



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:00 AM GMT

PDB ID : 3KIN
Title : KINESIN (DIMERIC) FROM RATTUS NORVEGICUS
Authors : Kozielski, F.; Sack, S.; Marx, A.; Thormahlen, M.; Schonbrunn, E.; Biou, V.;
Thompson, A.; Mandelkow, E.-M.; Mandelkow, E.
Deposited on : 1997-08-25
Resolution : 3.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

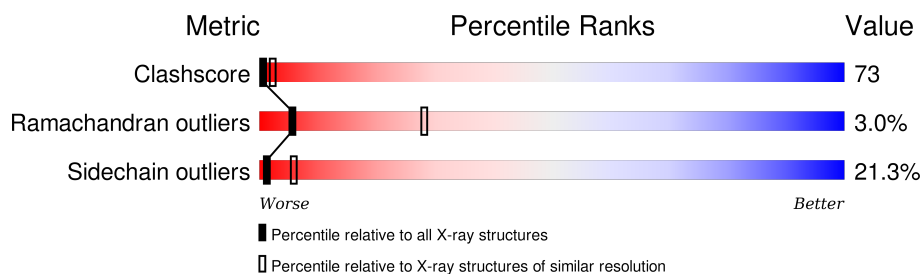
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	
1	C	238	
2	B	117	
2	D	117	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	401	X	-	X	-
3	ADP	C	400	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5743 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.

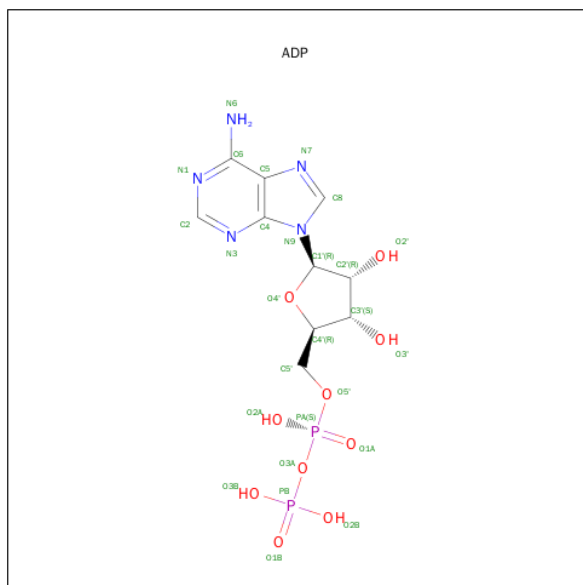
- Molecule 1 is a protein called KINESIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1899	1201	325	363	10			
1	C	238	Total	C	N	O	S	0	0	0
			1899	1201	325	363	10			

- Molecule 2 is a protein called KINESIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			925	576	167	177	5			
2	D	115	Total	C	N	O	S	0	0	0
			906	566	161	174	5			

- 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	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

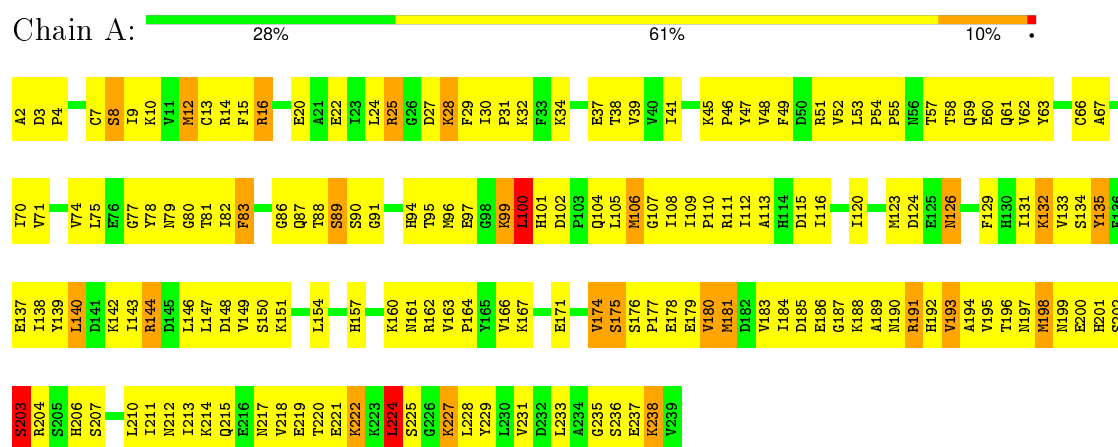
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	11	Total	O	0	0
			11	11		
4	C	18	Total	O	0	0
			18	18		
4	D	8	Total	O	0	0
			8	8		

3 Residue-property plots

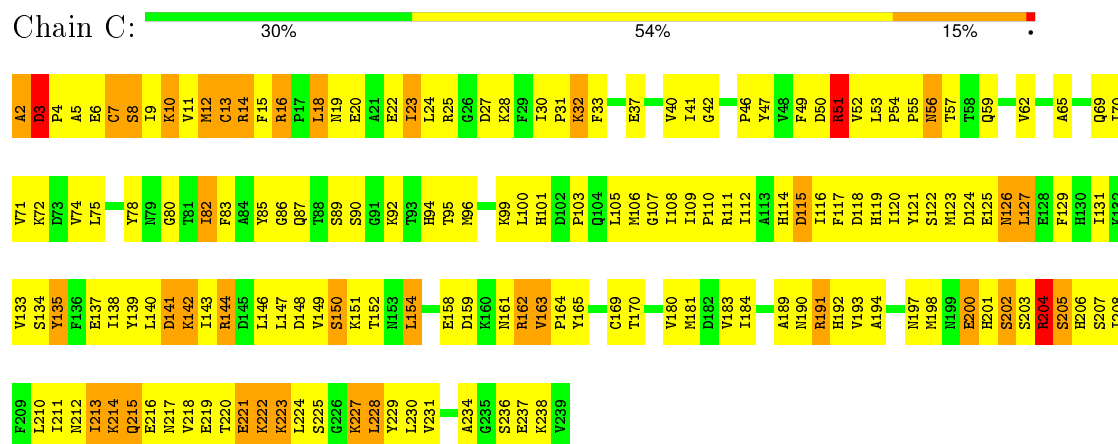
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

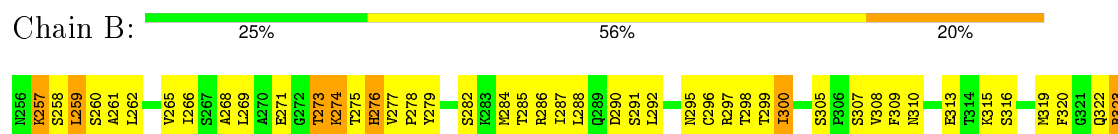
• Molecule 1: KINESIN HEAVY CHAIN



• Molecule 1: KINESIN HEAVY CHAIN



• Molecule 2: KINESIN HEAVY CHAIN



A324	A325	T326	T327	K328	T330	V331	S332	V333	N334	L335	E336	L337	T338	A339	E340	E341	N342	K343	K344	K345	Y346	E347	K348	E349	K350	E351	K352	N353	K354	K355	L356	K357	S358	V359	I360	K361	K362	L363	E364	V365	E366	L367	N368	R369	W370	R371	N372
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● Molecule 2: KINESIN HEAVY CHAIN



N256	K257	S258	L259	S260	A261	L262	G263	N264	V265	L266	S267	A268	L269	A270	T273	K274	T275	H276	V277	P278	Y279	R280	D281	S282	K283	N284	T285	R286	L287	L288	Q289	D290	S291	L292	G293	G294	N295	C296	R297	I300	V301	I302	C303	C304	S305	P306	S307	V308	F309	N310	E311	A312	E313	T314	K315	L318
A324	K325	T326	K328	N329	T330	V331	S332	V333	N334	L335	E336	L337	T338	A339	E340	E341	W342	K343	K344	K345	Y346	E347	K348	E349	K350	E351	K352	N353	K354	K355	A356	L356	K357	S358	V359	I360	Q361	K362	L363	E364	V365	E366	L367	N368	R369	W370	ARG	ASN								

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.15Å 91.85Å 141.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.289 , 0.362	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5743	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/1936	0.98	4/2612 (0.2%)
1	C	0.74	4/1936 (0.2%)	1.13	13/2612 (0.5%)
2	B	2.25	4/936 (0.4%)	1.16	7/1257 (0.6%)
2	D	0.36	0/917	0.97	0/1232
All	All	1.04	8/5725 (0.1%)	1.06	24/7713 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	372	ASN	C-O	65.63	2.48	1.23
1	C	2	ALA	CA-CB	22.42	1.99	1.52
1	C	2	ALA	C-O	12.80	1.47	1.23
2	B	371	ARG	C-O	11.08	1.44	1.23
2	B	372	ASN	N-CA	10.53	1.67	1.46
1	C	3	ASP	CA-CB	8.30	1.72	1.53
2	B	372	ASN	CA-CB	7.40	1.72	1.53
1	C	3	ASP	N-CA	6.40	1.59	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	ASN	CA-C-O	-16.45	85.55	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	ASP	N-CA-C	15.22	152.10	111.00
1	C	2	ALA	CB-CA-C	-13.90	89.25	110.10
1	C	2	ALA	O-C-N	-13.45	101.18	122.70
1	C	2	ALA	N-CA-C	12.10	143.67	111.00
2	B	371	ARG	O-C-N	10.86	140.07	122.70
1	C	3	ASP	CB-CA-C	-9.78	90.83	110.40
1	C	2	ALA	CA-C-N	9.68	138.50	117.20
1	C	204	ARG	CD-NE-CZ	9.19	136.46	123.60
2	B	372	ASN	N-CA-CB	-7.99	96.23	110.60
2	B	372	ASN	CB-CA-C	7.83	126.06	110.40
1	A	83	PHE	CA-CB-CG	7.81	132.65	113.90
1	C	3	ASP	N-CA-CB	-7.74	96.67	110.60
1	A	162	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	C	14	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	371	ARG	CA-C-N	-6.58	102.72	117.20
1	C	14	ARG	CD-NE-CZ	6.07	132.10	123.60
2	B	372	ASN	N-CA-C	5.94	127.04	111.00
1	C	51	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	371	ARG	N-CA-C	-5.61	95.85	111.00
1	C	3	ASP	CA-CB-CG	-5.42	101.49	113.40
1	A	162	ARG	CD-NE-CZ	5.27	130.97	123.60
1	A	224	LEU	CA-CB-CG	5.06	126.94	115.30
1	C	14	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	3	ASP	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	1899	0	1888	266	4
1	C	1899	0	1888	313	0
2	B	925	0	955	219	13

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	906	0	938	219	2
3	A	27	0	11	12	1
3	C	27	0	12	1	0
4	A	23	0	0	11	0
4	B	11	0	0	6	0
4	C	18	0	0	12	0
4	D	8	0	0	9	0
All	All	5743	0	5692	835	15

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 73.

All (835) 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:2:ALA:N	2:D:350:LYS:HZ1	0.97	1.43
1:C:2:ALA:CA	1:C:2:ALA:CB	1.99	1.40
1:A:157:HIS:CE1	1:A:167:LYS:HZ1	1.40	1.37
1:A:2:ALA:N	2:D:350:LYS:NZ	1.73	1.35
1:A:200:GLU:OE2	1:A:204:ARG:CZ	1.75	1.33
1:A:200:GLU:OE2	1:A:204:ARG:NH2	1.61	1.33
2:B:369:ARG:O	2:B:372:ASN:ND2	1.59	1.32
1:A:160:LYS:CE	1:C:221:GLU:OE1	1.78	1.32
2:B:366:GLU:O	2:B:370:TRP:N	1.61	1.30
1:A:181:MET:HE3	1:A:184:ILE:CD1	1.60	1.29
1:A:157:HIS:CE1	1:A:167:LYS:NZ	2.05	1.24
2:D:269:LEU:CD2	2:D:274:LYS:HE2	1.67	1.24
2:B:366:GLU:HG2	2:B:370:TRP:CE3	1.54	1.23
2:B:259:LEU:HB3	4:B:31:HOH:O	1.07	1.22
2:B:266:ILE:CD1	2:B:292:LEU:HD11	1.69	1.21
2:B:364:GLU:OE1	2:D:363:LEU:HD21	1.05	1.20
2:B:366:GLU:CG	2:B:370:TRP:CE3	2.10	1.19
1:C:197:ASN:HA	4:C:408:HOH:O	1.42	1.18
1:A:8:SER:OG	2:B:328:LYS:NZ	1.76	1.18
1:C:227:LYS:O	4:C:404:HOH:O	1.62	1.17
1:A:12:MET:HG2	1:A:66:CYS:SG	1.83	1.17
2:D:269:LEU:HD23	2:D:274:LYS:CE	1.73	1.17
1:A:96:MET:CE	1:A:231:VAL:O	1.91	1.16
2:B:343:LYS:HG3	2:D:342:TRP:CZ2	1.81	1.16
1:C:74:VAL:HG21	1:C:228:LEU:HD22	1.26	1.15
1:A:96:MET:HE2	1:A:231:VAL:O	1.42	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MET:CE	1:A:184:ILE:HD12	1.76	1.15
1:A:160:LYS:NZ	1:C:221:GLU:OE1	1.78	1.15
2:D:356:LEU:O	2:D:360:ILE:HD12	1.48	1.14
2:B:367:LEU:O	2:B:371:ARG:HB3	1.46	1.13
1:C:117:PHE:O	1:C:121:TYR:CD2	2.01	1.13
1:A:215:GLN:HG3	4:A:417:HOH:O	1.49	1.13
1:C:216:GLU:HG3	1:C:223:LYS:CG	1.80	1.12
1:C:191:ARG:NH2	1:C:202:SER:HB3	1.65	1.11
2:B:343:LYS:HG3	2:D:342:TRP:CE2	1.85	1.10
1:A:181:MET:CE	1:A:184:ILE:CD1	2.28	1.10
1:C:180:VAL:O	1:C:184:ILE:HD12	1.51	1.09
1:A:75:LEU:O	1:A:215:GLN:NE2	1.83	1.09
2:D:337:LEU:HD13	2:D:341:GLU:OE2	1.52	1.09
2:B:364:GLU:OE1	2:D:363:LEU:CD2	1.99	1.09
2:D:258:SER:OG	4:D:56:HOH:O	1.66	1.08
2:B:345:LYS:NZ	2:D:346:TYR:HE2	1.52	1.08
1:A:160:LYS:HE3	1:C:221:GLU:OE1	1.49	1.07
1:C:30:ILE:HG13	1:C:31:PRO:HD3	1.28	1.07
1:C:191:ARG:HH22	1:C:202:SER:HB3	0.90	1.06
1:C:216:GLU:CG	1:C:223:LYS:HG3	1.85	1.05
1:C:120:ILE:HA	1:C:123:MET:HG3	1.37	1.05
1:C:222:LYS:HZ1	2:D:335:LEU:HD22	1.21	1.05
1:C:216:GLU:HG3	1:C:223:LYS:HG3	1.07	1.04
2:B:259:LEU:CB	4:B:31:HOH:O	1.74	1.04
1:C:204:ARG:NH2	1:C:237:GLU:OE2	1.89	1.04
2:D:269:LEU:HD23	2:D:274:LYS:HE2	1.06	1.04
1:A:78:TYR:HA	4:B:7:HOH:O	1.57	1.03
2:B:266:ILE:HD13	2:B:292:LEU:HD11	1.32	1.03
1:A:2:ALA:N	2:D:350:LYS:CE	2.23	1.02
1:C:22:GLU:HG2	1:C:27:ASP:OD2	1.60	1.02
1:C:224:LEU:HD23	2:D:335:LEU:HD13	1.36	1.02
2:D:274:LYS:HA	2:D:277:VAL:HG13	1.42	1.02
2:B:266:ILE:HD13	2:B:292:LEU:CD1	1.89	1.02
1:C:137:GLU:OE2	1:C:144:ARG:NE	1.91	1.01
1:C:10:LYS:CB	1:C:50:ASP:OD2	2.08	1.01
2:B:338:THR:HG23	2:B:341:GLU:OE1	1.60	1.01
2:B:279:TYR:O	2:B:285:THR:OG1	1.79	1.00
1:C:18:LEU:CD2	1:C:22:GLU:HB3	1.91	1.00
1:A:2:ALA:O	2:D:350:LYS:HE2	1.61	1.00
1:A:79:ASN:ND2	1:A:227:LYS:H	1.60	1.00
1:C:151:LYS:HB3	1:C:154:LEU:HD21	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:CD2	2:D:335:LEU:HD13	1.91	1.00
1:A:233:LEU:CD2	2:B:284:MET:HE1	1.92	0.99
1:A:157:HIS:ND1	1:A:167:LYS:NZ	2.10	0.99
1:A:58:THR:O	1:A:62:VAL:HG23	1.61	0.99
1:A:181:MET:HE3	1:A:184:ILE:HD12	1.02	0.99
1:A:233:LEU:HD22	2:B:284:MET:HE1	1.41	0.98
1:A:195:VAL:HG11	1:A:198:MET:HE1	1.45	0.98
1:C:19:ASN:O	1:C:23:ILE:HG12	1.62	0.98
1:A:195:VAL:HG11	1:A:198:MET:CE	1.93	0.98
2:B:271:GLU:HB3	2:B:273:THR:HG22	1.45	0.98
2:D:357:LYS:HA	2:D:360:ILE:CD1	1.92	0.98
1:C:10:LYS:HB3	1:C:50:ASP:OD2	1.63	0.98
1:A:100:LEU:HD21	1:A:184:ILE:HG21	1.45	0.97
1:A:206:HIS:HD2	1:A:233:LEU:CD2	1.77	0.97
1:C:224:LEU:CD2	2:D:335:LEU:HB2	1.93	0.97
1:C:191:ARG:HH22	1:C:202:SER:CB	1.76	0.97
2:B:369:ARG:HH21	2:B:372:ASN:CG	1.67	0.97
1:A:200:GLU:OE2	1:A:204:ARG:NH1	1.98	0.97
1:C:148:ASP:OD1	1:C:150:SER:HB3	1.66	0.96
1:A:79:ASN:HD22	1:A:227:LYS:H	1.10	0.96
1:C:214:LYS:HG2	4:C:407:HOH:O	1.65	0.95
1:C:20:GLU:O	1:C:23:ILE:HB	1.67	0.95
2:B:369:ARG:NH2	2:B:372:ASN:CG	2.18	0.95
2:D:269:LEU:CD2	2:D:274:LYS:CE	2.38	0.95
2:B:351:GLU:O	2:B:354:LYS:HG3	1.68	0.94
1:C:138:ILE:HG21	4:D:56:HOH:O	1.67	0.94
2:D:355:ALA:O	2:D:359:VAL:HG23	1.68	0.94
1:C:222:LYS:NZ	2:D:335:LEU:HD22	1.83	0.93
1:C:4:PRO:HB2	2:D:330:THR:HG23	1.50	0.93
2:B:365:VAL:O	2:B:369:ARG:N	2.01	0.93
1:C:83:PHE:CZ	2:D:300:ILE:HD11	2.03	0.93
1:A:12:MET:CG	1:A:66:CYS:SG	2.57	0.93
1:C:143:ILE:HD12	2:D:283:LYS:HD2	1.52	0.92
1:A:157:HIS:CD2	1:A:167:LYS:HZ1	1.87	0.91
1:C:25:ARG:NH1	2:D:309:PHE:CG	2.39	0.91
1:A:151:LYS:HB3	1:A:154:LEU:HD11	1.51	0.91
2:D:274:LYS:HA	2:D:277:VAL:CG1	2.01	0.91
2:D:340:GLU:OE2	4:D:32:HOH:O	1.88	0.91
1:C:210:LEU:HD13	1:C:229:TYR:CE1	2.05	0.91
1:A:211:ILE:HG22	1:A:213:ILE:HD13	1.52	0.90
2:B:367:LEU:O	2:B:371:ARG:CB	2.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:HG21	1:C:228:LEU:CD2	2.01	0.90
1:A:100:LEU:CD2	1:A:184:ILE:HG21	2.02	0.90
2:B:367:LEU:HD11	2:D:367:LEU:HD23	1.51	0.90
2:B:366:GLU:HG2	2:B:370:TRP:HE3	0.83	0.89
1:A:215:GLN:HG2	1:A:224:LEU:HD12	1.54	0.89
1:C:83:PHE:CZ	2:D:300:ILE:CD1	2.55	0.89
1:C:110:PRO:HA	1:C:181:MET:CE	2.03	0.88
1:A:157:HIS:CG	1:A:167:LYS:NZ	2.41	0.88
1:A:181:MET:CE	1:A:184:ILE:HD13	2.04	0.88
2:B:271:GLU:CB	2:B:273:THR:HG22	2.04	0.88
2:D:269:LEU:HD23	2:D:274:LYS:CD	2.02	0.88
1:C:86:GLY:O	1:C:92:LYS:HE2	1.74	0.88
1:C:208:ILE:HG12	1:C:231:VAL:HG22	1.54	0.88
1:C:222:LYS:NZ	2:D:335:LEU:CD2	2.37	0.87
1:C:25:ARG:NH1	2:D:309:PHE:CD2	2.41	0.87
1:C:14:ARG:HD3	4:C:401:HOH:O	1.73	0.87
1:A:206:HIS:HD2	1:A:233:LEU:HD22	1.39	0.87
1:C:181:MET:SD	1:C:184:ILE:HD13	2.15	0.87
1:A:211:ILE:HG22	1:A:213:ILE:CD1	2.03	0.86
1:A:9:ILE:HG23	2:B:298:THR:HB	1.58	0.86
2:B:366:GLU:C	2:B:370:TRP:H	1.79	0.85
1:C:158:GLU:OE2	2:D:286:ARG:NH1	2.09	0.85
1:C:224:LEU:HD22	2:D:335:LEU:HB2	1.57	0.85
2:B:363:LEU:HD21	2:D:364:GLU:HG3	1.58	0.85
1:A:9:ILE:HD12	2:B:327:ILE:HB	1.58	0.85
1:C:191:ARG:NH2	1:C:202:SER:CB	2.37	0.84
1:A:146:LEU:HD13	1:A:187:GLY:O	1.77	0.84
1:A:199:ASN:O	1:A:203:SER:OG	1.94	0.84
1:A:157:HIS:CG	1:A:167:LYS:HZ2	1.94	0.84
2:B:366:GLU:CG	2:B:370:TRP:HE3	1.65	0.84
2:B:266:ILE:HD11	2:B:292:LEU:HD11	1.58	0.84
1:C:78:TYR:CZ	2:D:333:VAL:HG12	2.12	0.84
1:C:10:LYS:HB2	1:C:50:ASP:OD2	1.77	0.84
2:D:357:LYS:HA	2:D:360:ILE:HD12	1.57	0.84
1:C:30:ILE:HG13	1:C:31:PRO:CD	2.08	0.83
1:C:224:LEU:HD23	2:D:335:LEU:CD1	2.08	0.83
1:A:53:LEU:HD13	1:A:62:VAL:HG13	1.58	0.83
2:B:342:TRP:HZ3	2:D:346:TYR:CD2	1.97	0.82
1:A:109:ILE:HB	1:A:110:PRO:HD3	1.62	0.82
2:D:357:LYS:HA	2:D:360:ILE:HD13	1.59	0.82
1:A:195:VAL:HG21	1:A:198:MET:HE1	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:HIS:CD2	1:A:233:LEU:HD22	2.14	0.82
2:B:365:VAL:O	2:B:369:ARG:HB2	1.78	0.82
1:A:174:VAL:HG12	1:A:179:GLU:HB2	1.59	0.82
1:C:40:VAL:HG22	1:C:46:PRO:HA	1.62	0.81
1:A:16:ARG:NH1	2:B:305:SER:HB2	1.94	0.81
2:B:364:GLU:CD	2:D:363:LEU:HD21	1.99	0.81
2:B:366:GLU:CG	2:B:370:TRP:CD2	2.63	0.81
1:C:222:LYS:HG3	2:D:335:LEU:HD11	1.62	0.81
1:C:18:LEU:HD23	1:C:22:GLU:CB	2.11	0.81
1:A:87:GLN:HE22	2:B:310:ASN:HB3	1.45	0.81
1:A:8:SER:HA	2:B:328:LYS:HD3	1.61	0.81
1:C:164:PRO:HG2	2:D:286:ARG:O	1.81	0.81
2:B:266:ILE:HG13	2:B:320:PHE:CE1	2.15	0.81
1:C:222:LYS:HZ1	2:D:335:LEU:CD2	1.93	0.80
1:C:41:ILE:HD11	2:D:318:LEU:HD11	1.63	0.80
2:B:367:LEU:CD1	2:D:367:LEU:HD23	2.11	0.80
2:B:365:VAL:O	2:B:369:ARG:CB	2.30	0.79
1:C:110:PRO:HA	1:C:181:MET:HE2	1.63	0.79
1:A:139:TYR:CZ	1:A:140:LEU:HD21	2.18	0.79
1:A:2:ALA:N	2:D:350:LYS:HE2	1.96	0.79
1:C:28:LYS:HG2	2:D:308:VAL:HG11	1.64	0.79
2:B:371:ARG:O	2:B:372:ASN:CG	2.21	0.79
1:C:19:ASN:OD1	1:C:22:GLU:HB2	1.83	0.79
2:B:271:GLU:CB	2:B:273:THR:CG2	2.61	0.79
1:C:151:LYS:HB3	1:C:154:LEU:CD2	2.12	0.78
1:A:157:HIS:CD2	1:A:167:LYS:NZ	2.50	0.78
1:A:61:GLN:C	4:A:406:HOH:O	2.21	0.78
1:A:2:ALA:CA	2:D:350:LYS:HE2	2.13	0.78
2:B:343:LYS:CG	2:D:342:TRP:CZ2	2.65	0.78
1:C:224:LEU:CD2	2:D:335:LEU:CB	2.61	0.78
1:A:147:LEU:HD11	1:A:183:VAL:HG13	1.63	0.78
2:B:371:ARG:O	2:B:372:ASN:HB2	1.84	0.77
1:C:70:ILE:HG13	1:C:82:ILE:HD11	1.65	0.77
1:A:89:SER:HA	3:A:401:ADP:O2A	1.83	0.77
2:B:369:ARG:C	2:B:372:ASN:ND2	2.37	0.77
1:C:28:LYS:HG2	2:D:308:VAL:CG1	2.14	0.77
1:C:2:ALA:CB	1:C:2:ALA:C	2.53	0.77
1:A:77:GLY:O	2:B:334:ASN:ND2	2.17	0.77
1:C:140:LEU:O	1:C:142:LYS:HG2	1.83	0.77
1:A:204:ARG:O	4:A:407:HOH:O	2.02	0.77
1:A:38:THR:OG1	1:A:48:VAL:HG22	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:ASN:ND2	4:B:7:HOH:O	2.18	0.76
1:A:195:VAL:CG1	1:A:198:MET:HE1	2.13	0.76
1:A:200:GLU:CG	1:A:204:ARG:NH1	2.48	0.76
2:D:356:LEU:C	2:D:360:ILE:HD12	2.06	0.76
2:D:275:THR:CG2	2:D:276:HIS:HD2	1.97	0.76
1:A:2:ALA:C	2:D:350:LYS:HE2	2.05	0.76
2:B:371:ARG:O	2:B:372:ASN:CB	2.32	0.76
2:D:275:THR:HG22	2:D:276:HIS:HD2	1.47	0.76
1:C:159:ASP:OD2	1:C:163:VAL:HG23	1.86	0.76
2:D:315:LYS:HA	2:D:318:LEU:HD12	1.67	0.76
1:A:59:GLN:HB3	1:A:111:ARG:HH12	1.47	0.76
1:C:120:ILE:CA	1:C:123:MET:HG3	2.14	0.76
2:B:259:LEU:HG	4:B:31:HOH:O	1.81	0.75
1:C:211:ILE:CD1	1:C:230:LEU:HD11	2.17	0.75
2:B:369:ARG:NH2	2:B:372:ASN:OD1	2.16	0.75
1:A:181:MET:HE1	1:A:184:ILE:HD13	1.68	0.75
2:D:369:ARG:HG2	2:D:370:TRP:CD1	2.21	0.75
2:D:324:ALA:HA	2:D:327:ILE:HD13	1.69	0.75
2:D:275:THR:HG22	2:D:276:HIS:CD2	2.22	0.75
1:C:4:PRO:HB2	2:D:330:THR:CG2	2.16	0.75
1:A:94:HIS:CB	3:A:401:ADP:H3'	2.17	0.74
2:D:269:LEU:CD2	2:D:274:LYS:HD3	2.17	0.74
1:C:117:PHE:O	1:C:121:TYR:CE2	2.40	0.74
1:A:112:ILE:O	1:A:116:ILE:HG13	1.87	0.74
1:A:206:HIS:CD2	1:A:233:LEU:CD2	2.67	0.74
1:A:79:ASN:ND2	1:A:227:LYS:N	2.36	0.74
1:A:8:SER:HG	2:B:328:LYS:HZ2	1.32	0.74
2:D:356:LEU:O	2:D:360:ILE:CD1	2.33	0.74
1:C:18:LEU:HD23	1:C:22:GLU:HB3	1.69	0.74
1:C:18:LEU:CD2	1:C:22:GLU:CB	2.66	0.73
2:D:357:LYS:CA	2:D:360:ILE:HD12	2.17	0.73
2:D:294:GLY:O	2:D:329:ASN:HB3	1.89	0.73
2:D:280:ARG:HG3	2:D:286:ARG:HD3	1.70	0.73
1:C:151:LYS:CB	1:C:154:LEU:HD21	2.18	0.73
1:A:104:GLN:HG2	1:A:105:LEU:HG	1.70	0.73
1:A:206:HIS:HD2	1:A:233:LEU:HD23	1.52	0.73
1:A:96:MET:O	1:A:109:ILE:HG12	1.88	0.73
1:C:159:ASP:OD1	1:C:163:VAL:HG23	1.87	0.73
1:C:37:GLU:OE1	1:C:50:ASP:O	2.07	0.72
1:C:159:ASP:CG	1:C:163:VAL:HG23	2.09	0.72
2:B:342:TRP:CZ2	2:D:343:LYS:HG3	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:GLU:OE1	2:B:273:THR:HG21	1.90	0.72
2:B:366:GLU:CG	2:B:370:TRP:HB2	2.20	0.72
2:D:269:LEU:CD2	2:D:274:LYS:CD	2.67	0.72
2:B:342:TRP:CZ3	2:B:345:LYS:HD3	2.25	0.72
1:A:134:SER:OG	4:A:416:HOH:O	2.07	0.72
1:A:60:GLU:O	4:A:406:HOH:O	2.07	0.72
2:B:345:LYS:NZ	2:D:346:TYR:CE2	2.38	0.72
1:A:147:LEU:HD11	1:A:183:VAL:CG1	2.19	0.72
1:A:215:GLN:CG	1:A:224:LEU:HD12	2.20	0.71
1:C:143:ILE:CD1	2:D:283:LYS:HD2	2.20	0.71
1:C:119:HIS:O	1:C:123:MET:HG2	1.90	0.71
1:C:50:ASP:OD1	2:D:325:LYS:HD2	1.91	0.71
1:C:95:THR:OG1	4:C:401:HOH:O	2.08	0.71
1:A:96:MET:CE	1:A:231:VAL:C	2.58	0.71
2:B:366:GLU:HG3	2:B:370:TRP:HB2	1.74	0.70
2:D:311:GLU:OE1	4:D:87:HOH:O	2.08	0.70
1:C:228:LEU:HA	4:C:404:HOH:O	1.92	0.70
1:C:222:LYS:HZ2	2:D:335:LEU:HD21	1.56	0.70
2:B:342:TRP:HZ3	2:D:346:TYR:HD2	1.38	0.70
1:C:200:GLU:O	1:C:203:SER:HB2	1.91	0.70
2:B:261:ALA:HB1	2:B:285:THR:HG21	1.73	0.70
1:A:34:LYS:HD2	1:A:38:THR:HG21	1.72	0.70
2:B:269:LEU:HD22	2:B:274:LYS:HE2	1.72	0.70
1:C:19:ASN:OD1	1:C:22:GLU:CB	2.40	0.70
2:B:342:TRP:CZ3	2:D:346:TYR:HD2	2.08	0.69
1:C:51:ARG:HG2	1:C:53:LEU:HD21	1.73	0.69
2:D:279:TYR:CD2	2:D:289:GLN:HG3	2.27	0.69
1:C:30:ILE:HG21	2:D:308:VAL:HG23	1.74	0.69
1:C:18:LEU:HD22	1:C:22:GLU:HB3	1.73	0.69
1:A:200:GLU:HG3	1:A:204:ARG:NH1	2.08	0.69
1:C:224:LEU:CD2	2:D:335:LEU:CD1	2.67	0.69
2:B:271:GLU:HB2	2:B:273:THR:CG2	2.22	0.69
4:A:403:HOH:O	2:B:258:SER:OG	2.10	0.69
2:B:369:ARG:HA	2:B:369:ARG:NE	2.09	0.68
1:C:110:PRO:HA	1:C:181:MET:HE1	1.75	0.68
2:B:258:SER:O	2:B:262:LEU:N	2.18	0.68
2:B:342:TRP:CE3	2:B:345:LYS:HD3	2.29	0.68
1:C:190:ASN:O	1:C:192:HIS:N	2.26	0.68
1:A:202:SER:O	1:A:204:ARG:N	2.27	0.68
1:C:154:LEU:O	4:C:405:HOH:O	2.11	0.68
1:A:28:LYS:HE2	2:B:308:VAL:CG1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLU:HA	1:C:23:ILE:HG13	1.75	0.68
1:A:198:MET:SD	1:A:201:HIS:ND1	2.64	0.68
1:C:216:GLU:HG3	1:C:223:LYS:CD	2.24	0.67
1:A:52:VAL:O	1:A:54:PRO:HD3	1.94	0.67
1:A:94:HIS:HB2	3:A:401:ADP:H3'	1.76	0.67
1:A:195:VAL:CG2	1:A:198:MET:HE1	2.25	0.67
1:C:123:MET:HE2	1:C:129:PHE:HZ	1.59	0.67
1:C:147:LEU:HD21	1:C:183:VAL:HG12	1.77	0.67
1:C:110:PRO:CA	1:C:181:MET:CE	2.71	0.67
1:C:143:ILE:HD11	2:D:283:LYS:HB3	1.77	0.67
1:C:30:ILE:HG23	2:D:308:VAL:HB	1.75	0.67
1:A:148:ASP:HB3	1:A:151:LYS:HD3	1.76	0.67
1:C:208:ILE:HG23	1:C:231:VAL:HG22	1.77	0.67
1:C:25:ARG:HD2	2:D:309:PHE:CZ	2.30	0.66
1:A:81:THR:OG1	2:B:291:SER:OG	2.12	0.66
2:B:369:ARG:HA	2:B:372:ASN:ND2	2.10	0.66
1:C:126:ASN:CG	1:C:219:GLU:HB2	2.16	0.66
1:C:222:LYS:CG	2:D:335:LEU:HD11	2.25	0.66
1:C:224:LEU:HD21	2:D:335:LEU:HD22	1.77	0.66
1:A:233:LEU:HD21	2:B:284:MET:HE1	1.78	0.66
1:A:91:GLY:CA	3:A:401:ADP:O1A	2.43	0.66
1:C:6:GLU:O	1:C:7:CYS:HB3	1.96	0.66
2:D:337:LEU:CD1	2:D:341:GLU:OE2	2.39	0.66
1:C:159:ASP:OD1	1:C:163:VAL:N	2.28	0.66
1:C:56:ASN:H	1:C:56:ASN:HD22	1.44	0.66
1:A:62:VAL:O	1:A:66:CYS:HB2	1.95	0.66
2:B:367:LEU:HD11	2:D:367:LEU:CD2	2.25	0.66
1:C:237:GLU:HA	2:D:313:GLU:OE1	1.95	0.66
1:C:110:PRO:CA	1:C:181:MET:HE1	2.26	0.66
1:A:63:TYR:OH	1:A:115:ASP:OD2	2.09	0.66
1:A:233:LEU:CD2	2:B:284:MET:CE	2.73	0.66
1:C:210:LEU:HD13	1:C:229:TYR:CZ	2.31	0.66
2:B:369:ARG:HH21	2:B:372:ASN:ND2	1.92	0.65
1:A:195:VAL:CG1	1:A:198:MET:CE	2.72	0.65
1:C:224:LEU:HD21	2:D:335:LEU:HB2	1.77	0.65
1:A:200:GLU:CD	1:A:204:ARG:NH1	2.49	0.65
1:A:195:VAL:CB	1:A:198:MET:HE1	2.27	0.65
1:A:133:VAL:HG11	1:A:180:VAL:CG1	2.27	0.65
1:C:5:ALA:O	2:D:331:VAL:HG22	1.96	0.65
2:B:257:LYS:HA	2:B:260:SER:HB2	1.79	0.64
2:D:348:LYS:HA	2:D:351:GLU:CG	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:GLU:HB3	2:B:273:THR:CG2	2.23	0.64
1:C:117:PHE:O	1:C:121:TYR:HD2	1.73	0.64
1:A:27:ASP:OD1	2:B:309:PHE:HE2	1.80	0.64
1:C:236:SER:HA	2:D:259:LEU:CD2	2.26	0.64
1:C:217:ASN:ND2	1:C:220:THR:HG23	2.13	0.64
1:C:205:SER:O	1:C:234:ALA:HB2	1.97	0.64
1:A:94:HIS:HB3	3:A:401:ADP:H3'	1.80	0.64
2:B:319:MET:CE	2:B:322:GLN:HG3	2.27	0.64
1:C:222:LYS:HE3	1:C:224:LEU:HD21	1.77	0.64
1:C:11:VAL:O	1:C:49:PHE:HB3	1.98	0.64
1:A:222:LYS:HE3	1:A:224:LEU:HD21	1.80	0.63
1:C:83:PHE:CE1	2:D:300:ILE:HG12	2.34	0.63
2:D:275:THR:CG2	2:D:276:HIS:CD2	2.81	0.63
2:D:348:LYS:HD2	2:D:351:GLU:OE1	1.98	0.63
1:A:30:ILE:N	1:A:31:PRO:HD2	2.13	0.63
1:A:96:MET:HE3	1:A:231:VAL:C	2.19	0.63
1:C:224:LEU:HD21	2:D:335:LEU:HD13	1.79	0.63
2:D:337:LEU:HA	2:D:341:GLU:OE2	1.98	0.63
1:C:14:ARG:CD	4:C:401:HOH:O	2.37	0.63
1:A:126:ASN:OD1	1:A:219:GLU:HB2	1.99	0.62
1:A:157:HIS:NE2	1:A:167:LYS:NZ	2.30	0.62
2:D:269:LEU:HD13	2:D:292:LEU:O	1.99	0.62
1:C:16:ARG:O	2:D:306:PRO:HD3	1.99	0.62
1:A:63:TYR:CD1	1:A:67:ALA:HB3	2.34	0.62
2:B:367:LEU:O	2:B:372:ASN:N	2.32	0.62
1:A:100:LEU:CD2	1:A:184:ILE:CG2	2.77	0.62
2:B:266:ILE:HG23	2:B:327:ILE:HD11	1.80	0.62
1:A:100:LEU:HD23	1:A:181:MET:HE2	1.82	0.62
1:C:109:ILE:HB	1:C:110:PRO:HD3	1.81	0.62
1:C:71:VAL:HG12	1:C:75:LEU:HD11	1.80	0.62
2:D:269:LEU:HD22	2:D:274:LYS:CE	2.26	0.62
1:C:141:ASP:O	2:D:283:LYS:NZ	2.22	0.62
2:B:343:LYS:CG	2:D:342:TRP:CE2	2.73	0.61
1:A:29:PHE:CE2	1:A:31:PRO:HG2	2.35	0.61
1:A:7:CYS:SG	2:B:331:VAL:HG13	2.39	0.61
1:C:80:GLY:N	4:C:404:HOH:O	2.28	0.61
1:C:22:GLU:OE2	2:D:307:SER:HB3	2.00	0.61
2:B:258:SER:O	2:B:261:ALA:HB3	2.00	0.61
1:C:201:HIS:O	1:C:205:SER:OG	2.16	0.61
1:A:87:GLN:O	1:A:90:SER:HB3	2.00	0.61
1:C:71:VAL:O	1:C:75:LEU:HD12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:ASN:CB	2:D:353:ASN:HD21	2.13	0.61
1:C:217:ASN:OD1	1:C:219:GLU:HB3	2.00	0.61
2:B:337:LEU:HD12	2:B:342:TRP:CE2	2.36	0.61
1:C:216:GLU:CB	1:C:223:LYS:HG3	2.29	0.61
1:A:94:HIS:HD2	4:A:423:HOH:O	1.84	0.61
2:B:298:THR:HG22	2:B:300:ILE:CD1	2.31	0.61
1:C:117:PHE:C	1:C:121:TYR:CE2	2.74	0.61
1:C:222:LYS:HE3	1:C:224:LEU:CD2	2.30	0.61
2:B:369:ARG:HE	2:B:372:ASN:ND2	1.98	0.60
2:D:338:THR:O	2:D:341:GLU:HB3	2.00	0.60
1:C:16:ARG:NH2	1:C:22:GLU:OE1	2.33	0.60
1:A:16:ARG:NH2	1:A:22:GLU:OE2	2.33	0.60
1:A:139:TYR:CE2	1:A:140:LEU:HD11	2.37	0.60
1:C:85:TYR:HB3	2:D:302:ILE:HG22	1.83	0.60
2:B:297:ARG:NH2	2:B:331:VAL:HG21	2.16	0.60
1:A:100:LEU:HD21	1:A:184:ILE:CG2	2.26	0.60
2:D:284:MET:HB2	4:D:56:HOH:O	2.01	0.60
1:A:28:LYS:HE2	2:B:308:VAL:HG13	1.84	0.60
1:C:114:HIS:O	1:C:118:ASP:HB2	2.02	0.60
2:B:266:ILE:HD13	2:B:292:LEU:HD12	1.78	0.60
1:C:180:VAL:O	1:C:184:ILE:CD1	2.40	0.60
1:A:91:GLY:HA2	3:A:401:ADP:O1A	2.01	0.60
2:D:348:LYS:HA	2:D:351:GLU:HG3	1.84	0.60
1:C:197:ASN:CB	4:C:408:HOH:O	2.49	0.59
1:C:217:ASN:OD1	1:C:219:GLU:N	2.35	0.59
2:B:337:LEU:HD12	2:B:342:TRP:CZ2	2.35	0.59
1:C:28:LYS:CG	2:D:308:VAL:HG11	2.31	0.59
1:A:30:ILE:HG21	2:B:308:VAL:HG12	1.82	0.59
1:A:94:HIS:ND1	3:A:401:ADP:H2'	2.18	0.59
2:B:366:GLU:C	2:B:370:TRP:HB2	2.23	0.59
2:D:262:LEU:O	2:D:266:ILE:HG12	2.01	0.59
1:A:78:TYR:CZ	2:B:333:VAL:HG12	2.37	0.59
1:A:176:SER:OG	1:A:179:GLU:HG3	2.02	0.59
2:B:369:ARG:NH2	2:B:372:ASN:ND2	2.49	0.59
1:C:12:MET:HG3	1:C:51:ARG:HB3	1.85	0.59
1:C:53:LEU:HB3	1:C:57:THR:HG21	1.83	0.59
1:C:208:ILE:HG12	1:C:231:VAL:CG2	2.29	0.59
1:A:99:LYS:HE3	1:A:105:LEU:CD1	2.32	0.59
2:D:269:LEU:HB3	2:D:327:ILE:HG13	1.85	0.59
1:C:40:VAL:HG22	1:C:46:PRO:CA	2.32	0.59
1:C:99:LYS:HB2	1:C:105:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ARG:CA	2:B:372:ASN:ND2	2.65	0.59
1:C:190:ASN:C	1:C:192:HIS:H	2.06	0.59
1:C:87:GLN:O	1:C:90:SER:HB3	2.02	0.59
1:A:140:LEU:O	1:A:142:LYS:HG2	2.01	0.58
2:B:366:GLU:HG2	2:B:370:TRP:CD2	2.27	0.58
1:C:141:ASP:OD1	2:D:257:LYS:HD3	2.02	0.58
1:A:147:LEU:HD23	1:A:186:GLU:HG2	1.85	0.58
1:C:56:ASN:ND2	1:C:56:ASN:H	2.01	0.58
1:A:12:MET:CE	2:B:299:THR:HG23	2.33	0.58
1:C:108:ILE:HG22	1:C:112:ILE:HD12	1.85	0.58
1:A:131:ILE:HG23	1:A:213:ILE:HD11	1.83	0.58
1:C:28:LYS:NZ	2:D:308:VAL:HG11	2.18	0.58
1:C:20:GLU:O	1:C:23:ILE:CB	2.49	0.58
1:C:14:ARG:NE	4:C:401:HOH:O	2.35	0.58
1:A:100:LEU:HD23	1:A:181:MET:CE	2.33	0.58
2:D:264:ASN:ND2	4:D:76:HOH:O	2.36	0.58
1:A:212:ASN:ND2	1:A:227:LYS:HE2	2.19	0.58
1:C:211:ILE:HD12	1:C:230:LEU:HD11	1.85	0.58
1:C:190:ASN:O	1:C:193:VAL:N	2.33	0.58
2:B:269:LEU:HD22	2:B:274:LYS:CE	2.33	0.58
1:C:137:GLU:HA	1:C:206:HIS:O	2.03	0.58
1:C:47:TYR:CD2	2:D:318:LEU:HB3	2.39	0.58
1:A:88:THR:O	1:A:89:SER:HB2	2.03	0.58
2:D:286:ARG:O	2:D:289:GLN:HB2	2.04	0.58
1:C:181:MET:HA	1:C:184:ILE:HD13	1.86	0.58
1:A:166:VAL:CG2	2:B:287:ILE:HD11	2.33	0.58
1:C:131:ILE:HG13	1:C:213:ILE:HG23	1.86	0.58
2:D:257:LYS:O	2:D:260:SER:HB2	2.04	0.57
1:C:19:ASN:C	1:C:23:ILE:HG12	2.24	0.57
2:B:271:GLU:HB2	2:B:273:THR:HG23	1.85	0.57
1:C:202:SER:HA	1:C:205:SER:OG	2.04	0.57
1:A:179:GLU:O	1:A:183:VAL:HG23	2.04	0.57
1:C:41:ILE:HD11	2:D:318:LEU:CD1	2.32	0.57
2:D:311:GLU:O	2:D:314:THR:OG1	2.22	0.57
1:C:137:GLU:OE2	1:C:144:ARG:CZ	2.52	0.57
2:B:351:GLU:O	2:B:354:LYS:CG	2.48	0.57
2:B:273:THR:O	2:B:275:THR:N	2.38	0.57
2:D:355:ALA:O	2:D:359:VAL:CG2	2.47	0.57
1:C:86:GLY:O	1:C:92:LYS:CE	2.51	0.57
2:B:348:LYS:C	2:B:350:LYS:H	2.07	0.57
2:B:366:GLU:O	2:B:370:TRP:CA	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:CG	1:A:151:LYS:HD2	2.25	0.56
1:A:81:THR:HG21	2:B:291:SER:OG	2.05	0.56
2:B:366:GLU:HG3	2:B:370:TRP:CB	2.35	0.56
2:B:266:ILE:HG13	2:B:320:PHE:CZ	2.40	0.56
1:C:212:ASN:ND2	1:C:227:LYS:HD2	2.19	0.56
1:A:174:VAL:HG12	1:A:179:GLU:CB	2.33	0.56
1:C:134:SER:OG	1:C:170:THR:O	2.11	0.56
1:A:13:CYS:SG	1:A:15:PHE:CE2	2.99	0.56
1:A:157:HIS:CE1	1:A:167:LYS:HZ3	2.16	0.56
2:B:337:LEU:HB3	2:B:341:GLU:HB2	1.86	0.56
2:B:353:ASN:HB2	2:D:353:ASN:HD21	1.70	0.56
2:B:261:ALA:HB1	2:B:285:THR:CG2	2.36	0.56
1:C:110:PRO:CB	1:C:181:MET:CE	2.84	0.56
1:A:74:VAL:HA	1:A:78:TYR:O	2.06	0.56
2:D:359:VAL:O	2:D:363:LEU:HB2	2.05	0.55
2:D:265:VAL:CG1	2:D:279:TYR:HE1	2.19	0.55
2:D:267:SER:O	2:D:270:ALA:HB3	2.06	0.55
2:B:299:THR:O	2:B:300:ILE:HD12	2.05	0.55
1:C:190:ASN:C	1:C:192:HIS:N	2.59	0.55
2:B:362:HIS:O	2:B:365:VAL:HG12	2.06	0.55
1:C:110:PRO:HB3	1:C:181:MET:HE2	1.88	0.55
1:C:51:ARG:HG3	1:C:52:VAL:N	2.20	0.55
2:B:365:VAL:CG1	2:B:366:GLU:N	2.70	0.55
2:D:266:ILE:CD1	2:D:292:LEU:HD22	2.37	0.55
1:C:25:ARG:HD2	2:D:309:PHE:CE1	2.41	0.55
2:B:269:LEU:CD2	2:B:274:LYS:HE2	2.37	0.55
2:D:273:THR:O	2:D:274:LYS:C	2.45	0.55
1:A:231:VAL:HG21	2:B:288:LEU:HD21	1.87	0.55
1:C:78:TYR:CE2	2:D:297:ARG:NH2	2.74	0.55
1:C:71:VAL:HG12	1:C:75:LEU:CD1	2.37	0.55
2:B:358:SER:O	2:B:362:HIS:N	2.40	0.55
2:B:369:ARG:NE	2:B:372:ASN:ND2	2.55	0.55
1:C:189:ALA:O	1:C:192:HIS:ND1	2.36	0.55
1:C:25:ARG:NE	1:C:27:ASP:OD1	2.40	0.54
2:B:353:ASN:HD22	2:D:353:ASN:ND2	2.05	0.54
2:B:324:ALA:HA	2:B:327:ILE:HD12	1.89	0.54
1:A:109:ILE:HB	1:A:110:PRO:CD	2.35	0.54
2:B:275:THR:HG23	2:B:276:HIS:CE1	2.42	0.54
1:C:107:GLY:O	1:C:110:PRO:HD2	2.07	0.54
2:D:310:ASN:HA	4:D:67:HOH:O	2.08	0.54
1:C:15:PHE:CD1	1:C:33:PHE:HE1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:O	1:C:123:MET:HB2	2.08	0.54
1:A:212:ASN:ND2	1:A:227:LYS:CE	2.71	0.54
1:A:99:LYS:HE3	1:A:105:LEU:HD12	1.89	0.54
1:C:217:ASN:HD21	1:C:220:THR:HG23	1.72	0.54
2:D:269:LEU:HD22	2:D:274:LYS:HE2	1.73	0.54
1:C:135:TYR:O	1:C:146:LEU:HB2	2.08	0.54
1:C:110:PRO:CA	1:C:181:MET:HE2	2.33	0.54
1:C:75:LEU:O	1:C:215:GLN:NE2	2.41	0.54
1:A:8:SER:CA	2:B:328:LYS:HD3	2.33	0.54
1:C:137:GLU:HG2	1:C:146:LEU:HD21	1.89	0.54
2:D:278:PRO:O	2:D:281:ASP:HB2	2.08	0.54
1:C:40:VAL:CG2	1:C:46:PRO:HA	2.36	0.54
2:D:266:ILE:HD11	2:D:292:LEU:HD22	1.88	0.54
1:A:62:VAL:N	4:A:406:HOH:O	2.02	0.54
2:B:356:LEU:O	2:B:359:VAL:HG22	2.07	0.54
1:A:181:MET:HE1	1:A:184:ILE:CD1	2.25	0.53
1:C:78:TYR:CE1	2:D:333:VAL:HG12	2.43	0.53
1:A:131:ILE:HG23	1:A:213:ILE:CD1	2.37	0.53
1:C:126:ASN:O	1:C:218:VAL:HG13	2.08	0.53
1:C:216:GLU:HG3	1:C:223:LYS:HD2	1.89	0.53
1:A:88:THR:OG1	1:A:237:GLU:OE2	2.23	0.53
1:A:139:TYR:CE1	1:A:140:LEU:HD21	2.43	0.53
1:C:211:ILE:HD11	1:C:230:LEU:HD11	1.90	0.53
1:C:115:ASP:HA	1:C:118:ASP:HB3	1.90	0.53
2:B:342:TRP:CZ3	2:D:346:TYR:CD2	2.83	0.53
1:C:126:ASN:OD1	1:C:219:GLU:HB2	2.09	0.53
2:D:264:ASN:ND2	2:D:281:ASP:OD2	2.39	0.53
2:D:287:ILE:C	2:D:289:GLN:H	2.12	0.53
2:B:295:ASN:O	2:B:296:CYS:HB2	2.09	0.53
2:B:366:GLU:HG3	2:B:370:TRP:CG	2.43	0.53
1:C:99:LYS:O	1:C:106:MET:HA	2.08	0.53
1:A:137:GLU:OE1	1:A:191:ARG:HD2	2.09	0.53
1:A:13:CYS:HB3	1:A:52:VAL:HG22	1.91	0.52
2:B:319:MET:HE2	2:B:322:GLN:HG3	1.91	0.52
2:B:372:ASN:O	2:B:372:ASN:C	2.48	0.52
1:A:106:MET:O	1:A:111:ARG:NH1	2.43	0.52
1:C:217:ASN:OD1	1:C:219:GLU:CB	2.58	0.52
1:A:94:HIS:HB3	3:A:401:ADP:C3'	2.39	0.52
1:A:131:ILE:HG13	1:A:213:ILE:HG13	1.91	0.52
2:D:348:LYS:O	2:D:352:LYS:HG3	2.09	0.52
2:B:366:GLU:HG3	2:B:370:TRP:CD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:LEU:CD1	2:D:367:LEU:CD2	2.86	0.52
1:C:237:GLU:HA	2:D:313:GLU:CD	2.30	0.52
4:A:403:HOH:O	2:B:258:SER:CB	2.58	0.52
1:C:32:LYS:HA	1:C:32:LYS:NZ	2.23	0.52
1:A:202:SER:C	1:A:204:ARG:N	2.64	0.52
2:B:268:ALA:O	2:B:273:THR:HG23	2.09	0.52
1:A:9:ILE:HG23	2:B:298:THR:O	2.10	0.52
2:D:337:LEU:HD12	2:D:341:GLU:HG2	1.91	0.52
1:C:193:VAL:O	1:C:194:ALA:HB3	2.10	0.52
1:A:214:LYS:HE3	2:B:336:GLU:OE1	2.10	0.52
1:A:13:CYS:O	1:A:53:LEU:N	2.43	0.52
1:C:74:VAL:HA	1:C:78:TYR:O	2.09	0.52
1:C:14:ARG:HD2	1:C:62:VAL:HG21	1.91	0.52
1:C:13:CYS:SG	1:C:15:PHE:CE1	3.03	0.52
1:A:189:ALA:O	1:A:191:ARG:N	2.43	0.52
1:A:8:SER:HG	2:B:328:LYS:NZ	1.99	0.52
1:A:14:ARG:HH22	1:A:59:GLN:NE2	2.08	0.51
1:C:208:ILE:CG1	1:C:231:VAL:HG22	2.34	0.51
1:C:101:HIS:O	1:C:103:PRO:HD3	2.10	0.51
1:A:4:PRO:HB3	2:B:332:SER:HB2	1.92	0.51
2:B:274:LYS:HA	2:B:277:VAL:HG22	1.93	0.51
1:C:138:ILE:CG2	4:D:56:HOH:O	2.40	0.51
1:A:16:ARG:HG3	3:A:401:ADP:O4'	2.10	0.51
1:A:59:GLN:HE21	1:A:59:GLN:HA	1.74	0.51
1:C:110:PRO:HB3	1:C:181:MET:CE	2.41	0.51
1:A:139:TYR:CE1	1:A:140:LEU:CD2	2.93	0.51
1:C:143:ILE:HD11	2:D:283:LYS:CB	2.40	0.51
2:D:280:ARG:CG	2:D:286:ARG:HD3	2.38	0.51
2:D:264:ASN:HB3	2:D:278:PRO:HG2	1.91	0.51
1:C:119:HIS:O	1:C:123:MET:CG	2.58	0.51
2:B:271:GLU:OE1	2:B:273:THR:CG2	2.59	0.51
1:A:206:HIS:CD2	1:A:233:LEU:HD23	2.38	0.51
1:A:34:LYS:HD3	1:A:38:THR:HB	1.93	0.51
1:A:12:MET:HG3	1:A:53:LEU:HD11	1.93	0.51
2:B:343:LYS:CD	2:D:342:TRP:CZ2	2.93	0.51
1:C:18:LEU:HG	2:D:306:PRO:HG2	1.92	0.51
1:A:148:ASP:OD2	1:A:151:LYS:HD2	2.10	0.51
2:D:260:SER:O	2:D:263:GLY:N	2.44	0.51
1:A:206:HIS:CE1	2:B:258:SER:OG	2.64	0.51
1:A:120:ILE:CD1	1:A:131:ILE:HD11	2.40	0.51
1:A:70:ILE:CG2	1:A:80:GLY:HA3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:ARG:HH21	2:B:331:VAL:HG21	1.74	0.50
1:C:15:PHE:CD1	1:C:33:PHE:CE1	3.00	0.50
1:C:30:ILE:N	1:C:31:PRO:HD2	2.26	0.50
2:B:276:HIS:N	2:B:276:HIS:ND1	2.59	0.50
1:C:137:GLU:HG3	1:C:144:ARG:HB3	1.93	0.50
1:A:212:ASN:HD21	1:A:227:LYS:CE	2.24	0.50
1:C:202:SER:C	1:C:204:ARG:N	2.61	0.50
1:A:164:PRO:HB2	2:B:286:ARG:O	2.11	0.50
1:C:9:ILE:HD12	2:D:327:ILE:HB	1.94	0.50
1:A:9:ILE:CG2	2:B:298:THR:HB	2.35	0.50
2:B:342:TRP:HZ3	2:D:346:TYR:CE2	2.28	0.50
1:C:16:ARG:NH1	2:D:305:SER:HB2	2.27	0.50
1:C:222:LYS:HE3	1:C:224:LEU:CG	2.41	0.50
1:A:70:ILE:HG23	1:A:80:GLY:HA3	1.93	0.50
1:A:238:LYS:HD2	2:B:313:GLU:OE2	2.11	0.50
1:C:222:LYS:CG	2:D:335:LEU:CD1	2.90	0.50
2:B:274:LYS:HA	2:B:277:VAL:CG2	2.42	0.50
1:C:70:ILE:HG22	1:C:228:LEU:HD21	1.94	0.50
1:A:198:MET:SD	1:A:201:HIS:HB3	2.52	0.50
1:A:12:MET:HE2	2:B:299:THR:HG23	1.93	0.50
2:D:328:LYS:NZ	2:D:328:LYS:HB2	2.27	0.50
1:A:90:SER:C	3:A:401:ADP:O1A	2.51	0.49
1:A:71:VAL:HG13	1:A:116:ILE:HG12	1.94	0.49
1:C:222:LYS:HE3	1:C:224:LEU:HG	1.95	0.49
1:A:110:PRO:O	1:A:113:ALA:HB3	2.13	0.49
1:A:30:ILE:HG21	2:B:308:VAL:CG1	2.42	0.49
1:A:217:ASN:O	1:A:221:GLU:HA	2.13	0.49
1:C:83:PHE:CE1	2:D:300:ILE:CD1	2.95	0.49
2:D:339:ALA:C	2:D:341:GLU:H	2.16	0.49
1:C:127:LEU:HD12	1:C:129:PHE:CE1	2.47	0.49
1:A:235:GLY:O	2:B:259:LEU:HD21	2.13	0.49
1:C:140:LEU:O	1:C:142:LYS:N	2.45	0.49
1:A:211:ILE:HD12	1:A:228:LEU:HD23	1.95	0.49
1:C:125:GLU:HG2	1:C:125:GLU:O	2.13	0.49
1:A:138:ILE:HG12	1:A:143:ILE:HG12	1.93	0.49
1:C:110:PRO:CB	1:C:181:MET:HE2	2.43	0.49
2:D:257:LYS:HE3	2:D:281:ASP:O	2.13	0.49
1:C:116:ILE:O	1:C:120:ILE:HG13	2.12	0.49
2:B:366:GLU:O	2:B:367:LEU:C	2.51	0.49
1:C:224:LEU:HD21	2:D:335:LEU:CD2	2.43	0.49
1:C:19:ASN:OD1	1:C:22:GLU:CG	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HH12	2:B:305:SER:HB2	1.77	0.49
1:C:224:LEU:HD22	2:D:335:LEU:CB	2.36	0.48
2:D:268:ALA:O	2:D:273:THR:HG23	2.13	0.48
1:C:148:ASP:OD1	1:C:150:SER:CB	2.50	0.48
1:A:107:GLY:O	1:A:110:PRO:HD2	2.13	0.48
1:C:181:MET:HA	1:C:184:ILE:CD1	2.44	0.48
2:D:338:THR:N	2:D:341:GLU:HB3	2.28	0.48
1:C:51:ARG:HG3	1:C:52:VAL:H	1.78	0.48
1:C:224:LEU:HD21	2:D:335:LEU:CG	2.43	0.48
1:C:158:GLU:C	1:C:165:TYR:HE1	2.17	0.48
1:C:158:GLU:CA	1:C:165:TYR:HE1	2.26	0.48
1:A:101:HIS:HE1	1:A:185:ASP:OD1	1.97	0.48
2:D:360:ILE:O	2:D:364:GLU:N	2.46	0.48
1:C:9:ILE:HB	2:D:324:ALA:O	2.14	0.48
2:B:365:VAL:O	2:B:369:ARG:CA	2.61	0.48
2:D:342:TRP:O	2:D:345:LYS:HB2	2.14	0.48
2:B:337:LEU:HD22	2:B:341:GLU:HB3	1.96	0.48
2:B:350:LYS:HG3	2:D:349:GLU:OE2	2.13	0.48
2:B:342:TRP:CE2	2:D:343:LYS:HG3	2.48	0.48
2:B:282:SER:O	2:B:286:ARG:HG3	2.14	0.48
1:A:161:ASN:ND2	2:D:340:GLU:HG2	2.28	0.48
2:B:367:LEU:O	2:B:371:ARG:N	2.46	0.48
1:C:30:ILE:N	1:C:31:PRO:CD	2.77	0.48
1:A:81:THR:CB	2:B:291:SER:OG	2.62	0.48
1:C:224:LEU:CD2	2:D:335:LEU:CG	2.92	0.48
2:D:278:PRO:HB2	2:D:281:ASP:CG	2.34	0.48
1:C:133:VAL:HA	1:C:210:LEU:O	2.14	0.48
1:C:180:VAL:HG12	1:C:184:ILE:HD11	1.95	0.47
1:A:176:SER:HB2	1:A:177:PRO:HD2	1.95	0.47
1:A:225:SER:O	2:B:334:ASN:HB2	2.14	0.47
1:A:193:VAL:O	1:A:194:ALA:HB3	2.14	0.47
1:A:16:ARG:HG3	3:A:401:ADP:C1'	2.44	0.47
1:A:211:ILE:CG2	1:A:213:ILE:CD1	2.86	0.47
1:A:210:LEU:HD13	1:A:229:TYR:CE1	2.49	0.47
1:A:2:ALA:O	2:D:350:LYS:CE	2.49	0.47
2:B:261:ALA:CB	2:B:282:SER:HB3	2.45	0.47
1:C:211:ILE:HD11	1:C:230:LEU:CD1	2.43	0.47
1:A:25:ARG:HD2	2:B:309:PHE:CE2	2.49	0.47
1:C:108:ILE:CG2	1:C:112:ILE:CD1	2.92	0.47
2:B:337:LEU:HB2	2:B:342:TRP:NE1	2.29	0.47
2:D:282:SER:OG	2:D:285:THR:OG1	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:SER:C	1:A:204:ARG:H	2.17	0.47
1:A:58:THR:O	1:A:62:VAL:CG2	2.50	0.47
2:B:351:GLU:C	2:B:354:LYS:HG3	2.34	0.47
1:C:211:ILE:CD1	1:C:230:LEU:CD1	2.88	0.47
1:C:7:CYS:H	2:D:328:LYS:HG3	1.79	0.47
2:B:269:LEU:HB3	2:B:327:ILE:HG12	1.96	0.47
1:A:161:ASN:O	1:A:163:VAL:HG23	2.14	0.47
2:B:362:HIS:O	2:B:363:LEU:C	2.53	0.47
1:A:57:THR:HG22	1:A:61:GLN:HB2	1.97	0.47
1:A:200:GLU:CG	1:A:204:ARG:HH12	2.28	0.46
1:C:204:ARG:HA	1:C:204:ARG:HD3	1.77	0.46
2:D:264:ASN:HB3	2:D:278:PRO:CG	2.45	0.46
1:C:18:LEU:HD23	1:C:22:GLU:CD	2.35	0.46
1:C:10:LYS:HB2	1:C:50:ASP:CG	2.35	0.46
1:A:175:SER:N	1:A:179:GLU:OE1	2.47	0.46
2:D:265:VAL:HG13	2:D:279:TYR:HE1	1.80	0.46
1:A:8:SER:OG	2:B:328:LYS:CD	2.63	0.46
2:D:342:TRP:O	2:D:345:LYS:N	2.48	0.46
2:B:365:VAL:HG13	2:B:366:GLU:N	2.29	0.46
1:A:235:GLY:O	2:B:259:LEU:CD2	2.63	0.46
1:A:192:HIS:O	1:A:193:VAL:C	2.54	0.46
1:A:148:ASP:CG	1:A:151:LYS:CD	2.84	0.46
1:C:208:ILE:HG12	1:C:231:VAL:HG13	1.98	0.46
1:C:208:ILE:HG23	1:C:231:VAL:CG2	2.46	0.46
1:A:139:TYR:CD1	1:A:140:LEU:HG	2.49	0.46
1:A:139:TYR:CZ	1:A:140:LEU:CD2	2.96	0.46
1:C:221:GLU:O	1:C:222:LYS:C	2.53	0.46
1:A:83:PHE:CE1	2:B:300:ILE:HG13	2.51	0.46
2:B:345:LYS:CE	2:D:346:TYR:CE2	2.99	0.46
1:C:16:ARG:NH2	1:C:22:GLU:CD	2.69	0.46
1:C:202:SER:C	1:C:204:ARG:H	2.19	0.46
1:A:27:ASP:OD1	2:B:309:PHE:CE2	2.66	0.46
1:A:181:MET:SD	1:A:184:ILE:HD12	2.56	0.46
1:C:87:GLN:HE22	2:D:310:ASN:HB3	1.81	0.46
2:B:266:ILE:O	2:B:269:LEU:N	2.47	0.46
1:C:12:MET:CE	1:C:65:ALA:O	2.64	0.46
2:D:275:THR:HG23	2:D:276:HIS:HD2	1.79	0.46
1:C:106:MET:HE3	1:C:111:ARG:HA	1.97	0.46
1:C:191:ARG:NH2	1:C:202:SER:OG	2.49	0.45
1:C:202:SER:O	1:C:204:ARG:N	2.49	0.45
1:A:206:HIS:HE1	2:B:258:SER:OG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PHE:CZ	2:D:300:ILE:HD13	2.45	0.45
1:A:215:GLN:CG	4:A:417:HOH:O	2.28	0.45
1:C:208:ILE:CG2	1:C:231:VAL:HG22	2.46	0.45
2:B:257:LYS:CA	2:B:260:SER:HB2	2.46	0.45
2:D:360:ILE:O	2:D:361:GLN:C	2.54	0.45
1:C:144:ARG:NH2	1:C:191:ARG:HA	2.31	0.45
1:C:47:TYR:OH	2:D:315:LYS:HG3	2.16	0.45
1:A:233:LEU:HD21	2:B:284:MET:CE	2.44	0.45
3:A:401:ADP:H4'	3:A:401:ADP:O1A	2.17	0.45
2:D:295:ASN:HD21	2:D:332:SER:H	1.64	0.45
2:D:314:THR:OG1	2:D:315:LYS:N	2.48	0.45
1:A:67:ALA:HB2	1:A:82:ILE:CD1	2.47	0.45
1:A:12:MET:HG3	1:A:66:CYS:SG	2.48	0.45
1:A:15:PHE:CE2	1:A:39:VAL:HG21	2.52	0.45
1:A:30:ILE:CG2	2:B:308:VAL:CG1	2.94	0.45
1:A:81:THR:CB	2:B:291:SER:HG	2.30	0.45
1:A:144:ARG:NH2	1:A:191:ARG:O	2.49	0.45
1:C:191:ARG:O	1:C:198:MET:HE1	2.17	0.45
1:C:115:ASP:O	1:C:118:ASP:HB3	2.17	0.45
1:C:16:ARG:NH2	1:C:22:GLU:OE2	2.50	0.45
1:A:135:TYR:O	1:A:146:LEU:HB2	2.17	0.45
1:C:19:ASN:OD1	1:C:22:GLU:N	2.43	0.45
1:C:22:GLU:CG	1:C:27:ASP:OD2	2.48	0.45
2:B:290:ASP:HB3	4:B:45:HOH:O	2.17	0.44
2:D:357:LYS:O	2:D:360:ILE:HB	2.16	0.44
1:C:87:GLN:HE22	2:D:310:ASN:CB	2.30	0.44
1:C:54:PRO:CB	1:C:55:PRO:HD2	2.48	0.44
2:D:357:LYS:N	2:D:360:ILE:HD12	2.33	0.44
1:A:233:LEU:CD2	2:B:284:MET:SD	3.05	0.44
1:C:57:THR:HG22	1:C:62:VAL:HG23	1.99	0.44
1:A:166:VAL:HG23	2:B:287:ILE:CD1	2.48	0.44
1:C:217:ASN:CG	1:C:220:THR:H	2.21	0.44
1:C:197:ASN:CA	4:C:408:HOH:O	2.22	0.44
2:B:261:ALA:HB2	2:B:282:SER:HB3	1.99	0.44
1:A:192:HIS:O	1:A:195:VAL:N	2.47	0.44
2:D:295:ASN:ND2	2:D:332:SER:H	2.13	0.44
1:A:7:CYS:SG	2:B:331:VAL:CG1	3.04	0.44
1:C:32:LYS:HA	1:C:32:LYS:CE	2.47	0.44
2:B:275:THR:HG23	2:B:276:HIS:ND1	2.33	0.44
1:A:30:ILE:N	1:A:31:PRO:CD	2.78	0.44
1:A:106:MET:HG3	1:A:110:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:LYS:HZ3	2:B:343:LYS:HB3	1.81	0.44
2:B:265:VAL:HG21	2:B:285:THR:HB	1.99	0.44
1:C:210:LEU:HD13	1:C:229:TYR:CD1	2.51	0.44
1:A:176:SER:HB2	1:A:177:PRO:CD	2.48	0.44
1:A:177:PRO:HD2	1:A:178:GLU:OE1	2.18	0.44
1:A:49:PHE:HA	2:B:325:LYS:HD2	1.99	0.44
1:C:120:ILE:HA	1:C:123:MET:CG	2.28	0.44
2:B:273:THR:O	2:B:274:LYS:C	2.56	0.44
1:A:8:SER:OG	2:B:328:LYS:CE	2.60	0.44
1:C:80:GLY:O	1:C:228:LEU:HA	2.18	0.44
2:B:343:LYS:NZ	2:B:343:LYS:HB3	2.33	0.43
1:C:138:ILE:HG12	1:C:143:ILE:HG12	2.00	0.43
1:A:45:LYS:HA	1:A:46:PRO:HD3	1.84	0.43
1:A:139:TYR:CG	1:A:140:LEU:HG	2.53	0.43
1:A:166:VAL:CG2	2:B:287:ILE:CD1	2.96	0.43
1:A:123:MET:HE3	1:A:129:PHE:HZ	1.83	0.43
2:B:282:SER:OG	2:B:285:THR:HG23	2.18	0.43
1:A:195:VAL:CB	1:A:198:MET:CE	2.96	0.43
1:C:124:ASP:HB3	1:C:127:LEU:HD21	2.00	0.43
1:C:8:SER:N	2:D:328:LYS:HD3	2.33	0.43
1:C:78:TYR:CD2	2:D:297:ARG:NH1	2.87	0.43
1:C:161:ASN:O	1:C:162:ARG:HB2	2.17	0.43
1:C:30:ILE:CG2	2:D:308:VAL:HB	2.47	0.43
1:C:19:ASN:O	1:C:20:GLU:C	2.56	0.43
2:B:368:ASN:N	2:B:368:ASN:HD22	2.16	0.43
2:B:369:ARG:CZ	2:B:372:ASN:ND2	2.82	0.43
2:B:345:LYS:HZ3	2:D:346:TYR:HE2	0.67	0.43
1:A:34:LYS:CD	1:A:38:THR:HG21	2.46	0.43
1:A:99:LYS:HB3	1:A:102:ASP:HB3	1.99	0.43
2:B:360:ILE:HG12	2:D:360:ILE:HG13	2.01	0.43
1:A:94:HIS:CD2	4:A:423:HOH:O	2.65	0.43
1:C:139:TYR:CD1	1:C:204:ARG:O	2.72	0.43
1:A:139:TYR:O	1:A:140:LEU:C	2.56	0.43
1:A:30:ILE:CG2	2:B:308:VAL:HG13	2.49	0.43
2:B:348:LYS:O	2:B:350:LYS:N	2.51	0.43
1:A:86:GLY:O	1:A:236:SER:OG	2.34	0.43
2:B:266:ILE:HG13	2:B:320:PHE:HE1	1.78	0.43
1:C:108:ILE:CG2	1:C:112:ILE:HD12	2.48	0.43
2:D:348:LYS:HA	2:D:351:GLU:CD	2.39	0.43
2:D:274:LYS:HA	2:D:277:VAL:HG11	1.93	0.42
1:C:32:LYS:HA	1:C:32:LYS:HZ2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:THR:O	2:D:276:HIS:HB2	2.18	0.42
1:C:7:CYS:O	1:C:7:CYS:SG	2.76	0.42
2:B:366:GLU:O	2:B:369:ARG:N	2.52	0.42
1:C:217:ASN:O	1:C:221:GLU:N	2.52	0.42
1:C:59:GLN:NE2	1:C:94:HIS:CE1	2.87	0.42
1:C:223:LYS:O	2:D:335:LEU:HD12	2.19	0.42
2:D:260:SER:O	2:D:261:ALA:C	2.58	0.42
2:B:337:LEU:HB2	2:B:342:TRP:CD1	2.54	0.42
2:D:295:ASN:HA	2:D:330:THR:O	2.19	0.42
1:C:25:ARG:NH1	2:D:309:PHE:CB	2.81	0.42
2:B:354:LYS:O	2:B:357:LYS:HB2	2.19	0.42
1:A:161:ASN:HD22	2:D:340:GLU:HG2	1.85	0.42
1:C:149:VAL:HG21	1:C:193:VAL:HG21	2.02	0.42
1:C:216:GLU:HB2	1:C:223:LYS:HG3	2.01	0.42
2:D:265:VAL:HG13	2:D:279:TYR:CE1	2.54	0.42
1:C:222:LYS:HG2	2:D:335:LEU:CD1	2.49	0.42
1:C:137:GLU:OE2	1:C:144:ARG:NH2	2.53	0.42
2:D:313:GLU:O	2:D:314:THR:C	2.57	0.42
2:B:261:ALA:O	2:B:265:VAL:HG23	2.19	0.42
1:C:224:LEU:HD21	2:D:335:LEU:CD1	2.45	0.42
2:B:342:TRP:CH2	2:D:343:LYS:HG3	2.55	0.42
1:C:28:LYS:CG	2:D:308:VAL:CG1	2.91	0.42
1:C:89:SER:N	3:C:400:ADP:O2B	2.53	0.42
2:B:269:LEU:HG	2:B:277:VAL:HG11	2.02	0.42
1:C:14:ARG:HH12	1:C:59:GLN:HE21	1.66	0.42
1:A:132:LYS:NZ	1:A:171:GLU:OE2	2.52	0.42
1:A:14:ARG:HG3	1:A:53:LEU:HB2	2.01	0.42
2:D:257:LYS:O	2:D:260:SER:N	2.53	0.42
2:D:265:VAL:HG11	2:D:279:TYR:HE1	1.83	0.42
1:C:218:VAL:HG23	1:C:219:GLU:N	2.34	0.41
1:C:83:PHE:CE1	2:D:300:ILE:CG1	3.03	0.41
1:A:131:ILE:HG22	1:A:174:VAL:HG23	2.01	0.41
2:B:366:GLU:CG	2:B:370:TRP:CG	3.03	0.41
1:C:41:ILE:CD1	2:D:318:LEU:CD1	2.98	0.41
1:C:28:LYS:HG2	2:D:308:VAL:HG12	2.00	0.41
2:D:265:VAL:CG1	2:D:279:TYR:CE1	3.02	0.41
1:C:211:ILE:HD12	1:C:230:LEU:CD1	2.50	0.41
2:B:348:LYS:C	2:B:350:LYS:N	2.73	0.41
2:B:366:GLU:CA	2:B:370:TRP:H	2.34	0.41
1:C:148:ASP:OD2	1:C:151:LYS:HD2	2.20	0.41
2:D:290:ASP:OD1	2:D:295:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ASN:OD1	1:C:220:THR:N	2.50	0.41
1:A:59:GLN:CB	1:A:111:ARG:HH12	2.25	0.41
2:B:343:LYS:HG3	2:D:342:TRP:CH2	2.45	0.41
1:C:37:GLU:OE1	1:C:50:ASP:C	2.58	0.41
1:A:80:GLY:O	1:A:228:LEU:HA	2.21	0.41
1:C:140:LEU:C	1:C:142:LYS:H	2.24	0.41
1:A:34:LYS:HD2	1:A:38:THR:CG2	2.45	0.41
1:A:99:LYS:O	1:A:101:HIS:N	2.53	0.41
1:C:147:LEU:HD21	1:C:183:VAL:CG1	2.49	0.41
1:A:196:THR:OG1	1:A:197:ASN:N	2.54	0.41
1:C:112:ILE:O	1:C:116:ILE:HG13	2.21	0.41
1:C:12:MET:HE2	1:C:65:ALA:O	2.20	0.41
2:D:286:ARG:O	2:D:289:GLN:CB	2.67	0.40
1:A:99:LYS:HE3	1:A:105:LEU:HD13	2.00	0.40
1:A:28:LYS:HE2	2:B:308:VAL:HG11	2.01	0.40
1:A:29:PHE:CZ	1:A:55:PRO:HG2	2.56	0.40
1:A:25:ARG:HD2	2:B:309:PHE:CZ	2.55	0.40
2:B:344:LYS:O	2:B:347:GLU:HB2	2.20	0.40
1:C:117:PHE:O	1:C:118:ASP:C	2.59	0.40
1:A:195:VAL:HG11	1:A:198:MET:HE2	1.91	0.40
1:A:81:THR:CG2	2:B:291:SER:OG	2.68	0.40
1:C:108:ILE:HG23	1:C:112:ILE:HD11	2.04	0.40
1:C:51:ARG:C	1:C:52:VAL:HG23	2.42	0.40
1:A:200:GLU:CD	1:A:204:ARG:HH12	2.22	0.40
2:B:363:LEU:HD23	2:D:367:LEU:HG	2.03	0.40
2:B:346:TYR:CE1	2:D:345:LYS:HB3	2.56	0.40
2:D:295:ASN:ND2	4:D:59:HOH:O	2.54	0.40
1:C:164:PRO:O	1:C:165:TYR:HB3	2.21	0.40
1:A:126:ASN:OD1	1:A:219:GLU:N	2.51	0.40
2:D:314:THR:O	2:D:318:LEU:N	2.49	0.40

All (15) 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)
2:B:319:MET:C	2:B:371:ARG:NH2[3_556]	1.48	0.72
1:A:47:TYR:OH	2:B:372:ASN:O[3_556]	1.53	0.67
2:B:319:MET:O	2:B:371:ARG:NH2[3_556]	1.60	0.60
2:B:319:MET:SD	2:B:371:ARG:NE[3_556]	1.61	0.59
2:B:319:MET:CB	2:B:371:ARG:NH2[3_556]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:MET:CA	2:B:371:ARG:NH2[3_556]	1.72	0.48
2:B:319:MET:SD	2:B:371:ARG:CD[3_556]	1.82	0.38
2:B:319:MET:SD	2:B:371:ARG:CG[3_556]	1.94	0.26
2:B:319:MET:CE	2:B:371:ARG:CG[3_556]	2.10	0.10
2:B:319:MET:CB	2:B:371:ARG:CZ[3_556]	2.10	0.10
1:A:104:GLN:OE1	1:A:218:VAL:CG2[4_556]	2.11	0.09
2:B:323:ARG:NH2	2:D:370:TRP:CD1[3_556]	2.13	0.07
2:B:271:GLU:CG	2:D:370:TRP:CZ2[3_556]	2.14	0.06
1:A:45:LYS:CB	2:B:372:ASN:OD1[3_556]	2.17	0.03
1:A:124:ASP:OD2	3:A:401:ADP:C6[4_456]	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	236/238 (99%)	202 (86%)	28 (12%)	6 (2%)	7	32
1	C	236/238 (99%)	203 (86%)	27 (11%)	6 (2%)	7	32
2	B	115/117 (98%)	93 (81%)	18 (16%)	4 (4%)	4	24
2	D	113/117 (97%)	90 (80%)	18 (16%)	5 (4%)	3	18
All	All	700/710 (99%)	588 (84%)	91 (13%)	21 (3%)	5	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
2	B	274	LYS
1	C	7	CYS
2	D	274	LYS
2	D	275	THR
1	A	190	ASN
1	A	203	SER

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Mol	Chain	Res	Type
1	C	23	ILE
1	C	42	GLY
1	C	141	ASP
1	C	191	ARG
2	B	349	GLU
2	D	257	LYS
2	D	340	GLU
2	B	366	GLU
1	C	222	LYS
1	A	95	THR
1	A	193	VAL
2	D	293	GLY
1	A	108	ILE
2	B	278	PRO

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	213/213 (100%)	174 (82%)	39 (18%)	2	9
1	C	213/213 (100%)	170 (80%)	43 (20%)	1	7
2	B	105/105 (100%)	80 (76%)	25 (24%)	1	3
2	D	103/105 (98%)	75 (73%)	28 (27%)	0	1
All	All	634/636 (100%)	499 (79%)	135 (21%)	1	6

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	8	SER
1	A	10	LYS
1	A	12	MET
1	A	16	ARG
1	A	20	GLU
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	25	ARG
1	A	28	LYS
1	A	32	LYS
1	A	37	GLU
1	A	41	ILE
1	A	51	ARG
1	A	89	SER
1	A	97	GLU
1	A	99	LYS
1	A	100	LEU
1	A	106	MET
1	A	126	ASN
1	A	132	LYS
1	A	135	TYR
1	A	140	LEU
1	A	144	ARG
1	A	149	VAL
1	A	150	SER
1	A	174	VAL
1	A	175	SER
1	A	180	VAL
1	A	181	MET
1	A	188	LYS
1	A	191	ARG
1	A	198	MET
1	A	203	SER
1	A	207	SER
1	A	220	THR
1	A	222	LYS
1	A	224	LEU
1	A	227	LYS
1	A	238	LYS
2	B	257	LYS
2	B	259	LEU
2	B	273	THR
2	B	276	HIS
2	B	300	ILE
2	B	307	SER
2	B	315	LYS
2	B	316	SER
2	B	323	ARG
2	B	325	LYS

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Mol	Chain	Res	Type
2	B	326	THR
2	B	328	LYS
2	B	330	THR
2	B	333	VAL
2	B	336	GLU
2	B	340	GLU
2	B	345	LYS
2	B	350	LYS
2	B	354	LYS
2	B	356	LEU
2	B	357	LYS
2	B	364	GLU
2	B	365	VAL
2	B	368	ASN
2	B	369	ARG
1	C	3	ASP
1	C	8	SER
1	C	10	LYS
1	C	12	MET
1	C	13	CYS
1	C	16	ARG
1	C	18	LEU
1	C	24	LEU
1	C	32	LYS
1	C	51	ARG
1	C	56	ASN
1	C	69	GLN
1	C	72	LYS
1	C	82	ILE
1	C	96	MET
1	C	100	LEU
1	C	115	ASP
1	C	122	SER
1	C	126	ASN
1	C	127	LEU
1	C	135	TYR
1	C	142	LYS
1	C	144	ARG
1	C	150	SER
1	C	152	THR
1	C	154	LEU
1	C	162	ARG

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Mol	Chain	Res	Type
1	C	163	VAL
1	C	169	CYS
1	C	200	GLU
1	C	202	SER
1	C	204	ARG
1	C	205	SER
1	C	207	SER
1	C	213	ILE
1	C	214	LYS
1	C	215	GLN
1	C	221	GLU
1	C	223	LYS
1	C	225	SER
1	C	227	LYS
1	C	228	LEU
1	C	238	LYS
2	D	258	SER
2	D	267	SER
2	D	273	THR
2	D	274	LYS
2	D	285	THR
2	D	291	SER
2	D	301	VAL
2	D	302	ILE
2	D	304	CYS
2	D	307	SER
2	D	310	ASN
2	D	315	LYS
2	D	328	LYS
2	D	332	SER
2	D	333	VAL
2	D	338	THR
2	D	346	TYR
2	D	347	GLU
2	D	348	LYS
2	D	349	GLU
2	D	351	GLU
2	D	353	ASN
2	D	356	LEU
2	D	358	SER
2	D	361	GLN
2	D	365	VAL

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Mol	Chain	Res	Type
2	D	367	LEU
2	D	368	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	59	GLN
1	A	69	GLN
1	A	79	ASN
1	A	101	HIS
1	A	206	HIS
1	A	212	ASN
2	B	289	GLN
2	B	295	ASN
2	B	368	ASN
1	C	56	ASN
1	C	59	GLN
1	C	87	GLN
1	C	199	ASN
1	C	212	ASN
2	D	256	ASN
2	D	276	HIS
2	D	295	ASN
2	D	329	ASN
2	D	353	ASN
2	D	368	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	401	1	22,29,29	1.30	3 (13%)	27,45,45	2.85	13 (48%)
3	ADP	C	400	-	22,29,29	1.14	2 (9%)	27,45,45	2.75	14 (51%)

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	401	1	4/4/6/6	0/12/32/32	0/3/3/3
3	ADP	C	400	-	4/4/6/6	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	PB-O2B	-2.41	1.46	1.54
3	C	400	ADP	O4'-C1'	2.27	1.44	1.41
3	A	401	ADP	O4'-C1'	2.70	1.44	1.41
3	C	400	ADP	C2'-C3'	2.80	1.61	1.53
3	A	401	ADP	C2'-C3'	2.81	1.61	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	400	ADP	C1'-N9-C4	-6.46	117.20	126.94
3	C	400	ADP	N3-C2-N1	-6.10	124.23	128.89
3	A	401	ADP	N3-C2-N1	-4.54	125.42	128.89
3	C	400	ADP	O2B-PB-O3A	-3.15	90.80	105.09
3	C	400	ADP	O5'-C5'-C4'	-2.44	100.14	109.12
3	C	400	ADP	C5'-C4'-C3'	-2.40	105.69	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C5'-C4'-C3'	-2.29	106.11	115.21
3	A	401	ADP	PA-O3A-PB	-2.23	125.19	132.67
3	C	400	ADP	O2A-PA-O1A	-2.16	100.83	112.53
3	A	401	ADP	C4'-O4'-C1'	2.14	112.07	109.72
3	A	401	ADP	O3B-PB-O2B	2.26	116.00	107.38
3	C	400	ADP	N6-C6-N1	2.30	124.14	119.20
3	C	400	ADP	C2'-C1'-N9	2.38	117.93	114.29
3	A	401	ADP	C1'-N9-C4	2.47	130.67	126.94
3	A	401	ADP	C4-C5-N7	2.49	111.77	109.48
3	A	401	ADP	N6-C6-N1	2.59	124.77	119.20
3	C	400	ADP	C4-C5-N7	2.69	111.96	109.48
3	C	400	ADP	O4'-C4'-C3'	2.76	110.71	105.15
3	A	401	ADP	O3B-PB-O1B	2.87	119.83	110.58
3	A	401	ADP	C2-N1-C6	2.96	124.06	118.77
3	A	401	ADP	O2A-PA-O3A	3.04	118.88	105.09
3	A	401	ADP	O2'-C2'-C3'	3.17	122.14	111.83
3	C	400	ADP	O3B-PB-O1B	3.42	121.58	110.58
3	C	400	ADP	C2-N1-C6	3.43	124.90	118.77
3	C	400	ADP	O3A-PA-O5'	4.02	113.61	102.94
3	C	400	ADP	O2'-C2'-C3'	4.37	126.03	111.83
3	A	401	ADP	C2'-C1'-N9	10.03	129.62	114.29

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	401	ADP	C4'
3	A	401	ADP	C2'
3	A	401	ADP	C3'
3	A	401	ADP	C1'
3	C	400	ADP	C4'
3	C	400	ADP	C2'
3	C	400	ADP	C3'
3	C	400	ADP	C1'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	12	1
3	C	400	ADP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.