	D	218	ASN	2.8
1	A	37	THR	2.7
2	B	186	ASN	2.5
1	C	340	ASN	2.4
2	B	157	ILE	2.4
1	C	322	GLY	2.2
2	D	162	VAL	2.2

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

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(Å <sup>2</sup> )	Q<0.9
1	SEP	C	338	10/11	0.19	0.67	214,238,337,355	0
1	SEP	A	338	10/11	0.73	0.21	153,180,183,187	0
1	SEP	C	139	10/11	0.92	0.10	43,85,92,195	0
1	SEP	A	139	10/11	0.92	0.16	50,70,84,155	0
1	TPO	C	197	11/12	0.93	0.18	51,90,107,164	0
1	TPO	A	197	11/12	0.97	0.16	35,83,96,186	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

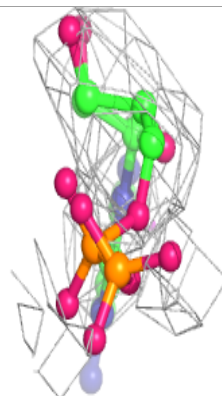
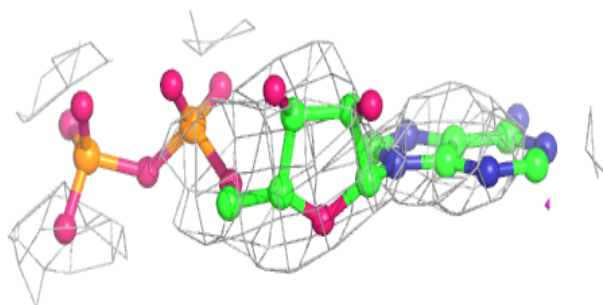
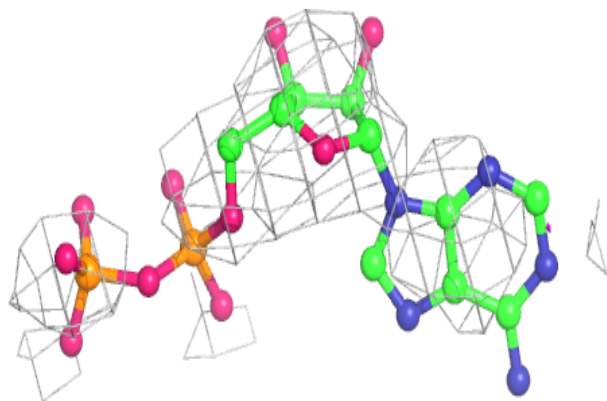
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	C	400	27/27	0.72	0.51	101,118,305,311	0
3	ADP	A	400	27/27	0.87	0.24	57,103,213,304	0

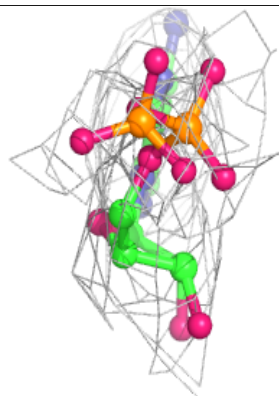
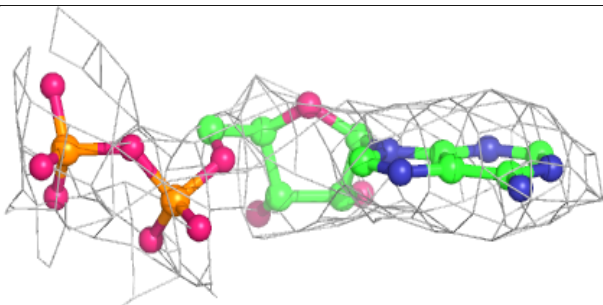
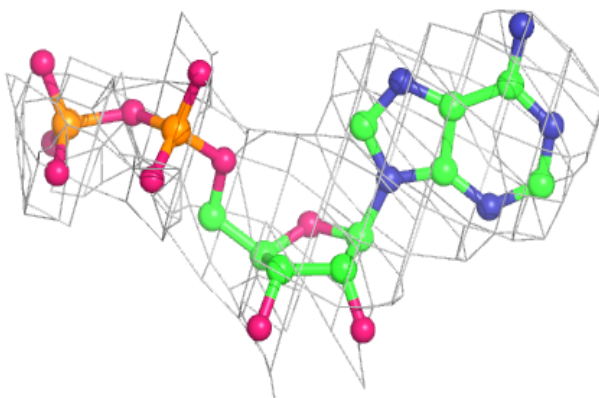
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP C 400:**

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

**Electron density around ADP A 400:**

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



## 6.5 Other polymers

There are no such residues in this entry.