



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DS5
Title : DIMERIC CRYSTAL STRUCTURE OF THE ALPHA SUBUNIT IN COMPLEX WITH TWO BETA PEPTIDES MIMICKING THE ARCHITECTURE OF THE TETRAMERIC PROTEIN KINASE CK2 HOLOENZYME.
Authors : Battistutta, R.; Sarno, S.; De Moliner, E.; Marin, O.; Zanotti, G.; Pinna, L.A.
Deposited on : 2000-01-07
Resolution : 3.16 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

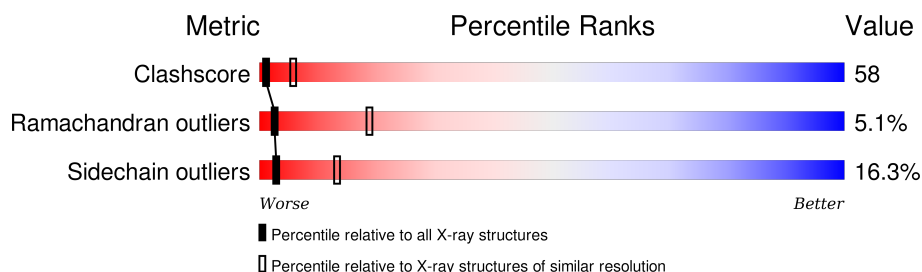
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)

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	332	
1	B	332	
1	C	332	
1	D	332	
2	E	23	
2	F	23	
2	G	23	

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Mol	Chain	Length	Quality of chain
2	H	23	

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
4	AMP	A	501	X	-	-	-
4	AMP	B	801	X	-	-	-
4	AMP	C	601	X	-	-	-
4	AMP	D	701	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11932 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 CASEIN KINASE, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2735	1762	471	490	12			
1	B	328	Total	C	N	O	S	0	0	0
			2735	1762	471	490	12			
1	C	328	Total	C	N	O	S	0	0	0
			2735	1762	471	490	12			
1	D	328	Total	C	N	O	S	0	0	0
			2735	1762	471	490	12			

- Molecule 2 is a protein called CASEIN KINASE, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	16	Total	C	N	O	S	0	0	0
			135	90	22	22	1			
2	F	18	Total	C	N	O	S	0	0	0
			154	102	27	24	1			
2	G	16	Total	C	N	O	S	0	0	0
			135	90	22	22	1			
2	H	16	Total	C	N	O	S	0	0	0
			135	90	22	22	1			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is water.

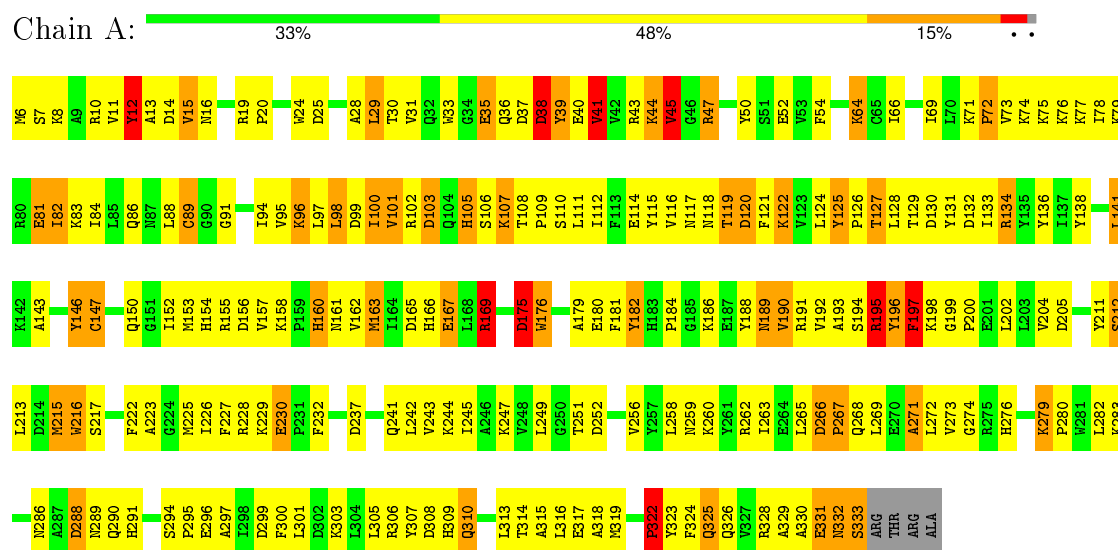
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	74	Total	O	0	0
			74	74		
5	C	89	Total	O	0	0
			89	89		
5	D	73	Total	O	0	0
			73	73		
5	E	6	Total	O	0	0
			6	6		
5	F	4	Total	O	0	0
			4	4		
5	G	6	Total	O	0	0
			6	6		
5	H	8	Total	O	0	0
			8	8		

3 Residue-property plots

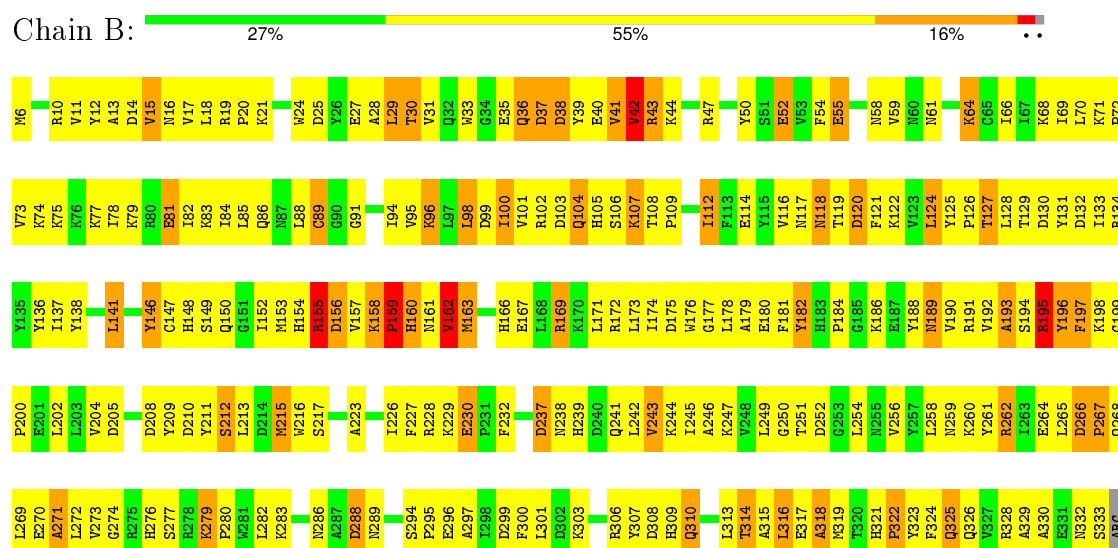
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



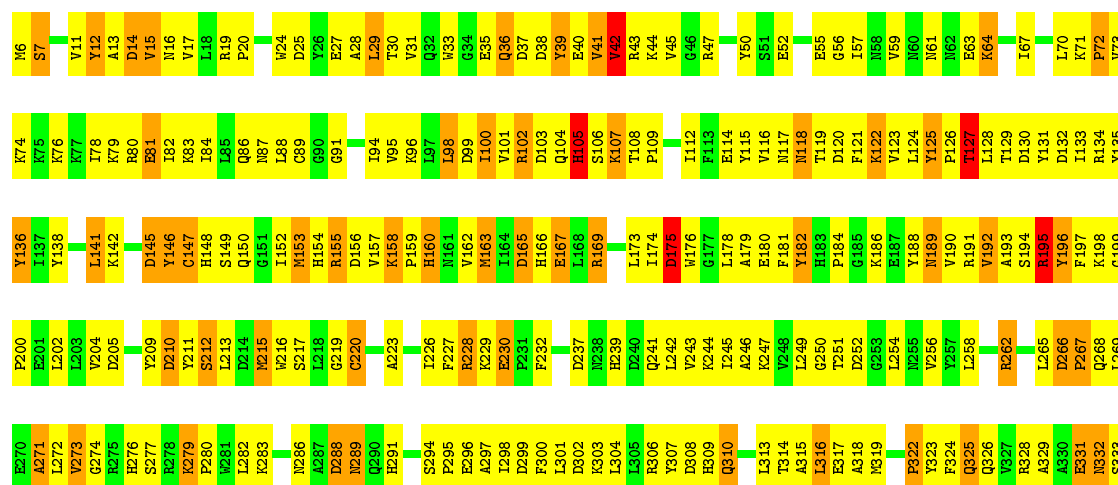
• Molecule 1: CASEIN KINASE, ALPHA CHAIN



THR
ARG
ALA

• Molecule 1: CASEIN KINASE, ALPHA CHAIN

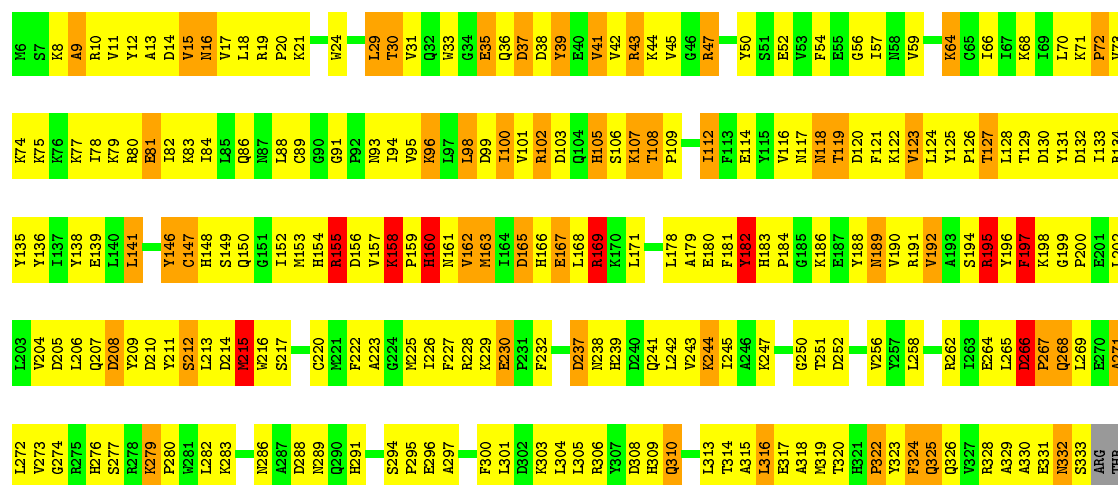
Chain C: 28% 53% 17% ..



ARG
THR
ARG
ALA

• Molecule 1: CASEIN KINASE, ALPHA CHAIN

Chain D: 29% 52% 15% ..



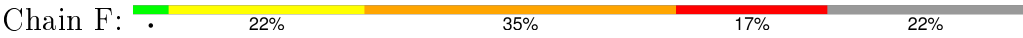
ARG
ALA

• Molecule 2: CASEIN KINASE, BETA CHAIN

Chain E: 9% 35% 22% 30%

ASN	GLN	PHE	VAL	PRO	ARG	LEU	Y188	G189	F190	K191	I192	H193	F194	M195	A196	Y197	Q198	L199	Q200	L201	Q202	A203
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● Molecule 2: CASEIN KINASE, BETA CHAIN



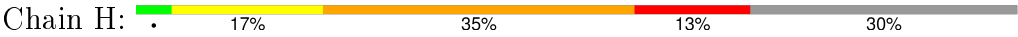
ASN	GLN	PHE	VAL	PRO	R186	L187	Y188	G189	F190	K191	I192	H193	F194	M195	A196	Y197	Q198	L199	Q200	L201	Q202	A203
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● Molecule 2: CASEIN KINASE, BETA CHAIN



ASN	GLN	PHE	VAL	PRO	ARG	LEU	Y188	G189	F190	K191	I192	H193	F194	M195	A196	Y197	Q198	L199	Q200	L201	Q202	A203
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● Molecule 2: CASEIN KINASE, BETA CHAIN



ASN	GLN	PHE	VAL	PRO	ARG	LEU	Y188	G189	F190	K191	I192	H193	F194	M195	A196	Y197	Q198	L199	Q200	L201	Q202	A203
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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	87.68 Å 119.85 Å 145.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.16	Depositor
% Data completeness (in resolution range)	95.3 (45.00-3.16)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.214 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11932	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: AMP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.40	18/2803 (0.6%)	1.23	13/3788 (0.3%)
1	B	1.30	7/2803 (0.2%)	1.21	11/3788 (0.3%)
1	C	1.34	10/2803 (0.4%)	1.24	18/3788 (0.5%)
1	D	1.29	10/2803 (0.4%)	1.20	11/3788 (0.3%)
2	E	1.78	2/139 (1.4%)	1.57	3/185 (1.6%)
2	F	1.74	4/158 (2.5%)	1.85	5/210 (2.4%)
2	G	1.55	1/139 (0.7%)	1.63	2/185 (1.1%)
2	H	1.84	3/139 (2.2%)	1.65	2/185 (1.1%)
All	All	1.35	55/11787 (0.5%)	1.25	65/15917 (0.4%)

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	A	0	4
1	B	0	2
1	C	0	4
1	D	0	3
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	16

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	VAL	CA-CB	-8.84	1.36	1.54
1	D	35	GLU	CB-CG	8.82	1.69	1.52
1	D	35	GLU	CG-CD	8.30	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	GLU	CG-CD	8.13	1.64	1.51
1	D	147	CYS	CB-SG	-8.10	1.68	1.82
1	A	40	GLU	CG-CD	8.06	1.64	1.51
1	A	147	CYS	CB-SG	-8.02	1.68	1.82
1	A	39	TYR	CD2-CE2	-7.75	1.27	1.39
1	D	230	GLU	CG-CD	7.61	1.63	1.51
1	B	230	GLU	CG-CD	7.33	1.62	1.51
1	B	167	GLU	CB-CG	7.24	1.66	1.52
1	A	39	TYR	CD1-CE1	-6.90	1.29	1.39
1	A	230	GLU	CG-CD	6.86	1.62	1.51
1	D	81	GLU	CG-CD	6.74	1.62	1.51
1	C	147	CYS	CB-SG	-6.72	1.70	1.82
1	C	153	MET	SD-CE	-6.63	1.40	1.77
1	A	190	VAL	CA-CB	-6.61	1.40	1.54
1	A	143	ALA	CA-CB	-6.31	1.39	1.52
1	C	136	TYR	CE1-CZ	-6.26	1.30	1.38
1	A	44	LYS	CD-CE	6.22	1.66	1.51
1	D	123	VAL	CB-CG1	-6.14	1.40	1.52
1	A	81	GLU	CB-CG	-6.14	1.40	1.52
1	C	36	GLN	CB-CG	-6.08	1.36	1.52
1	A	41	VAL	CA-CB	6.06	1.67	1.54
1	A	12	TYR	CE1-CZ	-6.04	1.30	1.38
1	B	318	ALA	CA-CB	-6.03	1.39	1.52
1	B	41	VAL	CB-CG2	-6.03	1.40	1.52
1	D	324	PHE	CB-CG	-6.00	1.41	1.51
1	C	81	GLU	CG-CD	5.97	1.60	1.51
2	F	197	TYR	CB-CG	-5.77	1.43	1.51
1	A	43	ARG	CG-CD	5.77	1.66	1.51
1	A	175	ASP	CB-CG	5.58	1.63	1.51
2	F	190	PHE	CE1-CZ	5.57	1.48	1.37
1	A	197	PHE	CE1-CZ	-5.48	1.26	1.37
2	G	197	TYR	CB-CG	-5.44	1.43	1.51
2	F	188	TYR	CD1-CE1	5.40	1.47	1.39
1	D	220	CYS	CB-SG	5.32	1.91	1.82
1	A	167	GLU	CG-CD	5.32	1.59	1.51
1	C	59	VAL	CA-CB	-5.30	1.43	1.54
1	D	244	LYS	CE-NZ	5.28	1.62	1.49
2	H	197	TYR	CD1-CE1	-5.26	1.31	1.39
2	E	188	TYR	CD1-CE1	5.26	1.47	1.39
1	A	176	TRP	CB-CG	-5.25	1.40	1.50
1	D	182	TYR	CE1-CZ	5.25	1.45	1.38
1	A	115	TYR	CB-CG	-5.22	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	194	PRO	CB-CG	5.21	1.76	1.50
1	C	220	CYS	CB-SG	5.19	1.91	1.82
1	A	216	TRP	CG-CD1	-5.14	1.29	1.36
2	E	190	PHE	CE2-CZ	5.10	1.47	1.37
1	C	230	GLU	CG-CD	5.08	1.59	1.51
1	C	115	TYR	CD2-CE2	-5.07	1.31	1.39
1	B	162	VAL	CB-CG1	-5.05	1.42	1.52
1	C	40	GLU	CG-CD	5.05	1.59	1.51
2	H	197	TYR	CB-CG	-5.03	1.44	1.51
2	F	197	TYR	CD2-CE2	-5.01	1.31	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	198	GLN	N-CA-C	8.81	134.78	111.00
1	B	124	LEU	CA-CB-CG	-8.31	96.19	115.30
1	A	134	ARG	NE-CZ-NH1	-7.92	116.34	120.30
2	F	198	GLN	N-CA-C	7.59	131.50	111.00
1	C	108	THR	N-CA-C	-6.92	92.31	111.00
1	C	228	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	C	14	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	145	ASP	CB-CG-OD2	6.54	124.18	118.30
2	F	193	HIS	C-N-CA	-6.47	94.83	122.00
2	F	188	TYR	CA-CB-CG	6.40	125.55	113.40
1	A	43	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	267	PRO	N-CA-C	-6.34	95.63	112.10
2	E	200	GLN	N-CA-C	-6.23	94.17	111.00
1	A	101	VAL	N-CA-C	6.20	127.74	111.00
1	B	167	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	C	29	LEU	CA-CB-CG	6.16	129.47	115.30
1	D	208	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	302	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	D	267	PRO	N-CA-C	-6.05	96.38	112.10
1	B	120	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	267	PRO	N-CA-C	-5.99	96.53	112.10
2	H	192	ILE	CG1-CB-CG2	-5.90	98.42	111.40
1	D	165	ASP	N-CA-C	-5.81	95.31	111.00
1	A	38	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	29	LEU	CA-CB-CG	5.68	128.36	115.30
1	D	163	MET	CG-SD-CE	5.67	109.28	100.20
1	D	215	MET	CG-SD-CE	5.66	109.26	100.20
1	D	80	ARG	NE-CZ-NH1	-5.65	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	LEU	CA-CB-CG	5.62	128.24	115.30
1	B	155	ARG	N-CA-C	5.62	126.17	111.00
1	C	267	PRO	N-CA-C	-5.59	97.57	112.10
1	A	45	VAL	CG1-CB-CG2	5.58	119.83	110.90
1	C	55	GLU	N-CA-C	-5.57	95.95	111.00
1	C	158	LYS	N-CA-C	-5.56	95.99	111.00
1	A	38	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	A	120	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	122	LYS	CD-CE-NZ	5.50	124.34	111.70
2	F	202	GLN	N-CA-C	5.48	125.79	111.00
1	C	266	ASP	N-CA-C	-5.45	96.28	111.00
2	E	200	GLN	C-N-CA	-5.41	108.17	121.70
1	A	266	ASP	N-CA-C	-5.41	96.41	111.00
1	C	127	THR	CB-CA-C	-5.41	97.01	111.60
1	C	175	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	42	VAL	CB-CA-C	-5.36	101.22	111.40
1	B	171	LEU	CA-CB-CG	5.34	127.57	115.30
1	D	155	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	210	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	207	GLN	N-CA-C	5.28	125.26	111.00
1	B	55	GLU	N-CA-C	-5.23	96.87	111.00
1	B	42	VAL	CB-CA-C	-5.21	101.49	111.40
1	C	165	ASP	N-CA-C	-5.21	96.92	111.00
1	B	266	ASP	N-CA-C	-5.21	96.94	111.00
2	F	193	HIS	N-CA-C	-5.19	97.00	111.00
1	A	169	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	314	THR	N-CA-C	-5.17	97.05	111.00
2	H	193	HIS	N-CA-C	-5.15	97.10	111.00
1	C	80	ARG	NE-CZ-NH1	-5.11	117.75	120.30
2	E	193	HIS	C-N-CA	-5.11	100.56	122.00
1	C	125	TYR	C-N-CD	5.10	139.11	128.40
1	A	47	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	158	LYS	CD-CE-NZ	5.09	123.40	111.70
1	A	101	VAL	CB-CA-C	-5.03	101.85	111.40
2	G	193	HIS	N-CA-C	-5.02	97.45	111.00
1	D	266	ASP	N-CA-C	-5.01	97.47	111.00
1	D	29	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain
1	A	125	TYR	Sidechain
1	A	182	TYR	Sidechain
1	A	307	TYR	Sidechain
1	B	182	TYR	Sidechain
1	B	307	TYR	Sidechain
1	C	12	TYR	Sidechain
1	C	182	TYR	Sidechain
1	C	307	TYR	Sidechain
1	C	39	TYR	Sidechain
1	D	182	TYR	Sidechain
1	D	197	PHE	Sidechain
1	D	39	TYR	Sidechain
2	F	188	TYR	Sidechain
2	G	197	TYR	Sidechain
2	H	197	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2735	0	2721	280	0
1	B	2735	0	2721	342	0
1	C	2735	0	2721	301	0
1	D	2735	0	2721	309	0
2	E	135	0	132	49	0
2	F	154	0	156	58	0
2	G	135	0	132	57	0
2	H	135	0	132	48	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
4	A	23	0	11	6	0
4	B	23	0	11	5	0
4	C	23	0	11	3	0
4	D	23	0	11	3	0
5	A	77	0	0	1	0
5	B	74	0	0	2	0
5	C	89	0	0	2	0
5	D	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	6	0	0	0	0
5	F	4	0	0	1	0
5	G	6	0	0	3	0
5	H	8	0	0	4	0
All	All	11932	0	11480	1344	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 58.

All (1344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:PRO:CB	2:H:194:PRO:CG	1.76	1.46
1:D:119:THR:HB	2:G:202:GLN:NE2	1.42	1.30
1:A:41:VAL:HG12	2:F:197:TYR:HB3	1.24	1.19
2:F:200:GLN:HB2	2:F:202:GLN:NE2	1.61	1.13
1:A:100:ILE:HD12	1:A:101:VAL:N	1.64	1.12
1:B:127:THR:HA	2:F:190:PHE:CE1	1.86	1.10
1:A:169:ARG:HG3	1:A:169:ARG:HH21	1.11	1.09
1:C:103:ASP:HB2	2:G:194:PRO:HB3	1.35	1.09
2:E:193:HIS:HB3	2:E:194:PRO:HD3	1.30	1.08
1:A:141:LEU:HD23	1:A:319:MET:HG2	1.32	1.08
1:C:141:LEU:HD23	1:C:319:MET:HG2	1.21	1.07
1:B:141:LEU:HD23	1:B:319:MET:HG2	1.18	1.07
1:C:84:ILE:HG23	1:C:152:ILE:HD13	1.34	1.07
2:H:200:GLN:HG2	5:H:208:HOH:O	1.55	1.05
1:B:43:ARG:HH11	1:B:43:ARG:HG2	0.93	1.04
1:B:36:GLN:OE1	1:B:103:ASP:HA	1.57	1.04
2:H:197:TYR:HD1	2:H:197:TYR:N	1.52	1.02
1:D:169:ARG:HG3	1:D:169:ARG:HH21	1.24	1.00
1:C:33:TRP:CE3	1:C:100:ILE:HD11	1.95	1.00
1:D:141:LEU:HD23	1:D:319:MET:HG2	1.41	0.99
1:D:314:THR:HB	1:D:317:GLU:HG3	1.44	0.99
1:D:124:LEU:HD12	1:D:127:THR:HG21	1.43	0.99
1:D:100:ILE:HD12	1:D:101:VAL:N	1.78	0.99
1:B:264:GLU:OE2	1:C:76:LYS:HB3	1.63	0.98
1:A:41:VAL:HG12	2:F:197:TYR:CB	1.93	0.98
1:B:84:ILE:HG23	1:B:152:ILE:HD13	1.46	0.98
1:D:36:GLN:OE1	2:H:194:PRO:HB2	1.63	0.98
1:C:100:ILE:HD12	1:C:101:VAL:N	1.79	0.97
2:F:200:GLN:HE21	2:F:202:GLN:NE2	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:THR:HB	2:G:202:GLN:HE21	1.15	0.97
2:E:193:HIS:CB	2:E:194:PRO:HD3	1.94	0.97
1:D:84:ILE:HG23	1:D:152:ILE:HD13	1.42	0.97
1:D:119:THR:CB	2:G:202:GLN:NE2	2.28	0.97
2:F:200:GLN:HE21	2:F:202:GLN:HE21	0.99	0.96
1:B:43:ARG:HG2	1:B:43:ARG:NH1	1.73	0.96
1:D:124:LEU:O	1:D:127:THR:HG22	1.66	0.96
1:D:36:GLN:CD	2:H:194:PRO:HB2	1.87	0.95
1:D:36:GLN:NE2	2:H:194:PRO:HB2	1.82	0.94
1:A:35:GLU:O	1:A:38:ASP:HB2	1.68	0.94
1:D:119:THR:CB	2:G:202:GLN:HE21	1.81	0.94
1:A:189:ASN:HD22	1:A:190:VAL:N	1.66	0.93
1:C:189:ASN:HD22	1:C:190:VAL:N	1.66	0.93
2:G:198:GLN:O	2:G:199:LEU:HD23	1.68	0.93
2:F:198:GLN:O	2:F:199:LEU:HD23	1.69	0.92
2:H:193:HIS:CB	2:H:194:PRO:HD3	1.99	0.92
2:H:197:TYR:CD1	2:H:197:TYR:N	2.30	0.92
1:C:100:ILE:C	1:C:100:ILE:HD12	1.90	0.92
1:A:120:ASP:OD1	1:B:44:LYS:HD3	1.71	0.91
2:G:188:TYR:N	2:G:190:PHE:HE1	1.68	0.91
1:C:44:LYS:NZ	1:C:52:GLU:OE2	2.02	0.90
1:A:169:ARG:HH21	1:A:169:ARG:CG	1.85	0.90
1:B:126:PRO:HB2	2:F:197:TYR:OH	1.70	0.90
1:B:169:ARG:HH21	1:B:169:ARG:HG3	1.36	0.90
2:G:193:HIS:CB	2:G:194:PRO:HD3	2.01	0.90
2:H:190:PHE:O	2:H:190:PHE:HD1	1.52	0.90
1:D:158:LYS:HG2	1:D:161:ASN:HD22	1.36	0.90
1:D:119:THR:HB	2:G:202:GLN:HE22	1.33	0.89
2:G:188:TYR:N	2:G:190:PHE:CE1	2.40	0.89
1:B:42:VAL:HB	1:B:43:ARG:NH1	1.87	0.89
1:B:33:TRP:CE3	1:B:100:ILE:HD11	2.06	0.89
1:B:127:THR:HA	2:F:190:PHE:HE1	1.35	0.89
1:C:89:CYS:SG	1:C:96:LYS:NZ	2.46	0.89
1:C:267:PRO:O	1:C:268:GLN:HB3	1.73	0.89
1:C:169:ARG:HH21	1:C:169:ARG:HG3	1.37	0.88
1:C:33:TRP:CZ2	1:C:102:ARG:HD3	2.08	0.88
1:A:44:LYS:HE2	1:A:47:ARG:CG	2.04	0.88
1:C:36:GLN:NE2	2:G:194:PRO:HB2	1.89	0.88
1:D:160:HIS:H	1:D:160:HIS:CD2	1.91	0.88
1:D:332:ASN:H	1:D:332:ASN:HD22	1.21	0.88
1:C:102:ARG:HH11	1:C:107:LYS:HD3	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASN:HD22	1:B:190:VAL:N	1.71	0.87
1:A:44:LYS:HE2	1:A:47:ARG:HG2	1.54	0.87
1:D:182:TYR:OH	1:D:184:PRO:HA	1.74	0.87
1:D:100:ILE:C	1:D:100:ILE:HD12	1.94	0.87
1:C:35:GLU:O	1:C:38:ASP:HB2	1.74	0.87
1:A:105:HIS:HD2	1:A:106:SER:N	1.73	0.86
1:B:36:GLN:CG	2:E:194:PRO:HB2	2.05	0.86
1:D:215:MET:HE1	1:D:315:ALA:HA	1.56	0.86
2:E:193:HIS:HB3	2:E:194:PRO:CD	2.05	0.86
1:A:169:ARG:HG3	1:A:169:ARG:NH2	1.90	0.85
1:A:89:CYS:SG	1:A:96:LYS:NZ	2.48	0.85
1:A:33:TRP:CE3	1:A:100:ILE:HD11	2.11	0.85
1:D:33:TRP:CE3	1:D:100:ILE:HD11	2.11	0.85
2:F:200:GLN:HB2	2:F:202:GLN:HE21	1.35	0.84
1:C:33:TRP:CZ3	1:C:100:ILE:HD11	2.12	0.84
1:D:155:ARG:NH1	1:D:209:TYR:OH	2.09	0.84
1:D:169:ARG:HH21	1:D:169:ARG:CG	1.90	0.84
1:A:136:TYR:OH	1:A:166:HIS:HD2	1.60	0.84
1:D:33:TRP:CZ3	1:D:100:ILE:HD11	2.12	0.84
1:B:33:TRP:CZ3	1:B:100:ILE:HD11	2.13	0.84
1:A:160:HIS:H	1:A:160:HIS:CD2	1.96	0.84
1:A:105:HIS:CD2	1:A:106:SER:N	2.46	0.84
1:C:103:ASP:HB2	2:G:194:PRO:CB	2.07	0.83
1:C:103:ASP:CB	2:G:194:PRO:HB3	2.08	0.83
1:B:36:GLN:OE1	1:B:102:ARG:O	1.97	0.83
2:F:194:PRO:HD2	2:F:195:MET:HG3	1.57	0.83
1:B:286:ASN:ND2	1:B:288:ASP:H	1.76	0.82
2:E:198:GLN:HG3	2:E:199:LEU:H	1.41	0.82
1:B:84:ILE:HD12	1:B:152:ILE:HD13	1.61	0.82
1:A:314:THR:HB	1:A:317:GLU:HG3	1.62	0.82
1:A:84:ILE:HG23	1:A:152:ILE:HD13	1.61	0.82
1:C:36:GLN:HE22	2:G:194:PRO:HB2	1.44	0.82
1:D:124:LEU:CD1	1:D:127:THR:HG21	2.09	0.81
1:B:35:GLU:HB3	1:B:38:ASP:OD2	1.80	0.81
1:A:33:TRP:CZ3	1:A:100:ILE:HD11	2.15	0.81
1:D:189:ASN:HD22	1:D:190:VAL:N	1.77	0.81
1:D:119:THR:OG1	1:D:124:LEU:HB2	1.80	0.81
2:H:198:GLN:C	2:H:199:LEU:HD23	2.00	0.81
1:A:267:PRO:O	1:A:268:GLN:HB3	1.80	0.81
1:B:160:HIS:H	1:B:160:HIS:CD2	1.96	0.81
1:D:267:PRO:O	1:D:268:GLN:HB3	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:MET:HE1	1:C:315:ALA:HA	1.59	0.81
1:B:156:ASP:OD1	1:B:158:LYS:HE2	1.79	0.81
1:C:102:ARG:NH1	1:C:107:LYS:HD3	1.94	0.81
1:D:66:ILE:HG13	4:D:701:AMP:C6	2.16	0.81
1:B:44:LYS:NZ	1:B:47:ARG:HD3	1.96	0.80
1:B:267:PRO:O	1:B:268:GLN:HB3	1.80	0.80
1:D:286:ASN:HD21	1:D:288:ASP:HB3	1.46	0.80
1:B:314:THR:HB	1:B:317:GLU:HG3	1.62	0.80
1:B:36:GLN:HG2	2:E:194:PRO:HB2	1.64	0.80
1:D:167:GLU:HG3	1:D:168:LEU:N	1.97	0.80
1:B:119:THR:HG22	1:B:124:LEU:HB2	1.64	0.79
1:D:223:ALA:HB2	1:D:301:LEU:HD11	1.62	0.79
1:C:160:HIS:H	1:C:160:HIS:CD2	1.96	0.79
1:D:42:VAL:HG23	1:D:56:GLY:HA2	1.64	0.79
1:B:325:GLN:HG3	1:B:326:GLN:H	1.47	0.79
1:C:136:TYR:OH	1:C:166:HIS:HD2	1.66	0.79
1:B:14:ASP:O	1:B:16:ASN:N	2.16	0.79
1:B:89:CYS:SG	1:B:96:LYS:NZ	2.55	0.79
2:G:193:HIS:HB2	2:G:194:PRO:HD3	1.62	0.79
1:A:33:TRP:CZ3	1:A:102:ARG:HG3	2.17	0.79
1:B:44:LYS:HZ2	1:B:47:ARG:HD3	1.46	0.78
1:B:64:LYS:HB2	1:B:64:LYS:NZ	1.99	0.78
1:C:36:GLN:NE2	2:G:194:PRO:C	2.37	0.78
1:D:242:LEU:HD23	1:D:269:LEU:HD21	1.65	0.78
1:C:169:ARG:CG	1:C:169:ARG:HH21	1.96	0.78
1:B:325:GLN:HG3	1:B:326:GLN:N	1.98	0.78
1:B:286:ASN:ND2	1:B:288:ASP:N	2.32	0.78
1:D:300:PHE:HE1	1:D:318:ALA:HB1	1.49	0.77
2:H:193:HIS:HB2	2:H:194:PRO:HD3	1.67	0.77
1:A:189:ASN:ND2	1:A:191:ARG:H	1.82	0.77
1:D:72:PRO:O	1:D:73:VAL:HG13	1.85	0.77
1:A:314:THR:HG22	1:A:315:ALA:N	1.97	0.77
1:A:288:ASP:OD2	1:A:289:ASN:N	2.17	0.77
1:B:36:GLN:CD	2:E:194:PRO:HB2	2.05	0.77
1:A:119:THR:OG1	1:A:124:LEU:HB2	1.84	0.77
1:A:331:GLU:C	1:A:333:SER:H	1.87	0.77
1:C:314:THR:HB	1:C:317:GLU:HG3	1.67	0.77
2:H:190:PHE:O	2:H:190:PHE:CD1	2.37	0.77
1:A:286:ASN:OD1	1:A:289:ASN:ND2	2.18	0.77
1:D:314:THR:HG22	1:D:315:ALA:N	2.00	0.76
1:B:169:ARG:HH21	1:B:169:ARG:CG	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LYS:CE	1:B:161:ASN:HD21	1.98	0.76
1:B:35:GLU:O	1:B:38:ASP:HB2	1.86	0.76
2:G:198:GLN:O	2:G:199:LEU:CD2	2.33	0.76
1:B:216:TRP:CZ2	1:B:245:ILE:HD13	2.20	0.76
1:A:72:PRO:O	1:A:73:VAL:HG13	1.84	0.76
1:A:41:VAL:CG1	2:F:197:TYR:HB3	2.12	0.76
1:B:212:SER:HB2	1:B:309:HIS:HB2	1.67	0.76
1:B:158:LYS:HE3	1:B:161:ASN:ND2	1.99	0.76
1:C:125:TYR:O	1:C:126:PRO:C	2.20	0.76
1:D:202:LEU:HD11	1:D:213:LEU:HD11	1.67	0.76
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.21	0.76
1:C:186:LYS:HD3	1:C:188:TYR:CE1	2.21	0.75
2:H:193:HIS:HB3	2:H:194:PRO:HD3	1.65	0.75
1:C:228:ARG:HD2	1:C:288:ASP:OD1	1.86	0.75
1:D:47:ARG:O	1:D:47:ARG:HG2	1.85	0.75
1:D:325:GLN:HG3	1:D:326:GLN:H	1.51	0.75
1:D:89:CYS:SG	1:D:96:LYS:NZ	2.60	0.74
2:G:192:ILE:O	2:G:194:PRO:N	2.20	0.74
2:F:192:ILE:O	2:F:194:PRO:N	2.20	0.74
2:F:191:LYS:HG2	2:F:196:ALA:HA	1.69	0.74
1:A:286:ASN:ND2	1:A:288:ASP:H	1.85	0.74
1:C:6:MET:O	1:C:7:SER:HB2	1.84	0.74
1:B:158:LYS:HE3	1:B:161:ASN:HD21	1.50	0.74
1:A:158:LYS:HG3	1:A:160:HIS:HD2	1.52	0.74
1:D:36:GLN:HE22	2:H:194:PRO:HB2	1.50	0.74
2:E:198:GLN:C	2:E:199:LEU:HD23	2.08	0.73
2:E:191:LYS:HA	2:E:197:TYR:CE1	2.22	0.73
1:D:325:GLN:HG3	1:D:326:GLN:N	2.04	0.73
1:B:300:PHE:HE1	1:B:318:ALA:HB1	1.53	0.73
1:B:189:ASN:ND2	1:B:191:ARG:H	1.87	0.73
1:A:215:MET:HE1	1:A:315:ALA:HA	1.69	0.73
1:B:215:MET:CE	1:B:315:ALA:HA	2.18	0.73
1:B:182:TYR:OH	1:B:184:PRO:HA	1.87	0.73
1:C:165:ASP:OD1	1:C:167:GLU:HB3	1.88	0.73
1:A:100:ILE:C	1:A:100:ILE:HD12	2.08	0.73
1:B:36:GLN:O	1:B:38:ASP:N	2.22	0.73
1:D:314:THR:HG22	1:D:316:LEU:H	1.53	0.72
1:A:33:TRP:CH2	1:A:102:ARG:HG3	2.25	0.72
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.24	0.72
1:B:286:ASN:HD21	1:B:288:ASP:CB	2.03	0.72
2:F:200:GLN:NE2	2:F:202:GLN:NE2	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASN:ND2	1:C:191:ARG:H	1.87	0.72
1:A:106:SER:OG	1:A:107:LYS:N	2.20	0.72
1:B:100:ILE:HD12	1:B:100:ILE:C	2.09	0.72
1:A:286:ASN:ND2	1:A:288:ASP:N	2.38	0.72
1:D:91:GLY:HA3	1:D:146:TYR:CE2	2.25	0.72
1:B:202:LEU:HD11	1:B:213:LEU:HD11	1.71	0.72
1:B:98:LEU:O	1:B:99:ASP:HB2	1.89	0.71
1:D:70:LEU:HD12	1:D:78:ILE:HD13	1.71	0.71
1:B:136:TYR:OH	1:B:166:HIS:HD2	1.72	0.71
2:G:202:GLN:O	2:G:203:ALA:HB2	1.89	0.71
1:B:100:ILE:HD12	1:B:101:VAL:N	2.06	0.71
1:D:129:THR:H	1:D:132:ASP:HB2	1.56	0.71
1:C:215:MET:CE	1:C:315:ALA:HA	2.20	0.71
1:B:84:ILE:CD1	1:B:152:ILE:HD13	2.20	0.71
1:C:314:THR:HG22	1:C:315:ALA:N	2.06	0.71
1:B:161:ASN:O	1:B:174:ILE:HG12	1.91	0.71
1:A:129:THR:HG23	1:A:132:ASP:OD2	1.90	0.71
1:C:242:LEU:HD23	1:C:269:LEU:HD21	1.73	0.71
1:C:251:THR:HG21	1:C:274:GLY:O	1.91	0.71
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.26	0.70
1:B:124:LEU:O	1:B:127:THR:HB	1.91	0.70
1:A:182:TYR:OH	1:A:184:PRO:HA	1.91	0.70
1:A:19:ARG:HB3	1:A:20:PRO:HD2	1.72	0.70
1:D:121:PHE:HB2	1:D:125:TYR:CD2	2.26	0.70
1:D:166:HIS:O	1:D:166:HIS:CG	2.39	0.70
2:F:190:PHE:C	2:F:191:LYS:HG3	2.11	0.70
1:B:212:SER:CB	1:B:309:HIS:HB2	2.21	0.70
1:A:189:ASN:HD22	1:A:189:ASN:C	1.92	0.70
1:C:286:ASN:ND2	1:C:288:ASP:H	1.89	0.70
1:A:202:LEU:HD11	1:A:213:LEU:HD11	1.73	0.70
1:C:36:GLN:O	1:C:38:ASP:N	2.25	0.70
1:B:243:VAL:HG22	1:B:273:VAL:HA	1.73	0.70
1:C:243:VAL:HG22	1:C:273:VAL:HA	1.74	0.70
1:D:332:ASN:N	1:D:332:ASN:HD22	1.88	0.70
1:A:186:LYS:HD3	1:A:188:TYR:CZ	2.26	0.70
1:D:33:TRP:CE3	1:D:102:ARG:HB3	2.26	0.69
1:A:186:LYS:HD3	1:A:188:TYR:CE1	2.27	0.69
1:D:153:MET:HE2	1:D:182:TYR:HD1	1.58	0.69
1:C:6:MET:N	1:C:262:ARG:NH2	2.41	0.69
1:C:36:GLN:HE22	2:G:194:PRO:CB	2.04	0.69
1:C:16:ASN:ND2	1:C:182:TYR:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:O	1:C:82:ILE:HG13	1.93	0.69
1:D:314:THR:CB	1:D:317:GLU:HG3	2.21	0.69
1:A:215:MET:CE	1:A:315:ALA:HA	2.22	0.69
1:C:134:ARG:HG2	1:C:323:TYR:CZ	2.28	0.69
1:C:154:HIS:HE1	1:C:156:ASP:O	1.75	0.69
1:C:102:ARG:HD2	1:C:107:LYS:CD	2.23	0.69
1:A:331:GLU:C	1:A:333:SER:N	2.40	0.69
1:C:33:TRP:CE2	1:C:102:ARG:HD3	2.28	0.68
1:A:103:ASP:HB2	2:F:194:PRO:CG	2.23	0.68
1:C:212:SER:HB2	1:C:309:HIS:HB2	1.74	0.68
1:D:29:LEU:HD12	1:D:79:LYS:HG2	1.74	0.68
1:A:47:ARG:NH2	1:B:120:ASP:OD2	2.25	0.68
1:B:242:LEU:HD23	1:B:269:LEU:HD21	1.74	0.68
1:C:19:ARG:HB3	1:C:20:PRO:HD2	1.76	0.68
1:D:36:GLN:HE22	2:H:194:PRO:CB	2.07	0.68
1:D:124:LEU:O	1:D:127:THR:CG2	2.42	0.68
1:A:103:ASP:HB2	2:F:194:PRO:CB	2.24	0.68
2:G:190:PHE:N	2:G:190:PHE:CD1	2.62	0.68
1:A:105:HIS:HD2	1:A:106:SER:CA	2.07	0.68
1:B:103:ASP:HB2	2:E:194:PRO:HB3	1.76	0.68
2:H:200:GLN:CG	5:H:208:HOH:O	2.28	0.68
2:G:193:HIS:HB3	2:G:194:PRO:HD3	1.75	0.68
1:C:41:VAL:HG12	2:G:197:TYR:CB	2.24	0.67
2:H:197:TYR:H	2:H:197:TYR:HD1	1.40	0.67
1:B:126:PRO:CB	2:F:197:TYR:OH	2.41	0.67
1:B:33:TRP:CE3	1:B:102:ARG:HB2	2.28	0.67
1:B:36:GLN:OE1	1:B:103:ASP:CA	2.39	0.67
1:D:158:LYS:HG2	1:D:161:ASN:ND2	2.06	0.67
1:C:199:GLY:HA2	1:C:216:TRP:CD1	2.29	0.67
1:B:119:THR:CG2	1:B:124:LEU:HB2	2.25	0.67
2:F:198:GLN:HB2	2:F:199:LEU:HG	1.76	0.67
1:D:125:TYR:O	1:D:126:PRO:C	2.30	0.67
2:F:200:GLN:O	2:F:202:GLN:HG2	1.94	0.67
2:H:191:LYS:HA	2:H:197:TYR:HE1	1.59	0.67
1:D:112:ILE:HD12	1:D:112:ILE:N	2.10	0.67
1:B:125:TYR:O	1:B:126:PRO:C	2.30	0.67
1:B:325:GLN:HA	1:B:328:ARG:HH12	1.60	0.67
1:A:243:VAL:HG12	1:A:244:LYS:N	2.10	0.67
1:C:300:PHE:HE1	1:C:318:ALA:HB1	1.59	0.67
1:B:42:VAL:HB	1:B:43:ARG:HH12	1.58	0.67
1:D:186:LYS:HD3	1:D:188:TYR:CE1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:GLU:OE2	2:E:198:GLN:NE2	2.28	0.66
1:A:198:LYS:HB3	1:A:202:LEU:HD12	1.78	0.66
1:B:158:LYS:HD3	1:B:194:SER:HB2	1.77	0.66
1:C:157:VAL:HB	1:C:217:SER:HB2	1.77	0.66
1:B:55:GLU:OE2	1:B:64:LYS:HD3	1.96	0.66
1:D:124:LEU:C	1:D:126:PRO:HD2	2.16	0.66
1:A:269:LEU:O	1:A:273:VAL:HG23	1.95	0.66
1:A:44:LYS:CE	1:A:52:GLU:OE2	2.44	0.66
1:C:289:ASN:OD1	1:C:289:ASN:C	2.34	0.66
1:A:125:TYR:O	1:A:126:PRO:C	2.30	0.66
1:A:103:ASP:HB2	2:F:194:PRO:HG3	1.77	0.66
1:B:117:ASN:HD21	2:F:202:GLN:HB2	1.60	0.65
2:E:193:HIS:CB	2:E:194:PRO:CD	2.64	0.65
1:D:125:TYR:N	1:D:126:PRO:HD2	2.11	0.65
1:A:101:VAL:O	1:A:109:PRO:HA	1.96	0.65
1:A:272:LEU:H	1:A:272:LEU:HD12	1.61	0.65
1:B:64:LYS:HZ2	1:B:64:LYS:HB2	1.57	0.65
1:D:212:SER:HB2	1:D:309:HIS:HB2	1.79	0.65
1:B:314:THR:HG22	1:B:315:ALA:N	2.12	0.65
1:B:192:VAL:O	1:B:198:LYS:HE2	1.96	0.65
1:B:282:LEU:HD22	1:B:282:LEU:N	2.11	0.65
1:A:153:MET:HE2	1:A:182:TYR:HD1	1.61	0.65
1:A:192:VAL:O	1:A:198:LYS:HE2	1.97	0.65
1:C:41:VAL:HB	2:G:197:TYR:HB3	1.79	0.65
1:B:251:THR:HG21	1:B:274:GLY:O	1.95	0.65
2:H:200:GLN:CB	5:H:208:HOH:O	2.45	0.65
1:A:158:LYS:HG3	1:A:160:HIS:CD2	2.30	0.65
1:D:243:VAL:HG22	1:D:273:VAL:HA	1.77	0.65
1:D:50:TYR:O	1:D:71:LYS:HB2	1.96	0.65
1:C:120:ASP:OD1	1:D:44:LYS:HD2	1.96	0.65
1:B:105:HIS:CD2	1:B:106:SER:N	2.65	0.64
1:D:215:MET:CE	1:D:315:ALA:HA	2.24	0.64
1:C:189:ASN:ND2	1:C:190:VAL:N	2.44	0.64
1:C:41:VAL:HG21	2:G:192:ILE:CG2	2.26	0.64
1:B:279:LYS:HD2	1:B:283:LYS:HD2	1.80	0.64
1:D:154:HIS:ND1	1:D:154:HIS:O	2.31	0.64
1:C:102:ARG:HD2	1:C:107:LYS:HD2	1.79	0.64
2:H:199:LEU:HD23	2:H:199:LEU:N	2.12	0.64
1:B:158:LYS:CE	1:B:161:ASN:ND2	2.60	0.64
1:C:29:LEU:HD12	1:C:79:LYS:HG2	1.79	0.64
1:C:73:VAL:HG21	5:C:681:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191:LYS:C	2:H:197:TYR:OH	2.36	0.64
1:C:186:LYS:HD3	1:C:188:TYR:CZ	2.32	0.64
2:H:193:HIS:CB	2:H:194:PRO:CD	2.75	0.64
1:C:325:GLN:HA	1:C:328:ARG:HH12	1.61	0.64
1:A:300:PHE:HE1	1:A:318:ALA:HB1	1.62	0.64
1:A:268:GLN:O	1:A:272:LEU:HD13	1.97	0.64
1:D:212:SER:CB	1:D:309:HIS:HB2	2.27	0.63
1:C:286:ASN:ND2	1:C:288:ASP:N	2.47	0.63
1:B:29:LEU:O	1:B:79:LYS:HE3	1.97	0.63
1:B:239:HIS:CG	1:B:269:LEU:HD13	2.32	0.63
1:B:153:MET:HE2	1:B:182:TYR:HD1	1.63	0.63
1:A:103:ASP:OD1	2:F:194:PRO:HB3	1.98	0.63
1:D:189:ASN:ND2	1:D:191:ARG:H	1.95	0.63
1:A:251:THR:HG21	1:A:274:GLY:O	1.98	0.63
1:C:36:GLN:HE22	2:G:194:PRO:C	2.00	0.63
1:A:36:GLN:O	1:A:38:ASP:N	2.32	0.63
1:B:215:MET:HE2	1:B:315:ALA:HA	1.79	0.63
1:C:332:ASN:N	1:C:332:ASN:HD22	1.96	0.63
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.32	0.63
1:C:41:VAL:HG12	2:G:197:TYR:HB2	1.80	0.63
1:A:31:VAL:CG1	1:A:33:TRP:CE2	2.81	0.63
1:A:125:TYR:CD2	1:A:225:MET:HG2	2.33	0.63
2:G:188:TYR:O	2:G:189:GLY:C	2.35	0.63
1:B:286:ASN:HD22	1:B:288:ASP:H	1.44	0.63
1:C:130:ASP:O	1:C:134:ARG:HG3	1.97	0.63
1:D:45:VAL:O	1:D:45:VAL:HG12	1.97	0.63
1:D:169:ARG:HG3	1:D:169:ARG:NH2	2.00	0.63
1:B:288:ASP:O	1:B:288:ASP:OD2	2.16	0.63
1:A:242:LEU:HD23	1:A:269:LEU:HD21	1.81	0.63
1:C:189:ASN:C	1:C:189:ASN:HD22	2.01	0.63
1:C:189:ASN:HD22	1:C:190:VAL:H	1.46	0.62
1:D:16:ASN:HD22	1:D:183:HIS:CE1	2.17	0.62
1:B:243:VAL:HG12	1:B:244:LYS:N	2.14	0.62
1:D:72:PRO:O	1:D:73:VAL:CG1	2.48	0.62
1:C:36:GLN:C	1:C:38:ASP:H	2.02	0.62
2:F:200:GLN:CB	2:F:202:GLN:NE2	2.52	0.62
1:C:129:THR:H	1:C:132:ASP:HB2	1.64	0.62
1:C:72:PRO:O	1:C:73:VAL:HG13	1.99	0.62
1:D:105:HIS:CD2	1:D:106:SER:N	2.68	0.62
1:C:212:SER:CB	1:C:309:HIS:HB2	2.29	0.62
1:D:198:LYS:HB3	1:D:202:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:CD1	1:D:78:ILE:HD13	2.29	0.62
1:C:325:GLN:HA	1:C:328:ARG:NH1	2.15	0.62
1:B:196:TYR:HA	1:B:241:GLN:HE22	1.64	0.62
1:A:189:ASN:C	1:A:189:ASN:ND2	2.52	0.62
1:B:64:LYS:CB	1:B:64:LYS:NZ	2.62	0.62
1:B:72:PRO:O	1:B:73:VAL:HG13	1.98	0.62
2:F:186:ARG:O	2:F:188:TYR:N	2.33	0.62
1:C:202:LEU:HD11	1:C:213:LEU:HD11	1.82	0.62
1:A:272:LEU:N	1:A:272:LEU:HD12	2.15	0.62
1:A:78:ILE:O	1:A:82:ILE:HG13	2.00	0.62
1:B:16:ASN:OD1	1:B:24:TRP:HB3	2.00	0.62
1:C:119:THR:HB	1:C:124:LEU:HB2	1.82	0.61
1:D:325:GLN:HA	1:D:328:ARG:HH12	1.65	0.61
2:G:193:HIS:CB	2:G:194:PRO:CD	2.75	0.61
1:B:223:ALA:HB2	1:B:301:LEU:HD11	1.82	0.61
1:C:332:ASN:ND2	1:C:332:ASN:N	2.48	0.61
1:D:106:SER:C	1:D:107:LYS:HG3	2.20	0.61
1:D:216:TRP:CZ2	1:D:245:ILE:HD13	2.35	0.61
1:A:105:HIS:CD2	1:A:105:HIS:C	2.73	0.61
1:D:77:LYS:HD3	1:D:77:LYS:O	2.01	0.61
1:C:94:ILE:HG22	1:C:95:VAL:O	2.01	0.61
1:C:104:GLN:OE1	1:C:105:HIS:N	2.33	0.61
1:B:43:ARG:HH11	1:B:43:ARG:CG	1.85	0.61
1:B:216:TRP:HZ2	1:B:245:ILE:HD13	1.65	0.61
1:A:72:PRO:O	1:A:73:VAL:CG1	2.48	0.61
1:A:107:LYS:HE2	1:A:107:LYS:O	2.01	0.61
2:H:198:GLN:HG3	2:H:199:LEU:H	1.64	0.61
1:C:138:TYR:HE2	1:C:331:GLU:OE2	1.84	0.61
1:C:326:GLN:O	1:C:329:ALA:HB3	2.00	0.61
1:B:239:HIS:ND1	1:B:269:LEU:HD13	2.16	0.61
1:A:212:SER:HB2	1:A:309:HIS:HB2	1.82	0.61
1:A:289:ASN:OD1	1:A:289:ASN:C	2.39	0.61
1:B:325:GLN:HA	1:B:328:ARG:NH1	2.16	0.61
1:C:120:ASP:OD2	1:C:122:LYS:HB2	2.01	0.61
2:E:198:GLN:HG3	2:E:199:LEU:N	2.14	0.60
2:G:198:GLN:HB2	5:G:38:HOH:O	2.01	0.60
1:C:19:ARG:HH22	1:C:150:GLN:NE2	1.99	0.60
1:B:129:THR:O	1:B:130:ASP:C	2.39	0.60
1:B:19:ARG:HH22	1:B:150:GLN:NE2	1.99	0.60
1:B:163:MET:HE2	4:B:801:AMP:H2'	1.83	0.60
1:D:180:GLU:OE1	1:D:181:PHE:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:ILE:O	2:H:192:ILE:HG23	2.00	0.60
2:E:191:LYS:CA	2:E:197:TYR:HE1	2.14	0.60
1:A:44:LYS:O	1:A:45:VAL:HG23	2.01	0.60
1:B:288:ASP:OD2	1:B:288:ASP:C	2.40	0.60
1:C:127:THR:O	1:C:127:THR:HG22	2.00	0.60
1:D:215:MET:HG3	1:D:313:LEU:O	2.01	0.60
1:D:286:ASN:ND2	1:D:288:ASP:H	1.99	0.60
1:D:17:VAL:HG12	1:D:18:LEU:HD23	1.83	0.60
2:E:191:LYS:HA	2:E:197:TYR:HE1	1.66	0.60
1:D:112:ILE:CD1	1:D:112:ILE:N	2.65	0.60
1:A:98:LEU:O	1:A:99:ASP:HB2	2.01	0.60
1:B:41:VAL:HG12	1:B:42:VAL:N	2.16	0.60
1:D:158:LYS:HE2	1:D:161:ASN:ND2	2.17	0.60
1:C:154:HIS:ND1	1:C:154:HIS:O	2.34	0.60
1:A:64:LYS:HB2	1:A:64:LYS:NZ	2.17	0.60
1:B:266:ASP:C	1:B:267:PRO:O	2.36	0.60
1:C:165:ASP:OD1	1:C:167:GLU:CB	2.49	0.60
1:A:102:ARG:HD2	1:A:107:LYS:HD3	1.84	0.60
1:B:286:ASN:HD21	1:B:288:ASP:HB3	1.65	0.60
1:A:314:THR:CG2	1:A:315:ALA:N	2.65	0.60
1:B:81:GLU:HG3	1:B:177:GLY:HA2	1.83	0.60
1:D:11:VAL:O	1:D:12:TYR:HB2	2.02	0.60
1:B:106:SER:O	1:B:107:LYS:O	2.20	0.59
1:D:163:MET:HE2	4:D:701:AMP:N3	2.17	0.59
1:A:322:PRO:O	1:A:325:GLN:HG2	2.01	0.59
1:A:325:GLN:HG3	1:A:326:GLN:N	2.17	0.59
2:E:191:LYS:CA	2:E:197:TYR:CE1	2.85	0.59
1:D:186:LYS:HD3	1:D:188:TYR:CZ	2.37	0.59
1:C:163:MET:HE2	4:C:601:AMP:H2'	1.83	0.59
1:A:325:GLN:HG3	1:A:326:GLN:H	1.67	0.59
1:A:212:SER:CB	1:A:309:HIS:HB2	2.32	0.59
1:D:194:SER:O	1:D:195:ARG:C	2.40	0.59
1:D:314:THR:CG2	1:D:315:ALA:N	2.65	0.59
1:A:266:ASP:C	1:A:267:PRO:O	2.33	0.59
1:A:331:GLU:O	1:A:333:SER:N	2.36	0.59
2:H:192:ILE:O	2:H:194:PRO:N	2.35	0.59
1:A:154:HIS:O	1:A:154:HIS:ND1	2.36	0.59
1:B:189:ASN:HD22	1:B:190:VAL:H	1.47	0.59
1:D:286:ASN:ND2	1:D:288:ASP:N	2.50	0.59
1:B:13:ALA:O	1:B:184:PRO:HG3	2.02	0.59
1:D:121:PHE:HB2	1:D:125:TYR:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:192:ILE:O	2:F:193:HIS:C	2.41	0.59
1:A:199:GLY:HA2	1:A:216:TRP:CD1	2.37	0.59
1:B:44:LYS:CE	1:B:47:ARG:HD3	2.33	0.59
1:C:163:MET:HE2	4:C:601:AMP:N3	2.18	0.59
1:C:36:GLN:C	1:C:38:ASP:N	2.56	0.59
1:A:216:TRP:CZ2	1:A:245:ILE:HD13	2.38	0.59
1:A:243:VAL:HG22	1:A:273:VAL:HA	1.85	0.59
2:E:191:LYS:C	2:E:197:TYR:OH	2.41	0.58
1:C:286:ASN:OD1	1:C:289:ASN:ND2	2.37	0.58
1:C:71:LYS:O	1:C:73:VAL:HG22	2.02	0.58
1:C:44:LYS:HD3	1:D:120:ASP:OD2	2.03	0.58
1:B:199:GLY:HA2	1:B:216:TRP:CD1	2.37	0.58
1:D:19:ARG:HH22	1:D:150:GLN:NE2	2.00	0.58
1:A:36:GLN:C	1:A:38:ASP:H	2.07	0.58
1:C:198:LYS:HB3	1:C:202:LEU:HD12	1.84	0.58
1:D:36:GLN:NE2	2:H:194:PRO:CB	2.61	0.58
1:A:112:ILE:HD12	1:A:112:ILE:N	2.17	0.58
1:D:96:LYS:HG2	1:D:98:LEU:HD13	1.86	0.58
1:D:325:GLN:HA	1:D:328:ARG:NH1	2.18	0.58
1:A:35:GLU:OE1	1:A:36:GLN:N	2.36	0.58
1:C:243:VAL:HG12	1:C:244:LYS:N	2.17	0.58
1:C:169:ARG:NH2	1:C:169:ARG:HG3	2.15	0.58
1:C:42:VAL:HG23	1:C:56:GLY:HA2	1.85	0.58
1:D:197:PHE:N	1:D:197:PHE:CD2	2.71	0.58
1:A:10:ARG:O	1:A:11:VAL:CG2	2.51	0.58
1:C:174:ILE:HG13	1:C:175:ASP:N	2.19	0.58
1:D:242:LEU:CD2	1:D:269:LEU:HD21	2.34	0.58
2:F:188:TYR:CE1	2:F:191:LYS:HD3	2.39	0.58
1:A:129:THR:H	1:A:132:ASP:HB2	1.67	0.58
2:F:200:GLN:NE2	2:F:202:GLN:HE21	1.83	0.58
1:A:121:PHE:O	1:A:122:LYS:C	2.39	0.58
1:B:200:PRO:O	1:B:204:VAL:HG22	2.03	0.58
1:C:64:LYS:NZ	1:C:64:LYS:HB2	2.19	0.58
1:B:289:ASN:C	1:B:289:ASN:OD1	2.41	0.57
1:D:124:LEU:HD12	1:D:127:THR:CG2	2.26	0.57
1:D:314:THR:HG22	1:D:316:LEU:N	2.19	0.57
1:D:289:ASN:C	1:D:289:ASN:OD1	2.40	0.57
1:C:182:TYR:OH	1:C:184:PRO:HA	2.03	0.57
1:C:294:SER:O	1:C:295:PRO:C	2.40	0.57
1:D:300:PHE:CE1	1:D:318:ALA:HB1	2.36	0.57
1:B:36:GLN:C	1:B:38:ASP:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASN:ND2	1:B:190:VAL:N	2.47	0.57
1:C:322:PRO:O	1:C:325:GLN:HG2	2.04	0.57
1:D:196:TYR:HB2	1:D:197:PHE:CD2	2.40	0.57
1:B:264:GLU:OE2	1:C:76:LYS:CB	2.48	0.57
1:B:36:GLN:NE2	2:E:194:PRO:CB	2.67	0.57
1:B:141:LEU:CD2	1:B:319:MET:HG2	2.13	0.57
1:C:118:ASN:CG	1:C:163:MET:CE	2.72	0.57
2:H:188:TYR:N	2:H:188:TYR:HD2	2.02	0.57
1:C:268:GLN:O	1:C:272:LEU:HD13	2.05	0.56
2:H:188:TYR:CD2	2:H:188:TYR:N	2.73	0.56
1:C:91:GLY:HA3	1:C:146:TYR:CE2	2.40	0.56
1:C:267:PRO:O	1:C:268:GLN:CB	2.46	0.56
1:D:326:GLN:O	1:D:329:ALA:HB3	2.04	0.56
1:D:153:MET:HE2	1:D:182:TYR:CD1	2.39	0.56
1:A:124:LEU:O	1:A:127:THR:HB	2.04	0.56
1:A:294:SER:O	1:A:295:PRO:C	2.41	0.56
1:D:120:ASP:O	1:D:123:VAL:HG12	2.05	0.56
1:A:105:HIS:HD2	1:A:106:SER:HA	1.69	0.56
1:B:103:ASP:HB2	2:E:194:PRO:CB	2.34	0.56
1:B:103:ASP:CB	2:E:194:PRO:HB3	2.35	0.56
1:B:286:ASN:ND2	1:B:288:ASP:HB3	2.19	0.56
1:A:314:THR:HG22	1:A:315:ALA:H	1.67	0.56
1:C:314:THR:CG2	1:C:315:ALA:N	2.69	0.56
1:D:300:PHE:CZ	1:D:304:LEU:HD11	2.40	0.56
1:C:50:TYR:O	1:C:71:LYS:HB2	2.06	0.56
1:A:10:ARG:C	1:A:11:VAL:HG23	2.24	0.56
1:C:33:TRP:CE3	1:C:100:ILE:CD1	2.81	0.56
2:E:197:TYR:CD1	2:E:197:TYR:N	2.73	0.56
1:A:258:LEU:HD11	1:A:265:LEU:HD13	1.87	0.56
1:B:118:ASN:C	1:B:118:ASN:OD1	2.43	0.56
2:F:202:GLN:O	2:F:203:ALA:CB	2.53	0.56
1:C:123:VAL:HG13	2:H:197:TYR:HD2	1.70	0.56
1:D:332:ASN:H	1:D:332:ASN:ND2	1.99	0.56
1:B:286:ASN:OD1	1:B:289:ASN:ND2	2.38	0.56
1:C:155:ARG:NH1	1:C:209:TYR:OH	2.38	0.56
1:A:163:MET:HE2	4:A:501:AMP:C4	2.41	0.56
1:A:272:LEU:H	1:A:272:LEU:CD1	2.19	0.56
1:B:215:MET:HE2	1:B:315:ALA:CA	2.34	0.56
1:D:243:VAL:HG12	1:D:244:LYS:N	2.21	0.56
1:C:41:VAL:CB	2:G:197:TYR:HB3	2.36	0.56
2:F:202:GLN:O	2:F:203:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ASN:OD1	1:D:289:ASN:ND2	2.39	0.56
1:C:47:ARG:CG	1:C:47:ARG:O	2.53	0.56
1:C:36:GLN:CD	2:G:194:PRO:HB2	2.26	0.56
1:B:158:LYS:HE2	1:B:161:ASN:HD21	1.71	0.56
1:B:156:ASP:HB2	1:B:178:LEU:HD12	1.88	0.56
1:B:326:GLN:O	1:B:329:ALA:HB3	2.06	0.56
1:D:47:ARG:CG	1:D:47:ARG:O	2.54	0.56
1:C:33:TRP:CE3	1:C:102:ARG:HB2	2.41	0.55
1:C:33:TRP:CZ3	1:C:100:ILE:CD1	2.88	0.55
1:D:272:LEU:HD12	1:D:272:LEU:H	1.71	0.55
1:D:269:LEU:O	1:D:273:VAL:HG23	2.06	0.55
1:B:108:THR:HG22	1:B:108:THR:O	2.07	0.55
1:C:282:LEU:N	1:C:282:LEU:HD22	2.21	0.55
1:D:189:ASN:HD22	1:D:189:ASN:C	2.07	0.55
1:A:211:TYR:O	1:A:213:LEU:N	2.40	0.55
1:C:47:ARG:HG3	1:C:47:ARG:O	2.07	0.55
1:B:282:LEU:CD2	1:B:282:LEU:N	2.69	0.55
1:D:294:SER:O	1:D:295:PRO:C	2.43	0.55
1:B:15:VAL:HG11	1:B:149:SER:O	2.06	0.55
1:D:19:ARG:HB3	1:D:20:PRO:HD2	1.89	0.55
1:D:128:LEU:HB3	1:D:132:ASP:HB3	1.87	0.55
2:G:198:GLN:CB	5:G:38:HOH:O	2.55	0.55
1:A:197:PHE:N	1:A:197:PHE:CD2	2.74	0.55
1:A:116:VAL:HG12	1:A:117:ASN:O	2.06	0.55
1:A:189:ASN:ND2	1:A:190:VAL:N	2.46	0.55
1:C:192:VAL:HG23	1:C:202:LEU:HD13	1.88	0.55
1:D:199:GLY:HA2	1:D:216:TRP:CD1	2.42	0.55
1:A:282:LEU:HD22	1:A:282:LEU:N	2.22	0.55
1:B:36:GLN:NE2	2:E:194:PRO:HB2	2.21	0.55
1:C:269:LEU:O	1:C:273:VAL:HG23	2.06	0.55
1:B:189:ASN:C	1:B:189:ASN:HD22	2.09	0.55
2:F:193:HIS:HB3	2:F:194:PRO:HD3	1.89	0.55
1:C:125:TYR:O	1:C:126:PRO:O	2.23	0.55
1:C:325:GLN:HG3	1:C:326:GLN:H	1.72	0.55
1:D:200:PRO:O	1:D:204:VAL:HG22	2.06	0.55
1:C:314:THR:HG22	1:C:316:LEU:H	1.72	0.55
1:D:72:PRO:C	1:D:73:VAL:HG13	2.27	0.55
1:C:180:GLU:OE1	1:C:181:PHE:N	2.31	0.55
1:C:229:LYS:HD3	1:C:232:PHE:CD1	2.42	0.55
2:G:202:GLN:O	2:G:203:ALA:CB	2.55	0.54
1:D:186:LYS:O	1:D:208:ASP:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLN:CD	2:E:194:PRO:CB	2.73	0.54
2:E:192:ILE:O	2:E:194:PRO:N	2.41	0.54
1:D:303:LYS:HB3	1:D:313:LEU:HD21	1.89	0.54
1:D:84:ILE:HD12	1:D:152:ILE:HD13	1.88	0.54
1:B:186:LYS:HD3	1:B:188:TYR:CE1	2.42	0.54
1:D:37:ASP:N	1:D:37:ASP:OD2	2.38	0.54
1:B:77:LYS:O	1:B:77:LYS:HD3	2.08	0.54
1:D:36:GLN:NE2	2:H:194:PRO:C	2.61	0.54
1:D:136:TYR:OH	1:D:166:HIS:HD2	1.90	0.54
1:A:31:VAL:HG12	1:A:33:TRP:CE2	2.42	0.54
1:B:103:ASP:CG	2:E:194:PRO:HB3	2.28	0.54
1:B:88:LEU:O	1:B:89:CYS:C	2.44	0.54
1:D:182:TYR:HH	1:D:184:PRO:HA	1.69	0.54
1:A:128:LEU:HB3	1:A:132:ASP:CB	2.36	0.54
2:F:188:TYR:HD1	2:F:191:LYS:HD2	1.71	0.54
2:G:198:GLN:C	2:G:199:LEU:HG	2.28	0.54
1:B:158:LYS:HD3	1:B:194:SER:CB	2.37	0.54
1:A:157:VAL:O	1:A:217:SER:HB3	2.07	0.54
1:C:102:ARG:HD2	1:C:107:LYS:HD3	1.89	0.54
1:A:112:ILE:CD1	1:A:112:ILE:N	2.71	0.54
1:A:69:ILE:HG12	1:A:110:SER:OG	2.07	0.54
1:A:160:HIS:O	4:A:501:AMP:O3P	2.25	0.54
1:A:66:ILE:HG13	4:A:501:AMP:N6	2.23	0.54
1:B:133:ILE:O	1:B:134:ARG:C	2.46	0.54
1:D:267:PRO:O	1:D:268:GLN:CB	2.52	0.54
1:B:12:TYR:HB3	1:B:15:VAL:CG2	2.38	0.54
1:A:72:PRO:C	1:A:73:VAL:HG13	2.27	0.54
1:B:198:LYS:HB3	1:B:202:LEU:HD12	1.89	0.54
1:C:82:ILE:O	1:C:86:GLN:HG3	2.08	0.54
1:A:103:ASP:CG	2:F:194:PRO:HB3	2.28	0.54
1:D:153:MET:CE	1:D:182:TYR:HD1	2.20	0.54
1:A:153:MET:O	1:A:179:ALA:HA	2.08	0.54
1:D:29:LEU:O	1:D:79:LYS:HE3	2.08	0.54
1:D:308:ASP:OD1	1:D:310:GLN:HB2	2.08	0.54
1:B:82:ILE:O	1:B:86:GLN:HG3	2.08	0.54
1:C:258:LEU:HD11	1:C:265:LEU:HD13	1.89	0.54
1:C:133:ILE:O	1:C:134:ARG:C	2.45	0.54
1:C:325:GLN:HG3	1:C:326:GLN:N	2.23	0.54
1:D:272:LEU:N	1:D:272:LEU:HD12	2.23	0.54
1:B:127:THR:HA	2:F:190:PHE:CZ	2.40	0.54
1:D:160:HIS:N	1:D:160:HIS:CD2	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NH1	1:B:209:TYR:OH	2.40	0.54
1:A:103:ASP:HB2	2:F:194:PRO:HB3	1.89	0.54
1:D:266:ASP:C	1:D:267:PRO:O	2.40	0.54
1:A:128:LEU:HB3	1:A:132:ASP:HB3	1.90	0.54
1:A:154:HIS:O	1:A:156:ASP:N	2.41	0.54
1:A:101:VAL:O	1:A:101:VAL:HG23	2.08	0.53
1:B:121:PHE:HB2	1:B:125:TYR:CD2	2.42	0.53
1:A:136:TYR:OH	1:A:166:HIS:CD2	2.51	0.53
1:B:17:VAL:HG12	1:B:18:LEU:HD23	1.90	0.53
1:C:194:SER:O	1:C:195:ARG:C	2.47	0.53
1:B:264:GLU:HG3	1:C:76:LYS:HD3	1.90	0.53
1:C:246:ALA:O	1:C:250:GLY:N	2.39	0.53
1:D:36:GLN:O	1:D:38:ASP:N	2.41	0.53
2:E:189:GLY:O	2:E:191:LYS:HG2	2.08	0.53
1:C:98:LEU:O	1:C:99:ASP:HB2	2.08	0.53
1:C:138:TYR:CE2	1:C:331:GLU:OE2	2.61	0.53
1:B:322:PRO:O	1:B:325:GLN:HG2	2.09	0.53
1:C:121:PHE:CE1	1:C:159:PRO:HB2	2.44	0.53
1:D:21:LYS:HG3	1:D:24:TRP:CH2	2.44	0.53
1:C:266:ASP:C	1:C:267:PRO:O	2.41	0.53
1:D:107:LYS:O	1:D:109:PRO:HD3	2.09	0.53
1:C:103:ASP:O	1:C:107:LYS:HA	2.09	0.53
2:E:198:GLN:HA	2:E:198:GLN:HE21	1.74	0.53
1:A:158:LYS:HE2	1:A:160:HIS:HB2	1.90	0.53
1:B:42:VAL:CB	1:B:43:ARG:HH12	2.21	0.53
1:A:52:GLU:HG2	1:A:54:PHE:CE1	2.44	0.53
1:B:66:ILE:HG13	4:B:801:AMP:C6	2.44	0.53
1:A:10:ARG:O	1:A:11:VAL:HG23	2.09	0.53
1:D:237:ASP:OD1	1:D:238:ASN:N	2.42	0.53
1:C:116:VAL:HG12	1:C:117:ASN:O	2.09	0.53
1:A:33:TRP:CZ3	1:A:100:ILE:CD1	2.91	0.53
1:B:44:LYS:HE3	1:B:47:ARG:HD3	1.91	0.53
1:B:129:THR:HG23	1:B:132:ASP:OD2	2.09	0.53
1:C:44:LYS:CE	1:C:52:GLU:OE2	2.56	0.53
2:F:193:HIS:CB	2:F:194:PRO:HD3	2.39	0.53
1:A:120:ASP:OD2	1:A:120:ASP:C	2.47	0.53
1:C:296:GLU:O	1:C:297:ALA:C	2.47	0.53
1:D:251:THR:HG21	1:D:274:GLY:O	2.09	0.53
1:C:200:PRO:HD3	1:C:216:TRP:CE2	2.44	0.52
1:B:155:ARG:HD2	1:B:209:TYR:OH	2.09	0.52
1:B:252:ASP:O	1:B:256:VAL:HG23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:187:LEU:C	2:F:187:LEU:HD12	2.29	0.52
1:A:33:TRP:CE3	1:A:102:ARG:HG3	2.45	0.52
1:C:192:VAL:O	1:C:198:LYS:HE2	2.09	0.52
1:B:130:ASP:O	1:B:134:ARG:HG3	2.10	0.52
1:B:194:SER:O	1:B:195:ARG:C	2.48	0.52
1:B:175:ASP:HB2	4:B:801:AMP:O2P	2.09	0.52
1:D:128:LEU:HB3	1:D:132:ASP:CB	2.39	0.52
2:E:192:ILE:HB	2:E:197:TYR:CE2	2.45	0.52
2:E:198:GLN:CA	2:E:198:GLN:HE21	2.21	0.52
1:A:44:LYS:HD3	1:A:47:ARG:CZ	2.40	0.52
1:B:156:ASP:CG	1:B:158:LYS:HE2	2.30	0.52
1:D:192:VAL:O	1:D:198:LYS:HE2	2.08	0.52
1:A:82:ILE:O	1:A:86:GLN:HG3	2.09	0.52
1:C:36:GLN:NE2	2:G:194:PRO:O	2.42	0.52
1:A:44:LYS:HD2	1:B:120:ASP:OD2	2.09	0.52
2:G:191:LYS:HG2	2:G:196:ALA:HA	1.90	0.52
1:B:121:PHE:CD2	1:B:122:LYS:HG2	2.44	0.52
2:F:190:PHE:O	2:F:196:ALA:HA	2.10	0.52
1:D:258:LEU:HD11	1:D:265:LEU:HD13	1.90	0.52
1:A:19:ARG:HH22	1:A:150:GLN:NE2	2.07	0.52
1:B:229:LYS:HD3	1:B:232:PHE:CD1	2.44	0.52
1:C:154:HIS:O	1:C:154:HIS:CG	2.61	0.52
1:C:300:PHE:CE1	1:C:318:ALA:HB1	2.42	0.52
1:C:103:ASP:HB2	2:G:194:PRO:CG	2.39	0.52
1:A:215:MET:HG3	1:A:313:LEU:O	2.09	0.52
1:D:52:GLU:HG2	1:D:54:PHE:CE1	2.45	0.52
1:D:138:TYR:HE2	1:D:331:GLU:OE2	1.92	0.52
1:D:126:PRO:HG2	1:D:127:THR:H	1.74	0.52
1:B:29:LEU:HD12	1:B:79:LYS:HG2	1.91	0.52
1:D:134:ARG:HG2	1:D:323:TYR:CZ	2.45	0.52
1:C:112:ILE:N	1:C:112:ILE:HD12	2.25	0.52
1:C:41:VAL:O	2:G:197:TYR:HB2	2.09	0.52
1:A:36:GLN:O	1:A:39:TYR:N	2.37	0.52
1:C:136:TYR:OH	1:C:166:HIS:CD2	2.54	0.52
1:D:282:LEU:N	1:D:282:LEU:HD22	2.25	0.52
1:B:228:ARG:HD2	1:B:288:ASP:OD2	2.10	0.51
1:B:282:LEU:CD2	1:B:282:LEU:H	2.23	0.51
1:C:102:ARG:HH11	1:C:107:LYS:CD	2.16	0.51
1:B:103:ASP:O	1:B:104:GLN:C	2.49	0.51
2:H:190:PHE:O	2:H:197:TYR:HE1	1.93	0.51
1:D:33:TRP:CZ3	1:D:102:ARG:CB	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:HD21	1:B:288:ASP:CA	2.23	0.51
1:A:127:THR:O	1:A:127:THR:HG23	2.09	0.51
1:C:154:HIS:O	1:C:156:ASP:N	2.43	0.51
1:D:157:VAL:HB	1:D:217:SER:HB2	1.93	0.51
1:A:138:TYR:HB2	1:A:324:PHE:CD1	2.46	0.51
2:G:188:TYR:HE2	5:G:246:HOH:O	1.93	0.51
1:C:158:LYS:HD2	1:C:160:HIS:CD2	2.46	0.51
1:B:64:LYS:HZ3	1:B:64:LYS:CB	2.23	0.51
1:C:29:LEU:O	1:C:79:LYS:HE3	2.10	0.51
1:B:196:TYR:HA	1:B:241:GLN:NE2	2.25	0.51
1:C:41:VAL:HG21	2:G:192:ILE:HG21	1.91	0.51
1:B:157:VAL:HB	1:B:217:SER:CB	2.41	0.51
1:D:82:ILE:O	1:D:86:GLN:HG3	2.09	0.51
1:C:300:PHE:CZ	1:C:304:LEU:HD11	2.45	0.51
1:D:154:HIS:O	1:D:156:ASP:N	2.44	0.51
1:A:263:ILE:HD11	5:A:536:HOH:O	2.11	0.51
1:D:33:TRP:CZ3	1:D:102:ARG:HB2	2.46	0.51
1:B:189:ASN:C	1:B:189:ASN:ND2	2.64	0.51
1:B:19:ARG:HB3	1:B:20:PRO:HD2	1.93	0.51
1:B:42:VAL:HB	1:B:43:ARG:HH11	1.69	0.51
1:B:242:LEU:CD2	1:B:269:LEU:HD21	2.40	0.51
1:C:14:ASP:O	1:C:17:VAL:N	2.44	0.51
1:A:296:GLU:O	1:A:297:ALA:C	2.49	0.51
1:C:189:ASN:C	1:C:189:ASN:ND2	2.59	0.51
1:B:129:THR:H	1:B:132:ASP:HB2	1.76	0.51
1:A:44:LYS:HE2	1:A:47:ARG:HG3	1.86	0.51
1:B:12:TYR:HB3	1:B:15:VAL:HG21	1.92	0.51
1:D:106:SER:C	1:D:107:LYS:CG	2.79	0.51
1:C:118:ASN:CG	1:C:163:MET:HE3	2.30	0.51
1:A:29:LEU:O	1:A:79:LYS:HE3	2.11	0.51
1:A:308:ASP:OD1	1:A:310:GLN:HB2	2.11	0.51
1:A:105:HIS:O	1:A:106:SER:C	2.48	0.51
2:F:191:LYS:HA	2:F:195:MET:O	2.11	0.51
1:B:117:ASN:ND2	2:F:202:GLN:HB2	2.26	0.51
1:B:31:VAL:CG1	1:B:33:TRP:CE2	2.94	0.51
2:H:190:PHE:O	2:H:197:TYR:CE1	2.63	0.51
1:B:272:LEU:HD12	1:B:272:LEU:H	1.76	0.51
1:A:286:ASN:HD21	1:A:288:ASP:N	2.09	0.51
1:A:291:HIS:CD2	1:A:291:HIS:H	2.28	0.51
1:A:131:TYR:O	1:A:132:ASP:C	2.47	0.51
1:C:153:MET:HE2	1:C:182:TYR:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:HIS:CE1	1:C:156:ASP:O	2.60	0.51
1:C:45:VAL:HG22	1:C:45:VAL:O	2.11	0.51
1:D:103:ASP:HA	2:H:194:PRO:HB3	1.92	0.50
1:B:36:GLN:C	1:B:38:ASP:N	2.63	0.50
1:C:84:ILE:O	1:C:87:ASN:HB2	2.09	0.50
2:H:198:GLN:HG3	2:H:199:LEU:N	2.25	0.50
1:C:124:LEU:O	1:C:124:LEU:HD12	2.11	0.50
1:A:195:ARG:HH11	1:A:195:ARG:HG3	1.74	0.50
1:B:158:LYS:NZ	1:B:194:SER:OG	2.39	0.50
1:D:223:ALA:HB2	1:D:301:LEU:CD1	2.38	0.50
1:C:118:ASN:CG	1:C:163:MET:HE1	2.31	0.50
1:D:94:ILE:HG22	1:D:95:VAL:O	2.11	0.50
1:A:50:TYR:O	1:A:71:LYS:HB2	2.11	0.50
2:F:191:LYS:CG	2:F:196:ALA:HA	2.40	0.50
2:E:191:LYS:C	2:E:197:TYR:HH	2.14	0.50
1:B:96:LYS:N	1:B:114:GLU:OE2	2.44	0.50
1:C:11:VAL:O	1:C:12:TYR:HB2	2.10	0.50
1:D:318:ALA:C	1:D:320:THR:H	2.14	0.50
1:D:71:LYS:O	1:D:73:VAL:HG22	2.12	0.50
1:A:194:SER:O	1:A:195:ARG:C	2.47	0.50
2:H:197:TYR:C	2:H:198:GLN:O	2.47	0.50
1:B:210:ASP:OD1	1:B:212:SER:N	2.35	0.50
1:C:125:TYR:HA	1:C:128:LEU:HG	1.93	0.50
2:F:191:LYS:HG2	2:F:196:ALA:CA	2.39	0.50
1:A:29:LEU:HD12	1:A:79:LYS:HG2	1.93	0.50
1:D:129:THR:N	1:D:132:ASP:HB2	2.25	0.50
2:E:194:PRO:HD2	2:E:195:MET:SD	2.52	0.50
2:E:192:ILE:N	2:E:197:TYR:CZ	2.80	0.50
2:H:191:LYS:CA	2:H:197:TYR:HE1	2.23	0.50
1:D:119:THR:HG1	1:D:124:LEU:HB2	1.74	0.50
1:A:36:GLN:C	1:A:38:ASP:N	2.65	0.50
1:D:268:GLN:O	1:D:271:ALA:HB3	2.11	0.50
1:C:223:ALA:HB2	1:C:301:LEU:HD11	1.93	0.50
1:B:84:ILE:CD1	1:B:152:ILE:CD1	2.89	0.50
1:A:211:TYR:O	1:A:212:SER:C	2.48	0.50
1:A:286:ASN:HD22	1:A:288:ASP:H	1.57	0.49
1:C:272:LEU:HD12	1:C:272:LEU:H	1.77	0.49
1:C:286:ASN:HD22	1:C:288:ASP:H	1.59	0.49
1:D:12:TYR:O	1:D:15:VAL:HG23	2.12	0.49
1:C:118:ASN:CB	1:C:163:MET:HE3	2.41	0.49
1:D:279:LYS:HD3	1:D:280:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:HIS:HA	1:C:152:ILE:O	2.12	0.49
1:B:169:ARG:NH2	1:B:169:ARG:CG	2.68	0.49
1:B:169:ARG:NH2	1:B:169:ARG:HG3	2.13	0.49
1:A:77:LYS:HD3	1:A:77:LYS:O	2.12	0.49
1:D:291:HIS:H	1:D:291:HIS:CD2	2.29	0.49
1:B:264:GLU:H	1:C:76:LYS:NZ	2.10	0.49
1:C:24:TRP:HA	1:C:181:PHE:CZ	2.47	0.49
1:D:106:SER:OG	1:D:108:THR:HB	2.12	0.49
1:D:197:PHE:N	1:D:197:PHE:HD2	2.09	0.49
1:C:41:VAL:CG1	2:G:197:TYR:HB3	2.42	0.49
1:B:105:HIS:HD2	1:B:106:SER:N	2.09	0.49
1:B:200:PRO:HD3	1:B:216:TRP:CE2	2.47	0.49
1:D:106:SER:C	1:D:108:THR:H	2.15	0.49
1:B:33:TRP:CZ2	1:B:102:ARG:HD3	2.47	0.49
1:B:35:GLU:O	1:B:36:GLN:C	2.51	0.49
1:A:286:ASN:OD1	1:A:289:ASN:CG	2.51	0.49
1:D:216:TRP:HZ2	1:D:245:ILE:HD13	1.76	0.49
1:D:119:THR:HA	2:G:202:GLN:NE2	2.28	0.49
1:D:167:GLU:CG	1:D:168:LEU:N	2.72	0.49
1:D:98:LEU:HB2	1:D:112:ILE:O	2.12	0.49
1:B:14:ASP:O	1:B:15:VAL:C	2.46	0.49
1:A:326:GLN:O	1:A:329:ALA:HB3	2.13	0.49
1:A:154:HIS:CE1	1:A:156:ASP:HB3	2.47	0.49
1:C:121:PHE:CD1	1:C:159:PRO:HB2	2.48	0.49
1:A:19:ARG:CB	1:A:20:PRO:HD2	2.39	0.49
1:A:97:LEU:HD12	1:A:98:LEU:N	2.28	0.49
1:A:154:HIS:O	1:A:154:HIS:CG	2.65	0.49
1:D:138:TYR:CE2	1:D:331:GLU:OE2	2.66	0.49
1:A:31:VAL:HG11	1:A:33:TRP:CE2	2.47	0.49
1:D:163:MET:HE2	4:D:701:AMP:H2'	1.93	0.49
1:D:123:VAL:HG13	1:D:124:LEU:N	2.26	0.49
2:E:193:HIS:HB2	2:E:194:PRO:HD3	1.88	0.49
1:A:204:VAL:HG12	1:A:265:LEU:HD11	1.94	0.49
1:D:157:VAL:HB	1:D:217:SER:CB	2.43	0.49
1:D:36:GLN:OE1	2:H:194:PRO:CB	2.48	0.48
1:A:163:MET:HE2	4:A:501:AMP:N3	2.28	0.48
1:B:195:ARG:HG3	1:B:195:ARG:HH11	1.78	0.48
1:A:129:THR:O	1:A:130:ASP:C	2.51	0.48
1:B:262:ARG:HA	5:B:1070:HOH:O	2.12	0.48
1:C:33:TRP:CH2	1:C:102:ARG:HD3	2.47	0.48
2:H:200:GLN:NE2	2:H:201:LEU:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ILE:CG1	1:D:227:PHE:N	2.76	0.48
1:D:158:LYS:HD2	1:D:160:HIS:CD2	2.48	0.48
1:B:10:ARG:HG3	1:B:11:VAL:HG23	1.95	0.48
1:A:288:ASP:O	1:A:291:HIS:HD2	1.97	0.48
1:B:300:PHE:CE1	1:B:318:ALA:HB1	2.40	0.48
1:D:279:LYS:HD2	1:D:283:LYS:HD2	1.94	0.48
2:H:192:ILE:O	2:H:192:ILE:CG2	2.61	0.48
1:A:267:PRO:O	1:A:268:GLN:CB	2.53	0.48
1:A:300:PHE:CE1	1:A:318:ALA:HB1	2.47	0.48
1:D:196:TYR:HA	1:D:241:GLN:NE2	2.27	0.48
1:B:180:GLU:OE1	1:B:181:PHE:N	2.36	0.48
1:B:121:PHE:CE2	1:B:122:LYS:HG2	2.48	0.48
1:B:153:MET:O	1:B:179:ALA:HA	2.13	0.48
1:B:308:ASP:OD1	1:B:310:GLN:HB2	2.14	0.48
1:B:44:LYS:NZ	1:B:47:ARG:CD	2.71	0.48
1:C:169:ARG:CG	1:C:169:ARG:NH2	2.68	0.48
1:D:196:TYR:HA	1:D:241:GLN:HE22	1.78	0.48
2:E:202:GLN:O	2:E:202:GLN:CG	2.62	0.48
1:A:94:ILE:HG22	1:A:95:VAL:O	2.14	0.48
1:D:129:THR:O	1:D:130:ASP:C	2.51	0.48
1:D:134:ARG:HG2	1:D:323:TYR:CE2	2.48	0.48
1:D:129:THR:O	1:D:132:ASP:N	2.47	0.48
1:C:131:TYR:O	1:C:132:ASP:C	2.52	0.48
1:D:122:LYS:O	2:G:192:ILE:HD12	2.13	0.48
2:F:188:TYR:CD1	2:F:191:LYS:CD	2.96	0.48
1:C:153:MET:O	1:C:179:ALA:HA	2.13	0.48
1:A:242:LEU:CD2	1:A:269:LEU:HD21	2.44	0.48
1:B:78:ILE:O	1:B:82:ILE:HG13	2.13	0.48
1:B:52:GLU:HG2	1:B:54:PHE:CE1	2.48	0.48
1:D:119:THR:CA	2:G:202:GLN:NE2	2.77	0.48
1:D:98:LEU:O	1:D:99:ASP:HB2	2.14	0.48
1:D:222:PHE:O	1:D:223:ALA:C	2.53	0.48
1:A:286:ASN:ND2	1:A:289:ASN:H	2.12	0.48
1:A:192:VAL:HG23	1:A:202:LEU:HD13	1.96	0.48
1:A:223:ALA:HB2	1:A:301:LEU:HD11	1.96	0.48
1:B:138:TYR:HB2	1:B:324:PHE:CD1	2.49	0.48
1:A:33:TRP:HE3	1:A:101:VAL:HA	1.79	0.47
1:C:123:VAL:CG1	1:C:123:VAL:O	2.60	0.47
2:H:191:LYS:HA	2:H:197:TYR:CE1	2.45	0.47
1:B:96:LYS:CG	1:B:98:LEU:HD13	2.44	0.47
1:A:200:PRO:O	1:A:204:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:PHE:O	1:D:301:LEU:C	2.52	0.47
1:B:279:LYS:HD3	1:B:280:PRO:HD2	1.96	0.47
2:F:194:PRO:HD2	2:F:195:MET:CG	2.37	0.47
1:D:314:THR:HG22	1:D:315:ALA:H	1.77	0.47
1:A:44:LYS:HZ3	1:A:47:ARG:HE	1.63	0.47
1:C:124:LEU:HD11	1:C:128:LEU:HD21	1.96	0.47
1:C:247:LYS:HG2	1:C:276:HIS:CE1	2.48	0.47
1:B:249:LEU:HD12	1:B:249:LEU:N	2.29	0.47
1:B:100:ILE:CD1	1:B:100:ILE:C	2.77	0.47
1:B:132:ASP:OD1	1:B:169:ARG:NH1	2.46	0.47
1:D:182:TYR:CZ	1:D:184:PRO:HA	2.47	0.47
1:D:202:LEU:HD11	1:D:213:LEU:CD1	2.41	0.47
2:G:197:TYR:CD1	2:G:197:TYR:C	2.87	0.47
2:F:188:TYR:HE1	2:F:191:LYS:HD3	1.77	0.47
2:E:197:TYR:O	2:E:198:GLN:O	2.32	0.47
1:B:258:LEU:HD11	1:B:265:LEU:HD13	1.97	0.47
1:D:50:TYR:C	1:D:71:LYS:HB2	2.35	0.47
1:B:186:LYS:HD3	1:B:188:TYR:CZ	2.50	0.47
1:C:36:GLN:HE21	2:G:195:MET:HA	1.78	0.47
1:D:129:THR:HG23	1:D:132:ASP:OD2	2.14	0.47
1:C:166:HIS:O	1:C:169:ARG:HD2	2.14	0.47
1:B:254:LEU:O	1:B:258:LEU:HG	2.15	0.47
1:A:153:MET:HE2	1:A:182:TYR:CD1	2.45	0.47
1:A:74:LYS:HD3	1:D:264:GLU:HB2	1.97	0.47
1:C:98:LEU:HD22	1:C:114:GLU:N	2.29	0.47
1:D:189:ASN:C	1:D:189:ASN:ND2	2.68	0.47
1:B:154:HIS:HE1	1:B:156:ASP:O	1.97	0.47
1:B:157:VAL:HB	1:B:217:SER:HB2	1.96	0.47
1:A:134:ARG:HG2	1:A:323:TYR:CE2	2.49	0.47
1:B:175:ASP:C	1:B:177:GLY:H	2.18	0.47
1:A:196:TYR:HB2	1:A:197:PHE:CD2	2.50	0.47
1:C:11:VAL:HG12	1:C:12:TYR:CD2	2.50	0.47
1:A:288:ASP:O	1:A:291:HIS:CD2	2.68	0.47
1:A:129:THR:N	1:A:132:ASP:HB2	2.30	0.47
1:C:129:THR:O	1:C:130:ASP:C	2.53	0.47
1:D:196:TYR:HB2	1:D:197:PHE:HD2	1.79	0.47
1:C:229:LYS:HD3	1:C:232:PHE:HD1	1.78	0.47
1:B:121:PHE:HB2	1:B:125:TYR:CE2	2.49	0.47
1:C:158:LYS:HB2	1:C:197:PHE:CZ	2.49	0.47
1:D:44:LYS:HE3	1:D:52:GLU:OE2	2.15	0.47
1:A:81:GLU:O	1:A:82:ILE:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLU:HB2	1:D:171:LEU:HD13	1.97	0.47
1:A:103:ASP:CB	2:F:194:PRO:HB3	2.45	0.47
1:D:33:TRP:CZ3	1:D:102:ARG:HB3	2.50	0.47
1:A:268:GLN:O	1:A:271:ALA:HB3	2.15	0.47
1:B:14:ASP:O	1:B:17:VAL:N	2.47	0.47
1:C:216:TRP:CZ2	1:C:245:ILE:HD13	2.50	0.47
1:D:10:ARG:C	1:D:11:VAL:HG23	2.35	0.47
1:C:41:VAL:HG21	2:G:192:ILE:HG22	1.95	0.47
1:A:35:GLU:C	1:A:35:GLU:OE1	2.53	0.47
1:A:153:MET:CE	1:A:182:TYR:HD1	2.27	0.47
1:B:50:TYR:O	1:B:71:LYS:HB2	2.14	0.47
1:D:133:ILE:O	1:D:134:ARG:C	2.53	0.47
1:A:229:LYS:HD3	1:A:232:PHE:HD1	1.80	0.47
1:D:116:VAL:HG12	1:D:117:ASN:O	2.15	0.47
1:B:154:HIS:ND1	1:B:154:HIS:O	2.48	0.46
1:C:128:LEU:HB3	1:C:132:ASP:HB3	1.97	0.46
1:C:291:HIS:H	1:C:291:HIS:CD2	2.33	0.46
1:A:83:LYS:HD2	1:A:83:LYS:HA	1.71	0.46
1:A:102:ARG:HD2	1:A:107:LYS:CD	2.45	0.46
1:B:106:SER:O	1:B:107:LYS:C	2.53	0.46
2:E:191:LYS:N	2:E:197:TYR:HE1	2.13	0.46
1:A:268:GLN:O	1:A:272:LEU:CD1	2.63	0.46
1:C:157:VAL:HB	1:C:217:SER:CB	2.43	0.46
1:A:33:TRP:CE3	1:A:100:ILE:CD1	2.91	0.46
1:B:105:HIS:CD2	1:B:105:HIS:C	2.89	0.46
1:B:160:HIS:N	1:B:160:HIS:CD2	2.75	0.46
1:A:130:ASP:O	1:A:134:ARG:HG3	2.15	0.46
1:D:148:HIS:HE1	1:D:214:ASP:OD2	1.98	0.46
1:D:36:GLN:NE2	2:H:194:PRO:O	2.48	0.46
1:A:39:TYR:CE1	1:A:112:ILE:HG21	2.50	0.46
1:D:296:GLU:OE2	1:D:296:GLU:N	2.48	0.46
1:A:229:LYS:HD3	1:A:232:PHE:CD1	2.50	0.46
1:B:173:LEU:HD23	1:B:176:TRP:CH2	2.50	0.46
1:C:283:LYS:NZ	5:C:661:HOH:O	2.48	0.46
1:A:36:GLN:OE1	2:F:194:PRO:HG2	2.16	0.46
1:C:13:ALA:O	1:C:184:PRO:HG3	2.15	0.46
1:C:279:LYS:HD2	1:C:283:LYS:HD2	1.98	0.46
1:B:246:ALA:O	1:B:250:GLY:N	2.47	0.46
2:G:190:PHE:HD1	2:G:190:PHE:N	2.13	0.46
1:D:119:THR:CG2	2:G:202:GLN:HE21	2.29	0.46
1:B:33:TRP:CZ3	1:B:100:ILE:CD1	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:O	1:A:89:CYS:C	2.54	0.46
1:C:288:ASP:O	1:C:291:HIS:CD2	2.68	0.46
1:B:68:LYS:NZ	1:B:81:GLU:OE2	2.47	0.46
1:B:6:MET:HB3	1:B:261:TYR:CD2	2.51	0.46
1:C:226:ILE:CG1	1:C:227:PHE:N	2.79	0.46
1:C:210:ASP:OD1	1:C:212:SER:OG	2.34	0.46
1:B:314:THR:CG2	1:B:315:ALA:N	2.77	0.46
1:C:127:THR:CG2	1:C:127:THR:O	2.64	0.46
1:A:25:ASP:O	1:A:28:ALA:HB3	2.16	0.46
1:B:36:GLN:NE2	2:E:194:PRO:HB3	2.30	0.46
2:H:196:ALA:C	2:H:197:TYR:CD1	2.90	0.46
1:D:332:ASN:ND2	1:D:332:ASN:N	2.58	0.46
1:D:272:LEU:CD1	1:D:272:LEU:H	2.28	0.46
1:B:83:LYS:HD2	1:B:83:LYS:HA	1.63	0.46
2:F:200:GLN:HG3	2:F:200:GLN:H	1.24	0.46
2:E:192:ILE:N	2:E:197:TYR:OH	2.48	0.46
1:A:189:ASN:HD22	1:A:190:VAL:H	1.58	0.46
1:C:268:GLN:O	1:C:271:ALA:HB3	2.15	0.46
1:D:118:ASN:CB	1:D:163:MET:HE3	2.46	0.46
1:C:300:PHE:O	1:C:301:LEU:C	2.51	0.46
1:B:173:LEU:HD23	1:B:176:TRP:CZ2	2.50	0.46
1:D:84:ILE:CD1	1:D:152:ILE:HD13	2.46	0.45
1:C:145:ASP:HB2	1:C:315:ALA:HB3	1.98	0.45
1:C:242:LEU:CD2	1:C:269:LEU:HD21	2.44	0.45
1:D:13:ALA:O	1:D:184:PRO:HG3	2.15	0.45
1:B:192:VAL:HG23	1:B:202:LEU:HD13	1.99	0.45
1:B:72:PRO:O	1:B:73:VAL:CG1	2.63	0.45
1:D:68:LYS:NZ	1:D:81:GLU:OE2	2.48	0.45
1:D:83:LYS:HA	1:D:83:LYS:HD2	1.59	0.45
1:C:70:LEU:CD1	1:C:78:ILE:HD13	2.46	0.45
1:A:103:ASP:OD2	1:A:106:SER:OG	2.19	0.45
1:B:136:TYR:OH	1:B:166:HIS:CD2	2.62	0.45
1:D:24:TRP:HA	1:D:181:PHE:CZ	2.50	0.45
1:B:25:ASP:O	1:B:28:ALA:HB3	2.16	0.45
1:C:70:LEU:HD12	1:C:78:ILE:HD13	1.98	0.45
1:B:103:ASP:HB2	2:E:194:PRO:CG	2.47	0.45
1:C:136:TYR:HH	1:C:166:HIS:HD2	1.63	0.45
1:B:160:HIS:H	1:B:160:HIS:HD2	1.54	0.45
1:B:266:ASP:HA	1:C:74:LYS:HG2	1.98	0.45
1:C:158:LYS:HA	1:C:197:PHE:CE1	2.51	0.45
1:C:121:PHE:CD1	1:C:159:PRO:CB	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:TYR:O	1:D:213:LEU:N	2.48	0.45
1:C:296:GLU:N	1:C:296:GLU:OE2	2.47	0.45
1:D:126:PRO:HG2	2:G:197:TYR:OH	2.16	0.45
1:B:264:GLU:CG	1:C:76:LYS:HD3	2.46	0.45
1:B:148:HIS:HA	1:B:152:ILE:O	2.16	0.45
1:A:314:THR:CG2	1:A:315:ALA:H	2.29	0.45
1:B:146:TYR:O	1:B:149:SER:N	2.50	0.45
1:D:210:ASP:OD1	1:D:212:SER:N	2.40	0.45
1:B:153:MET:HE2	1:B:182:TYR:CD1	2.48	0.45
1:C:15:VAL:O	1:C:19:ARG:HG3	2.17	0.45
1:B:163:MET:CE	4:B:801:AMP:H2'	2.46	0.45
1:D:237:ASP:OD1	1:D:237:ASP:C	2.54	0.45
1:D:229:LYS:HD3	1:D:232:PHE:CD1	2.52	0.45
1:C:25:ASP:O	1:C:28:ALA:HB3	2.15	0.45
1:B:299:ASP:OD1	1:B:303:LYS:NZ	2.50	0.45
1:A:101:VAL:O	1:A:110:SER:N	2.48	0.45
2:E:190:PHE:C	2:E:197:TYR:HE1	2.20	0.45
1:B:211:TYR:O	1:B:212:SER:C	2.55	0.45
1:D:118:ASN:CG	1:D:163:MET:HE1	2.37	0.45
1:D:228:ARG:HD2	1:D:288:ASP:OD2	2.17	0.45
1:A:325:GLN:HA	1:A:328:ARG:NH1	2.32	0.45
1:A:332:ASN:ND2	1:A:332:ASN:C	2.67	0.45
1:B:294:SER:O	1:B:295:PRO:C	2.55	0.45
1:D:124:LEU:HD21	1:D:166:HIS:HB2	1.98	0.45
1:A:100:ILE:HD12	1:A:101:VAL:H	1.70	0.45
1:D:322:PRO:O	1:D:325:GLN:HG2	2.17	0.45
1:A:76:LYS:N	1:D:264:GLU:OE2	2.46	0.45
1:B:247:LYS:HG2	1:B:276:HIS:CE1	2.51	0.45
1:D:121:PHE:O	1:D:122:LYS:C	2.51	0.45
1:C:211:TYR:O	1:C:212:SER:C	2.55	0.45
1:C:211:TYR:O	1:C:213:LEU:N	2.50	0.45
1:D:265:LEU:HG	1:D:269:LEU:HD23	1.98	0.45
1:C:81:GLU:O	1:C:82:ILE:C	2.55	0.45
1:D:125:TYR:N	1:D:126:PRO:CD	2.80	0.45
1:D:154:HIS:CG	1:D:154:HIS:O	2.70	0.45
1:D:178:LEU:HA	1:D:178:LEU:HD23	1.75	0.45
1:D:43:ARG:NH1	2:G:203:ALA:O	2.41	0.45
1:B:131:TYR:O	1:B:132:ASP:C	2.54	0.45
1:A:44:LYS:HE2	1:A:52:GLU:OE2	2.14	0.45
1:D:153:MET:O	1:D:179:ALA:HA	2.17	0.45
1:A:98:LEU:HD22	1:A:114:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LYS:O	1:B:208:ASP:HA	2.16	0.45
1:D:119:THR:O	1:D:120:ASP:C	2.53	0.44
1:B:33:TRP:CD2	1:B:102:ARG:HB2	2.52	0.44
1:A:44:LYS:HG2	1:A:45:VAL:N	2.32	0.44
1:A:96:LYS:O	1:A:96:LYS:HG2	2.17	0.44
1:B:266:ASP:O	1:B:267:PRO:C	2.53	0.44
1:C:154:HIS:CE1	1:C:156:ASP:C	2.90	0.44
1:B:112:ILE:N	1:B:112:ILE:HD12	2.32	0.44
1:B:95:VAL:HA	1:B:172:ARG:HD2	2.00	0.44
1:A:15:VAL:HG22	1:A:16:ASN:N	2.32	0.44
1:B:33:TRP:CD1	1:B:33:TRP:N	2.82	0.44
2:E:199:LEU:N	2:E:199:LEU:HD23	2.31	0.44
1:D:165:ASP:C	1:D:167:GLU:H	2.21	0.44
1:A:120:ASP:OD2	1:A:121:PHE:N	2.50	0.44
1:D:158:LYS:CE	1:D:161:ASN:ND2	2.80	0.44
1:C:129:THR:O	1:C:132:ASP:N	2.50	0.44
1:D:211:TYR:O	1:D:212:SER:C	2.55	0.44
1:A:75:LYS:N	1:D:264:GLU:OE1	2.50	0.44
2:H:190:PHE:N	2:H:190:PHE:CD1	2.83	0.44
1:D:215:MET:HE1	1:D:315:ALA:CA	2.39	0.44
1:B:44:LYS:HE3	1:B:47:ARG:HB3	2.00	0.44
1:B:288:ASP:HB2	5:F:206:HOH:O	2.18	0.44
1:B:265:LEU:O	1:B:266:ASP:C	2.55	0.44
1:B:11:VAL:O	1:B:12:TYR:HB2	2.15	0.44
1:A:325:GLN:HA	1:A:328:ARG:HH12	1.82	0.44
1:D:10:ARG:O	1:D:11:VAL:CG2	2.66	0.44
1:A:11:VAL:O	1:A:12:TYR:HB2	2.18	0.44
1:B:85:LEU:HD21	1:B:176:TRP:CD1	2.52	0.44
1:C:303:LYS:HB3	1:C:313:LEU:HD21	1.98	0.44
1:B:126:PRO:CG	2:F:197:TYR:OH	2.65	0.44
2:E:198:GLN:HA	2:E:198:GLN:NE2	2.33	0.44
1:B:70:LEU:CD1	1:B:78:ILE:HD13	2.47	0.44
1:C:145:ASP:HB2	1:C:315:ALA:CB	2.47	0.44
1:B:21:LYS:HG3	1:B:24:TRP:CH2	2.53	0.44
1:B:300:PHE:O	1:B:301:LEU:C	2.56	0.44
1:A:10:ARG:C	1:A:11:VAL:CG2	2.84	0.44
1:C:308:ASP:OD1	1:C:310:GLN:HB2	2.18	0.44
1:A:41:VAL:O	2:F:197:TYR:HB2	2.18	0.44
1:B:286:ASN:OD1	1:B:289:ASN:HB3	2.16	0.44
1:B:19:ARG:CB	1:B:20:PRO:HD2	2.47	0.44
1:C:36:GLN:O	1:C:39:TYR:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:PHE:N	1:C:197:PHE:CD2	2.86	0.44
1:C:16:ASN:HB3	1:C:24:TRP:CD1	2.53	0.44
1:D:216:TRP:CE3	1:D:305:LEU:HD23	2.53	0.44
1:C:282:LEU:N	1:C:282:LEU:CD2	2.81	0.44
1:C:279:LYS:HD3	1:C:280:PRO:HD2	1.98	0.44
1:B:299:ASP:HB3	1:B:321:HIS:HE2	1.83	0.44
1:C:96:LYS:HG2	1:C:98:LEU:HD13	1.98	0.44
1:D:159:PRO:O	1:D:162:VAL:HG13	2.18	0.44
2:H:199:LEU:CD2	2:H:199:LEU:N	2.68	0.44
1:C:12:TYR:O	1:C:211:TYR:OH	2.29	0.44
1:A:241:GLN:O	1:A:245:ILE:HG13	2.17	0.44
1:A:266:ASP:O	1:A:267:PRO:C	2.53	0.44
1:C:72:PRO:O	1:C:73:VAL:CG1	2.63	0.44
1:D:8:LYS:O	1:D:9:ALA:O	2.36	0.44
2:F:190:PHE:O	2:F:191:LYS:HG3	2.18	0.44
1:A:216:TRP:HZ2	1:A:245:ILE:HD13	1.80	0.44
1:B:156:ASP:HA	1:B:193:ALA:HA	1.99	0.44
1:B:91:GLY:HA3	1:B:146:TYR:CD2	2.53	0.44
1:D:211:TYR:O	1:D:214:ASP:N	2.51	0.44
1:C:19:ARG:CB	1:C:20:PRO:HD2	2.40	0.44
1:D:305:LEU:HA	1:D:305:LEU:HD23	1.82	0.44
1:B:229:LYS:HG2	1:B:229:LYS:O	2.17	0.44
1:B:210:ASP:OD1	1:B:212:SER:OG	2.33	0.43
1:D:96:LYS:CG	1:D:98:LEU:HD13	2.48	0.43
1:D:169:ARG:NH2	1:D:169:ARG:CG	2.61	0.43
1:B:265:LEU:HG	1:B:269:LEU:HD23	2.00	0.43
1:D:258:LEU:CD1	1:D:265:LEU:HD13	2.48	0.43
1:B:196:TYR:HB2	1:B:197:PHE:CD2	2.53	0.43
1:D:14:ASP:O	1:D:18:LEU:HG	2.18	0.43
1:A:279:LYS:HD3	1:A:280:PRO:HD2	1.98	0.43
1:B:126:PRO:CB	2:F:197:TYR:HH	2.31	0.43
1:D:198:LYS:CB	1:D:202:LEU:HD12	2.48	0.43
1:D:328:ARG:CB	1:D:328:ARG:CZ	2.97	0.43
1:D:186:LYS:HB3	1:D:188:TYR:CE2	2.54	0.43
1:A:259:ASN:O	1:A:260:LYS:C	2.55	0.43
2:H:202:GLN:O	2:H:203:ALA:HB2	2.18	0.43
1:C:138:TYR:HB2	1:C:324:PHE:CD1	2.53	0.43
1:D:96:LYS:N	1:D:114:GLU:OE2	2.48	0.43
1:B:229:LYS:HD3	1:B:232:PHE:HD1	1.81	0.43
1:B:303:LYS:HB3	1:B:313:LEU:HD21	1.99	0.43
1:C:41:VAL:CG1	2:G:197:TYR:CB	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:GLN:HB3	5:H:208:HOH:O	2.16	0.43
1:C:239:HIS:CG	1:C:269:LEU:HD13	2.53	0.43
1:B:270:GLU:O	1:B:271:ALA:C	2.56	0.43
1:C:19:ARG:HH22	1:C:150:GLN:HE22	1.65	0.43
1:C:298:ILE:O	1:C:299:ASP:C	2.54	0.43
1:D:125:TYR:CE1	1:D:225:MET:HE1	2.52	0.43
1:B:40:GLU:HG3	1:B:59:VAL:HG13	2.00	0.43
1:B:84:ILE:HD13	1:B:152:ILE:CD1	2.49	0.43
1:C:142:LYS:NZ	1:C:331:GLU:OE1	2.37	0.43
1:A:314:THR:CB	1:A:317:GLU:HG3	2.39	0.43
1:C:153:MET:HE2	1:C:182:TYR:CD1	2.53	0.43
1:C:146:TYR:O	1:C:149:SER:N	2.51	0.43
1:A:310:GLN:OE1	1:A:310:GLN:HA	2.19	0.43
1:B:6:MET:HB3	1:B:261:TYR:HD2	1.84	0.43
1:D:64:LYS:HB2	1:D:64:LYS:NZ	2.33	0.43
1:C:98:LEU:CD2	1:C:114:GLU:HA	2.48	0.43
1:C:88:LEU:O	1:C:89:CYS:C	2.57	0.43
2:E:197:TYR:C	2:E:198:GLN:O	2.54	0.43
1:B:268:GLN:O	1:B:271:ALA:HB3	2.18	0.43
1:B:272:LEU:HD12	1:B:272:LEU:N	2.33	0.43
1:C:200:PRO:O	1:C:204:VAL:HG22	2.18	0.43
1:C:105:HIS:HB3	1:C:106:SER:H	1.38	0.43
1:C:175:ASP:OD1	4:C:601:AMP:O1P	2.36	0.43
1:C:195:ARG:HG3	1:C:195:ARG:HH11	1.84	0.43
1:C:98:LEU:HB2	1:C:112:ILE:O	2.19	0.43
1:B:36:GLN:O	1:B:39:TYR:N	2.47	0.43
2:E:192:ILE:HG23	2:E:192:ILE:O	2.19	0.43
1:C:254:LEU:O	1:C:258:LEU:HG	2.18	0.43
1:D:300:PHE:CE2	1:D:304:LEU:HD11	2.54	0.43
1:B:112:ILE:N	1:B:112:ILE:CD1	2.82	0.43
1:A:15:VAL:CG2	1:A:16:ASN:N	2.81	0.43
1:A:176:TRP:CD1	1:A:176:TRP:N	2.85	0.43
1:A:227:PHE:O	1:A:228:ARG:HB2	2.18	0.43
1:B:226:ILE:CG1	1:B:227:PHE:N	2.82	0.43
1:B:96:LYS:HG2	1:B:98:LEU:HD13	2.00	0.43
1:C:124:LEU:HD12	1:C:124:LEU:C	2.39	0.43
1:C:64:LYS:HZ2	1:C:64:LYS:HB2	1.83	0.43
1:A:222:PHE:O	1:A:223:ALA:C	2.56	0.43
1:C:61:ASN:OD1	1:C:63:GLU:HG3	2.18	0.43
1:B:125:TYR:HA	1:B:128:LEU:HG	2.00	0.43
1:B:33:TRP:CE3	1:B:100:ILE:CD1	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TYR:HE2	1:D:169:ARG:HB3	1.84	0.43
1:D:100:ILE:CD1	1:D:100:ILE:C	2.65	0.43
1:C:190:VAL:CG1	1:C:202:LEU:HA	2.49	0.43
1:A:265:LEU:O	1:A:266:ASP:C	2.54	0.43
1:B:279:LYS:HD3	1:B:279:LYS:HA	1.45	0.43
1:A:282:LEU:CD2	1:A:282:LEU:N	2.82	0.43
1:B:259:ASN:O	1:B:260:LYS:C	2.57	0.43
2:G:195:MET:C	2:G:196:ALA:O	2.54	0.42
1:A:268:GLN:HE21	1:A:268:GLN:HB2	1.51	0.42
1:B:158:LYS:O	1:B:159:PRO:C	2.57	0.42
1:A:129:THR:O	1:A:132:ASP:N	2.52	0.42
1:A:329:ALA:O	1:A:333:SER:HA	2.18	0.42
1:B:223:ALA:HB2	1:B:301:LEU:CD1	2.49	0.42
1:C:294:SER:O	1:C:296:GLU:N	2.52	0.42
1:B:94:ILE:HG22	1:B:95:VAL:O	2.19	0.42
1:C:39:TYR:CE2	1:C:112:ILE:HG12	2.54	0.42
1:C:44:LYS:HE3	1:C:52:GLU:OE2	2.19	0.42
1:D:125:TYR:HD1	1:D:128:LEU:HD11	1.83	0.42
1:D:266:ASP:O	1:D:267:PRO:C	2.57	0.42
1:B:14:ASP:C	1:B:16:ASN:N	2.73	0.42
1:D:11:VAL:HG12	1:D:12:TYR:CD2	2.54	0.42
1:D:296:GLU:O	1:D:297:ALA:C	2.57	0.42
1:A:279:LYS:HD2	1:A:283:LYS:HD2	2.01	0.42
1:A:249:LEU:N	1:A:249:LEU:HD12	2.34	0.42
1:B:237:ASP:OD1	1:B:238:ASN:N	2.52	0.42
2:H:193:HIS:HB3	2:H:194:PRO:CD	2.43	0.42
1:C:210:ASP:OD1	1:C:212:SER:N	2.44	0.42
1:B:316:LEU:O	1:B:316:LEU:HD12	2.19	0.42
1:D:108:THR:O	1:D:108:THR:HG22	2.19	0.42
1:B:70:LEU:HD12	1:B:78:ILE:HD13	2.01	0.42
1:C:252:ASP:O	1:C:256:VAL:HG23	2.19	0.42
1:C:178:LEU:HA	1:C:178:LEU:HD23	1.71	0.42
1:B:268:GLN:O	1:B:272:LEU:HD13	2.19	0.42
1:C:128:LEU:HB3	1:C:132:ASP:CB	2.49	0.42
1:B:116:VAL:HG23	4:B:801:AMP:HN62	1.83	0.42
1:A:279:LYS:HA	1:A:279:LYS:HD3	1.26	0.42
1:C:219:GLY:O	1:C:220:CYS:C	2.56	0.42
2:F:200:GLN:HE21	2:F:200:GLN:HB2	1.47	0.42
1:B:31:VAL:HG12	1:B:33:TRP:CE2	2.55	0.42
1:C:135:TYR:O	1:C:138:TYR:N	2.53	0.42
1:D:118:ASN:HB3	1:D:163:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:O	1:B:11:VAL:CG2	2.68	0.42
1:D:206:LEU:HD23	1:D:208:ASP:OD2	2.19	0.42
1:C:31:VAL:CG1	1:C:33:TRP:CE2	3.03	0.42
1:A:106:SER:O	1:A:107:LYS:HB2	2.20	0.42
1:B:122:LYS:O	2:F:192:ILE:HD12	2.20	0.42
2:F:198:GLN:OE1	2:F:201:LEU:HD11	2.19	0.42
1:D:239:HIS:CG	1:D:269:LEU:HD13	2.54	0.42
1:C:121:PHE:O	1:C:122:LYS:C	2.56	0.42
1:B:197:PHE:CD2	1:B:197:PHE:N	2.87	0.42
1:D:12:TYR:CD1	1:D:149:SER:HA	2.55	0.42
1:B:58:ASN:HB3	1:B:61:ASN:OD1	2.19	0.42
1:D:121:PHE:CG	1:D:159:PRO:HB3	2.55	0.42
1:B:126:PRO:O	1:B:128:LEU:N	2.52	0.42
1:B:148:HIS:HD2	5:B:1027:HOH:O	2.01	0.42
1:C:269:LEU:HA	1:C:269:LEU:HD12	1.76	0.42
1:B:12:TYR:CD1	1:B:149:SER:HA	2.55	0.42
1:C:288:ASP:O	1:C:291:HIS:HD2	2.02	0.42
1:C:64:LYS:CB	1:C:64:LYS:NZ	2.83	0.42
1:D:282:LEU:HD13	1:D:282:LEU:HA	1.87	0.42
1:D:226:ILE:HD11	1:D:227:PHE:CE2	2.54	0.42
1:D:116:VAL:HG12	1:D:117:ASN:N	2.34	0.42
1:C:173:LEU:HD23	1:C:176:TRP:CZ2	2.54	0.42
1:C:83:LYS:HA	1:C:83:LYS:HD2	1.75	0.42
2:G:202:GLN:H	2:G:202:GLN:HG2	1.45	0.42
1:C:123:VAL:HG22	1:D:41:VAL:HG11	2.01	0.42
1:D:66:ILE:O	1:D:112:ILE:HA	2.20	0.42
1:B:245:ILE:HG21	1:B:245:ILE:HD13	1.82	0.42
1:D:78:ILE:O	1:D:82:ILE:HG13	2.20	0.42
2:G:188:TYR:N	2:G:190:PHE:CD1	2.87	0.42
1:A:66:ILE:HG13	4:A:501:AMP:C6	2.55	0.42
1:C:265:LEU:HG	1:C:269:LEU:HD23	2.02	0.42
1:C:272:LEU:CD1	1:C:272:LEU:H	2.32	0.42
1:C:121:PHE:HB2	1:C:125:TYR:CG	2.55	0.42
1:C:199:GLY:HA2	1:C:216:TRP:NE1	2.34	0.42
1:D:15:VAL:HG11	1:D:149:SER:O	2.20	0.42
1:D:19:ARG:CB	1:D:20:PRO:HD2	2.49	0.42
1:D:138:TYR:HB2	1:D:324:PHE:CD1	2.54	0.42
1:A:24:TRP:HA	1:A:181:PHE:CZ	2.55	0.42
1:C:249:LEU:HD12	1:C:249:LEU:N	2.35	0.42
1:B:40:GLU:HA	2:E:196:ALA:O	2.20	0.42
1:B:137:ILE:HG22	1:B:141:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PRO:O	1:B:162:VAL:HG13	2.20	0.42
1:B:314:THR:HG22	1:B:316:LEU:H	1.85	0.42
1:D:237:ASP:O	1:D:238:ASN:C	2.55	0.42
1:C:39:TYR:HA	1:C:57:ILE:O	2.20	0.41
1:D:131:TYR:O	1:D:132:ASP:C	2.58	0.41
1:A:107:LYS:HB3	1:A:107:LYS:HE2	1.90	0.41
1:C:239:HIS:ND1	1:C:269:LEU:HD13	2.35	0.41
1:D:88:LEU:O	1:D:89:CYS:C	2.57	0.41
1:A:286:ASN:HD21	1:A:289:ASN:H	1.66	0.41
1:C:129:THR:N	1:C:132:ASP:HB2	2.33	0.41
1:B:69:ILE:HD13	2:E:193:HIS:CD2	2.56	0.41
2:F:198:GLN:C	2:F:199:LEU:HD23	2.36	0.41
1:D:118:ASN:CG	1:D:163:MET:CE	2.89	0.41
1:B:153:MET:CE	1:B:182:TYR:HD1	2.32	0.41
1:D:294:SER:O	1:D:296:GLU:N	2.53	0.41
1:A:252:ASP:O	1:A:256:VAL:HG23	2.20	0.41
1:D:31:VAL:CG1	1:D:33:TRP:CE2	3.03	0.41
1:B:264:GLU:H	1:C:76:LYS:HZ2	1.68	0.41
1:C:134:ARG:HG2	1:C:323:TYR:CE2	2.54	0.41
1:B:226:ILE:HD11	1:B:227:PHE:CE2	2.55	0.41
1:C:67:ILE:HG21	1:C:67:ILE:HD13	1.85	0.41
2:E:188:TYR:O	2:E:189:GLY:O	2.38	0.41
1:B:286:ASN:ND2	1:B:288:ASP:CB	2.77	0.41
1:C:286:ASN:ND2	1:C:288:ASP:OD2	2.53	0.41
1:D:29:LEU:HD22	1:D:30:THR:H	1.84	0.41
1:C:157:VAL:O	1:C:217:SER:HB3	2.19	0.41
1:B:29:LEU:HD22	1:B:30:THR:H	1.85	0.41
1:D:108:THR:HA	1:D:109:PRO:HD2	1.88	0.41
1:D:200:PRO:HD3	1:D:216:TRP:CE2	2.56	0.41
1:A:157:VAL:HB	1:A:217:SER:HB2	2.02	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.84	0.41
1:D:168:LEU:O	1:D:169:ARG:C	2.58	0.41
1:B:84:ILE:O	1:B:88:LEU:HG	2.20	0.41
1:D:189:ASN:HD22	1:D:190:VAL:H	1.62	0.41
1:A:200:PRO:HD3	1:A:216:TRP:CE2	2.56	0.41
1:C:119:THR:O	1:C:120:ASP:C	2.59	0.41
1:A:13:ALA:O	1:A:184:PRO:HG3	2.21	0.41
1:C:241:GLN:O	1:C:245:ILE:HG13	2.21	0.41
1:D:107:LYS:O	1:D:109:PRO:CD	2.69	0.41
2:G:190:PHE:HB2	2:G:197:TYR:OH	2.21	0.41
1:B:33:TRP:CE2	1:B:102:ARG:NE	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ARG:CB	1:C:169:ARG:HH21	2.34	0.41
1:A:156:ASP:OD2	1:A:161:ASN:ND2	2.53	0.41
1:A:301:LEU:HD11	1:A:305:LEU:HD12	2.02	0.41
1:A:299:ASP:OD1	1:A:303:LYS:NZ	2.54	0.41
1:D:35:GLU:O	1:D:38:ASP:HB2	2.21	0.41
2:E:188:TYR:CG	2:E:189:GLY:N	2.88	0.41
1:D:165:ASP:C	1:D:167:GLU:N	2.74	0.41
1:B:84:ILE:HG23	1:B:152:ILE:CD1	2.32	0.41
1:D:195:ARG:HH11	1:D:195:ARG:HG3	1.84	0.41
1:C:282:LEU:HA	1:C:282:LEU:HD13	1.78	0.41
1:A:195:ARG:NH1	1:A:195:ARG:HG3	2.35	0.41
1:D:247:LYS:HG2	1:D:276:HIS:CE1	2.56	0.41
1:A:14:ASP:N	1:A:14:ASP:OD2	2.39	0.41
1:D:39:TYR:HA	1:D:57:ILE:O	2.21	0.41
1:A:165:ASP:OD1	1:A:167:GLU:HB3	2.21	0.41
1:D:74:LYS:O	1:D:75:LYS:C	2.58	0.41
1:A:31:VAL:CG1	1:A:33:TRP:CD2	3.03	0.41
1:B:125:TYR:O	1:B:128:LEU:HG	2.21	0.41
1:A:36:GLN:OE1	2:F:194:PRO:HB2	2.20	0.41
1:D:189:ASN:ND2	1:D:190:VAL:N	2.57	0.41
1:B:11:VAL:HG12	1:B:12:TYR:CD2	2.56	0.41
1:A:289:ASN:OD1	1:A:290:GLN:N	2.54	0.41
1:C:72:PRO:C	1:C:73:VAL:HG13	2.39	0.41
1:A:251:THR:HG23	1:A:276:HIS:HB2	2.03	0.41
1:C:118:ASN:ND2	1:C:163:MET:HE1	2.36	0.41
1:A:294:SER:O	1:A:296:GLU:N	2.54	0.41
1:B:58:ASN:ND2	1:B:61:ASN:HD21	2.18	0.41
1:D:38:ASP:O	1:D:59:VAL:HG22	2.20	0.41
1:C:112:ILE:N	1:C:112:ILE:CD1	2.83	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.84	0.41
1:B:103:ASP:O	1:B:105:HIS:N	2.54	0.41
1:B:148:HIS:CE1	1:B:211:TYR:HB3	2.56	0.41
1:A:122:LYS:HE3	1:B:44:LYS:CD	2.51	0.41
1:A:120:ASP:OD2	1:A:122:LYS:N	2.51	0.41
1:B:286:ASN:OD1	1:B:289:ASN:CG	2.60	0.41
1:D:268:GLN:HE21	1:D:268:GLN:HB2	1.71	0.41
1:B:204:VAL:HG12	1:B:265:LEU:HD11	2.03	0.41
1:B:316:LEU:HA	1:B:316:LEU:HD13	1.79	0.41
1:A:286:ASN:OD1	1:A:289:ASN:HB3	2.21	0.41
1:A:127:THR:HG22	1:A:128:LEU:N	2.34	0.41
1:C:14:ASP:O	1:C:15:VAL:C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:PRO:HD3	1:C:216:TRP:CD2	2.56	0.41
1:B:279:LYS:CD	1:B:283:LYS:HD2	2.49	0.41
1:A:180:GLU:OE1	1:A:181:PHE:N	2.39	0.41
1:D:158:LYS:CE	1:D:161:ASN:HD21	2.34	0.41
1:A:44:LYS:HD3	1:A:47:ARG:NE	2.36	0.41
1:A:272:LEU:N	1:A:272:LEU:CD1	2.79	0.41
1:A:128:LEU:HB3	1:A:132:ASP:HB2	2.03	0.41
1:C:332:ASN:O	1:C:333:SER:HB2	2.21	0.41
1:A:74:LYS:HE2	1:D:264:GLU:O	2.21	0.41
2:E:200:GLN:CG	2:E:201:LEU:N	2.84	0.41
1:D:252:ASP:O	1:D:256:VAL:HG23	2.21	0.41
1:B:296:GLU:O	1:B:297:ALA:C	2.58	0.41
1:C:135:TYR:HE2	1:C:169:ARG:HB3	1.86	0.40
1:A:84:ILE:O	1:A:88:LEU:HG	2.21	0.40
1:B:216:TRP:O	1:B:217:SER:C	2.58	0.40
1:C:120:ASP:OD2	1:C:122:LYS:N	2.53	0.40
1:D:45:VAL:O	1:D:45:VAL:CG1	2.67	0.40
1:B:71:LYS:O	1:B:73:VAL:HG22	2.20	0.40
1:A:10:ARG:O	1:A:11:VAL:HG22	2.21	0.40
1:D:93:ASN:ND2	1:D:139:GLU:O	2.52	0.40
1:C:31:VAL:CG2	1:C:82:ILE:HD12	2.52	0.40
4:A:501:AMP:H5'2	1:B:47:ARG:NH2	2.36	0.40
1:D:160:HIS:H	1:D:160:HIS:HD2	1.61	0.40
1:C:265:LEU:O	1:C:266:ASP:C	2.57	0.40
1:B:267:PRO:O	1:B:268:GLN:CB	2.54	0.40
1:B:269:LEU:O	1:B:273:VAL:HG23	2.21	0.40
1:B:196:TYR:O	1:B:241:GLN:NE2	2.54	0.40
1:C:39:TYR:CD2	1:C:112:ILE:HG12	2.57	0.40
1:B:31:VAL:HG13	1:B:100:ILE:HG12	2.03	0.40
1:A:84:ILE:CD1	1:A:152:ILE:HD13	2.51	0.40
1:B:195:ARG:HG3	1:B:195:ARG:NH1	2.36	0.40
1:C:196:TYR:HB2	1:C:197:PHE:CD2	2.56	0.40
1:A:282:LEU:HA	1:A:282:LEU:HD13	1.86	0.40
1:D:238:ASN:N	1:D:238:ASN:ND2	2.70	0.40
2:H:195:MET:H	2:H:195:MET:HG2	1.59	0.40
1:B:101:VAL:O	1:B:109:PRO:HA	2.21	0.40
1:A:121:PHE:CG	1:A:122:LYS:N	2.89	0.40
1:A:331:GLU:O	1:A:332:ASN:C	2.55	0.40
1:B:74:LYS:O	1:B:75:LYS:C	2.59	0.40
1:B:103:ASP:C	1:B:103:ASP:OD1	2.58	0.40
1:A:332:ASN:ND2	1:A:333:SER:N	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LYS:HG2	1:A:276:HIS:CE1	2.57	0.40
1:D:279:LYS:HD3	1:D:279:LYS:HA	1.40	0.40
1:A:226:ILE:CG1	1:A:227:PHE:N	2.84	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	326/332 (98%)	271 (83%)	41 (13%)	14 (4%)	3	23
1	B	326/332 (98%)	270 (83%)	40 (12%)	16 (5%)	3	20
1	C	326/332 (98%)	268 (82%)	44 (14%)	14 (4%)	3	23
1	D	326/332 (98%)	268 (82%)	44 (14%)	14 (4%)	3	23
2	E	14/23 (61%)	8 (57%)	2 (14%)	4 (29%)	0	0
2	F	16/23 (70%)	12 (75%)	1 (6%)	3 (19%)	0	0
2	G	14/23 (61%)	10 (71%)	2 (14%)	2 (14%)	0	1
2	H	14/23 (61%)	10 (71%)	2 (14%)	2 (14%)	0	1
All	All	1362/1420 (96%)	1117 (82%)	176 (13%)	69 (5%)	2	19

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ARG
1	A	195	ARG
1	B	37	ASP
1	B	155	ARG
1	B	195	ARG
1	C	7	SER
1	C	105	HIS

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Mol	Chain	Res	Type
1	C	155	ARG
1	C	195	ARG
1	D	9	ALA
1	D	37	ASP
1	D	155	ARG
1	D	195	ARG
2	E	193	HIS
2	E	198	GLN
2	F	187	LEU
2	F	193	HIS
2	F	194	PRO
2	G	193	HIS
2	G	194	PRO
2	H	193	HIS
2	H	194	PRO
1	A	37	ASP
1	A	212	SER
1	A	331	GLU
1	B	15	VAL
1	B	127	THR
1	B	196	TYR
1	C	37	ASP
1	C	127	THR
1	C	175	ASP
1	C	212	SER
1	D	212	SER
2	E	189	GLY
2	E	194	PRO
1	A	196	TYR
1	B	104	GLN
1	B	107	LYS
1	B	212	SER
1	B	271	ALA
1	C	271	ALA
1	A	89	CYS
1	A	146	TYR
1	A	175	ASP
1	A	193	ALA
1	A	271	ALA
1	B	89	CYS
1	B	146	TYR
1	B	193	ALA

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Mol	Chain	Res	Type
1	B	330	ALA
1	C	193	ALA
1	D	160	HIS
1	A	330	ALA
1	B	156	ASP
1	B	159	PRO
1	C	146	TYR
1	C	196	TYR
1	D	108	THR
1	D	146	TYR
1	D	169	ARG
1	D	271	ALA
1	D	330	ALA
1	A	45	VAL
1	C	273	VAL
1	D	268	GLN
1	C	15	VAL
1	D	158	LYS
1	A	322	PRO
1	D	250	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/300 (99%)	249 (84%)	48 (16%)	3	13
1	B	297/300 (99%)	255 (86%)	42 (14%)	4	19
1	C	297/300 (99%)	257 (86%)	40 (14%)	5	22
1	D	297/300 (99%)	254 (86%)	43 (14%)	4	18
2	E	13/20 (65%)	3 (23%)	10 (77%)	0	0
2	F	15/20 (75%)	8 (53%)	7 (47%)	0	0
2	G	13/20 (65%)	8 (62%)	5 (38%)	0	0
2	H	13/20 (65%)	5 (38%)	8 (62%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1242/1280 (97%)	1039 (84%)	203 (16%)	3 13

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	7	SER
1	A	8	LYS
1	A	15	VAL
1	A	30	THR
1	A	35	GLU
1	A	38	ASP
1	A	41	VAL
1	A	45	VAL
1	A	64	LYS
1	A	72	PRO
1	A	82	ILE
1	A	96	LYS
1	A	98	LEU
1	A	100	ILE
1	A	103	ASP
1	A	105	HIS
1	A	107	LYS
1	A	108	THR
1	A	118	ASN
1	A	119	THR
1	A	122	LYS
1	A	127	THR
1	A	133	ILE
1	A	141	LEU
1	A	147	CYS
1	A	160	HIS
1	A	162	VAL
1	A	163	MET
1	A	169	ARG
1	A	175	ASP
1	A	189	ASN
1	A	195	ARG
1	A	197	PHE
1	A	205	ASP
1	A	215	MET
1	A	230	GLU

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Mol	Chain	Res	Type
1	A	237	ASP
1	A	262	ARG
1	A	279	LYS
1	A	288	ASP
1	A	306	ARG
1	A	310	GLN
1	A	316	LEU
1	A	322	PRO
1	A	325	GLN
1	A	332	ASN
1	A	333	SER
1	B	27	GLU
1	B	30	THR
1	B	36	GLN
1	B	37	ASP
1	B	38	ASP
1	B	42	VAL
1	B	43	ARG
1	B	52	GLU
1	B	64	LYS
1	B	81	GLU
1	B	96	LYS
1	B	98	LEU
1	B	100	ILE
1	B	112	ILE
1	B	118	ASN
1	B	141	LEU
1	B	147	CYS
1	B	158	LYS
1	B	159	PRO
1	B	160	HIS
1	B	162	VAL
1	B	163	MET
1	B	169	ARG
1	B	189	ASN
1	B	195	ARG
1	B	197	PHE
1	B	205	ASP
1	B	215	MET
1	B	230	GLU
1	B	237	ASP
1	B	243	VAL

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Mol	Chain	Res	Type
1	B	262	ARG
1	B	277	SER
1	B	279	LYS
1	B	288	ASP
1	B	306	ARG
1	B	310	GLN
1	B	316	LEU
1	B	322	PRO
1	B	325	GLN
1	B	332	ASN
1	B	333	SER
1	C	27	GLU
1	C	30	THR
1	C	41	VAL
1	C	42	VAL
1	C	43	ARG
1	C	64	LYS
1	C	72	PRO
1	C	98	LEU
1	C	100	ILE
1	C	102	ARG
1	C	105	HIS
1	C	107	LYS
1	C	109	PRO
1	C	118	ASN
1	C	141	LEU
1	C	147	CYS
1	C	160	HIS
1	C	162	VAL
1	C	163	MET
1	C	167	GLU
1	C	169	ARG
1	C	189	ASN
1	C	192	VAL
1	C	195	ARG
1	C	205	ASP
1	C	215	MET
1	C	230	GLU
1	C	237	ASP
1	C	262	ARG
1	C	277	SER
1	C	279	LYS

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Mol	Chain	Res	Type
1	C	288	ASP
1	C	289	ASN
1	C	306	ARG
1	C	310	GLN
1	C	316	LEU
1	C	322	PRO
1	C	325	GLN
1	C	331	GLU
1	C	332	ASN
1	D	15	VAL
1	D	16	ASN
1	D	30	THR
1	D	41	VAL
1	D	43	ARG
1	D	47	ARG
1	D	64	LYS
1	D	72	PRO
1	D	96	LYS
1	D	98	LEU
1	D	100	ILE
1	D	102	ARG
1	D	105	HIS
1	D	107	LYS
1	D	112	ILE
1	D	118	ASN
1	D	119	THR
1	D	127	THR
1	D	141	LEU
1	D	147	CYS
1	D	160	HIS
1	D	162	VAL
1	D	167	GLU
1	D	169	ARG
1	D	189	ASN
1	D	192	VAL
1	D	195	ARG
1	D	197	PHE
1	D	205	ASP
1	D	215	MET
1	D	230	GLU
1	D	237	ASP
1	D	262	ARG

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Mol	Chain	Res	Type
1	D	266	ASP
1	D	277	SER
1	D	279	LYS
1	D	306	ARG
1	D	310	GLN
1	D	316	LEU
1	D	322	PRO
1	D	325	GLN
1	D	332	ASN
1	D	333	SER
2	E	188	TYR
2	E	190	PHE
2	E	191	LYS
2	E	192	ILE
2	E	195	MET
2	E	197	TYR
2	E	198	GLN
2	E	199	LEU
2	E	200	GLN
2	E	202	GLN
2	F	187	LEU
2	F	188	TYR
2	F	190	PHE
2	F	191	LYS
2	F	199	LEU
2	F	200	GLN
2	F	201	LEU
2	G	188	TYR
2	G	190	PHE
2	G	195	MET
2	G	200	GLN
2	G	202	GLN
2	H	188	TYR
2	H	190	PHE
2	H	195	MET
2	H	197	TYR
2	H	198	GLN
2	H	199	LEU
2	H	200	GLN
2	H	202	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	160	HIS
1	A	166	HIS
1	A	189	ASN
1	A	238	ASN
1	A	268	GLN
1	A	291	HIS
1	A	325	GLN
1	A	326	GLN
1	A	332	ASN
1	B	105	HIS
1	B	148	HIS
1	B	150	GLN
1	B	160	HIS
1	B	161	ASN
1	B	166	HIS
1	B	189	ASN
1	B	238	ASN
1	B	241	GLN
1	B	268	GLN
1	B	276	HIS
1	B	291	HIS
1	B	325	GLN
1	B	326	GLN
1	C	36	GLN
1	C	118	ASN
1	C	150	GLN
1	C	160	HIS
1	C	166	HIS
1	C	189	ASN
1	C	238	ASN
1	C	259	ASN
1	C	291	HIS
1	C	325	GLN
1	C	326	GLN
1	C	332	ASN
1	D	36	GLN
1	D	105	HIS
1	D	148	HIS
1	D	150	GLN
1	D	160	HIS
1	D	161	ASN
1	D	166	HIS

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Mol	Chain	Res	Type
1	D	183	HIS
1	D	189	ASN
1	D	238	ASN
1	D	268	GLN
1	D	291	HIS
1	D	325	GLN
1	D	326	GLN
1	D	332	ASN
2	E	193	HIS
2	E	198	GLN
2	F	193	HIS
2	F	200	GLN
2	F	202	GLN
2	H	198	GLN
2	H	200	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	A	501	-	20,25,25	1.87	5 (25%)	22,38,38	2.84	8 (36%)
4	AMP	B	801	-	20,25,25	1.67	6 (30%)	22,38,38	2.85	8 (36%)
4	AMP	C	601	-	20,25,25	1.72	6 (30%)	22,38,38	2.74	7 (31%)
4	AMP	D	701	-	20,25,25	1.90	8 (40%)	22,38,38	2.59	7 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	A	501	-	1/1/5/5	0/6/26/26	0/3/3/3
4	AMP	B	801	-	1/1/5/5	0/6/26/26	0/3/3/3
4	AMP	C	601	-	1/1/5/5	0/6/26/26	0/3/3/3
4	AMP	D	701	-	1/1/5/5	0/6/26/26	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	AMP	O4'-C1'	-3.52	1.36	1.41
4	C	601	AMP	P-O5'	-2.46	1.52	1.60
4	A	501	AMP	P-O5'	-2.39	1.52	1.60
4	B	801	AMP	C4-N3	-2.36	1.32	1.35
4	A	501	AMP	C2'-C3'	-2.36	1.47	1.53
4	B	801	AMP	P-O2P	-2.20	1.46	1.54
4	D	701	AMP	P-O2P	-2.13	1.47	1.54
4	D	701	AMP	O3'-C3'	2.01	1.47	1.43
4	C	601	AMP	C4-N3	2.02	1.38	1.35
4	C	601	AMP	C2-N3	2.12	1.35	1.32
4	B	801	AMP	C3'-C4'	2.12	1.58	1.53
4	A	501	AMP	P-O3P	2.18	1.62	1.54
4	B	801	AMP	C5-C4	2.23	1.45	1.40
4	B	801	AMP	P-O3P	2.25	1.62	1.54
4	D	701	AMP	C2-N3	2.44	1.36	1.32
4	D	701	AMP	C5-C4	2.48	1.46	1.40
4	A	501	AMP	C3'-C4'	2.52	1.59	1.53
4	C	601	AMP	O5'-C5'	2.66	1.55	1.44
4	D	701	AMP	P-O3P	2.79	1.64	1.54
4	D	701	AMP	C5'-C4'	2.89	1.61	1.51
4	B	801	AMP	O5'-C5'	2.95	1.56	1.44
4	C	601	AMP	P-O3P	3.18	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	701	AMP	C3'-C4'	3.26	1.61	1.53
4	D	701	AMP	O5'-C5'	3.66	1.59	1.44
4	A	501	AMP	C4-N3	5.32	1.43	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	AMP	C4'-O4'-C1'	-6.18	102.93	109.72
4	A	501	AMP	C4'-O4'-C1'	-5.60	103.56	109.72
4	C	601	AMP	C4'-O4'-C1'	-3.35	106.04	109.72
4	C	601	AMP	O3P-P-O2P	-2.98	96.04	107.38
4	D	701	AMP	O3P-P-O2P	-2.95	96.15	107.38
4	B	801	AMP	C4-C5-N7	-2.54	107.15	109.48
4	A	501	AMP	C4-C5-N7	-2.47	107.21	109.48
4	A	501	AMP	O3P-P-O5'	-2.43	99.57	106.56
4	A	501	AMP	C1'-N9-C4	-2.32	123.44	126.94
4	D	701	AMP	C4'-O4'-C1'	-2.29	107.20	109.72
4	B	801	AMP	O3P-P-O2P	-2.22	98.94	107.38
4	C	601	AMP	C4-C5-N7	-2.06	107.58	109.48
4	A	501	AMP	O2P-P-O1P	2.09	117.32	110.58
4	D	701	AMP	O2P-P-O5'	2.19	112.88	106.56
4	D	701	AMP	O5'-C5'-C4'	2.20	117.22	109.12
4	B	801	AMP	O3'-C3'-C4'	2.28	117.89	111.05
4	B	801	AMP	O3P-P-O1P	2.45	118.45	110.58
4	B	801	AMP	O5'-C5'-C4'	2.75	119.24	109.12
4	C	601	AMP	O3P-P-O1P	3.15	120.71	110.58
4	C	601	AMP	O2P-P-O1P	3.17	120.78	110.58
4	A	501	AMP	O3P-P-O1P	3.29	121.16	110.58
4	D	701	AMP	O3P-P-O1P	3.66	122.35	110.58
4	C	601	AMP	O4'-C1'-N9	4.75	118.05	108.10
4	D	701	AMP	O4'-C1'-N9	5.83	120.30	108.10
4	B	801	AMP	C2'-C1'-N9	6.23	123.80	114.29
4	A	501	AMP	C2'-C1'-N9	6.64	124.44	114.29
4	A	501	AMP	O4'-C1'-N9	6.85	122.44	108.10
4	B	801	AMP	O4'-C1'-N9	7.54	123.88	108.10
4	D	701	AMP	C2'-C1'-N9	7.75	126.13	114.29
4	C	601	AMP	C2'-C1'-N9	9.10	128.19	114.29

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	501	AMP	C1'

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Mol	Chain	Res	Type	Atom
4	C	601	AMP	C1'
4	B	801	AMP	C1'
4	D	701	AMP	C1'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	AMP	6	0
4	B	801	AMP	5	0
4	C	601	AMP	3	0
4	D	701	AMP	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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