



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:41 AM UTC

PDB ID : 1DS5 / pdb_00001ds5
Title : DIMERIC CRYSTAL STRUCTURE OF THE ALPHA SUBUNIT IN COM-
PLEX WITH TWO BETA PEPTIDES MIMICKING THE ARCHITEC-
TURE 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

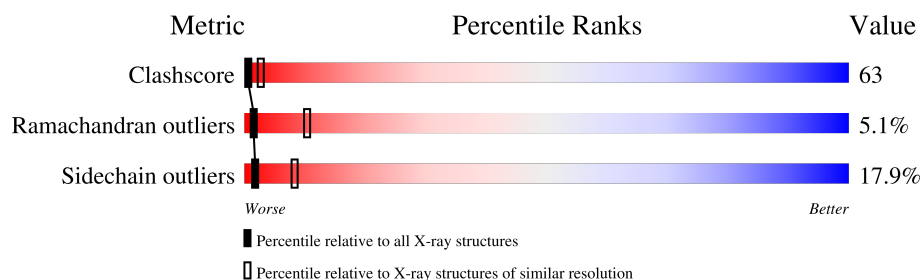
1 Overall quality at a glance

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	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	332	
1	B	332	
1	C	332	
1	D	332	
2	E	23	
2	F	23	
2	G	23	
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
3	AMP	A	501	X	-	X	-
3	AMP	B	801	X	-	-	-
3	AMP	C	601	X	-	-	-
3	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.

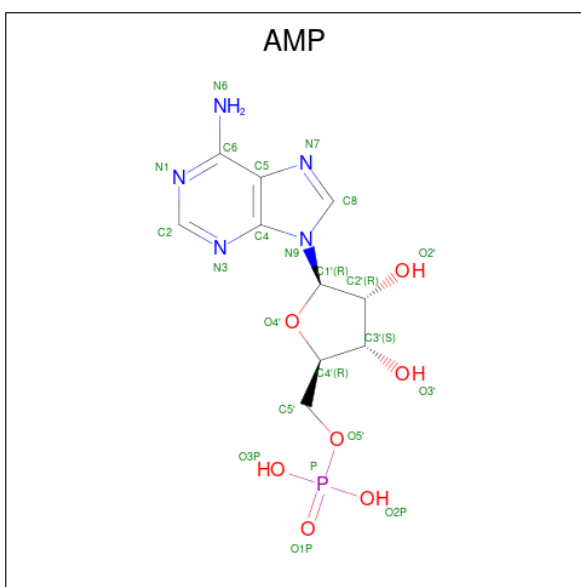
- Molecule 1 is a protein called CASEIN KINASE, ALPHA CHAIN.

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 ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- 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		

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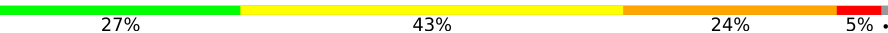
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	73	Total 73	O 73	0	0
5	E	6	Total 6	O 6	0	0
5	F	4	Total 4	O 4	0	0
5	G	6	Total 6	O 6	0	0
5	H	8	Total 8	O 8	0	0

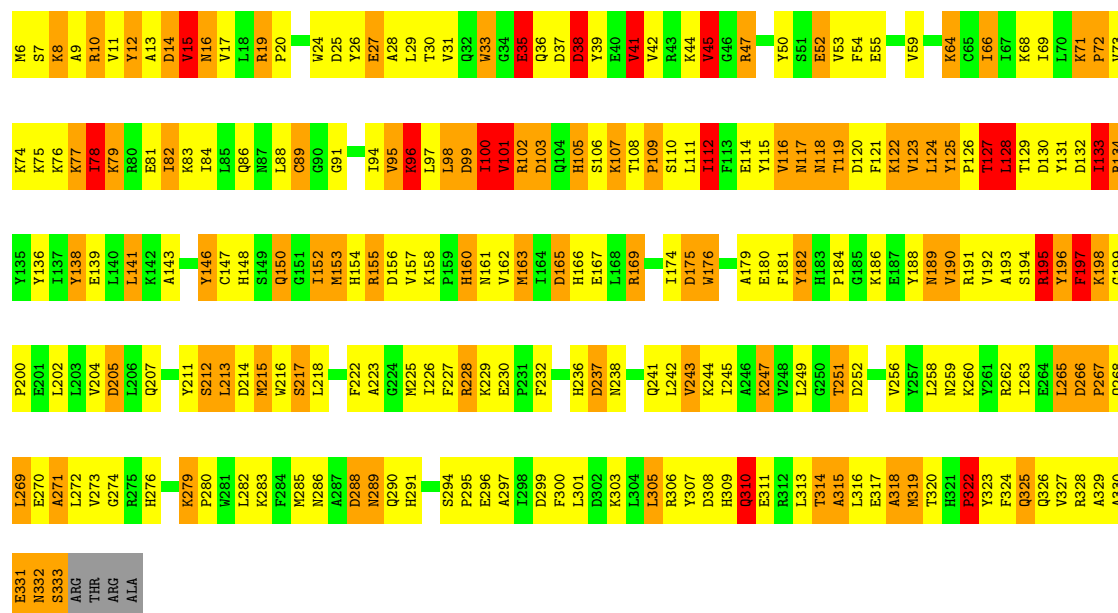
3 Residue-property plots

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

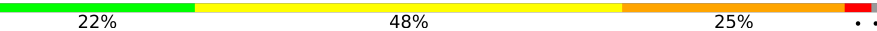
Note EDS was not executed.

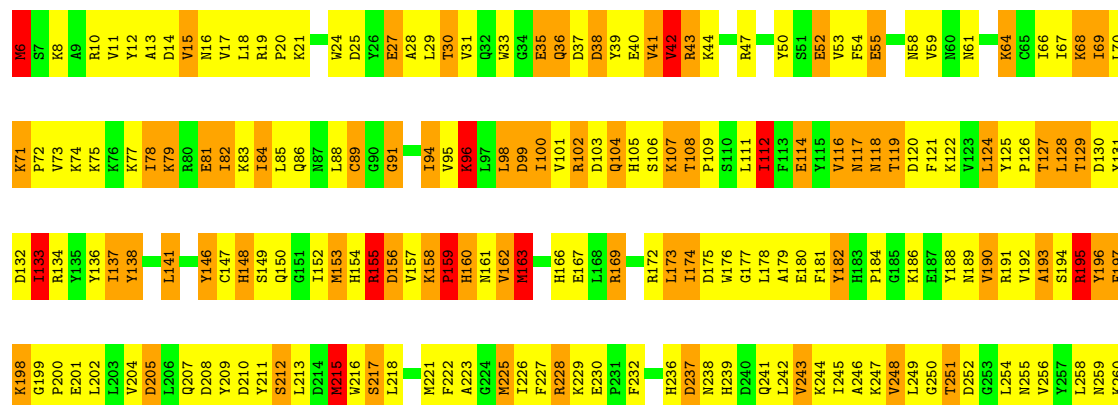
• Molecule 1: CASEIN KINASE, ALPHA CHAIN

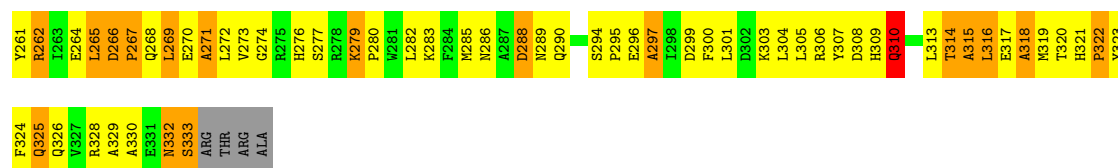
Chain A:  27% 43% 24% 5%



• Molecule 1: CASEIN KINASE, ALPHA CHAIN

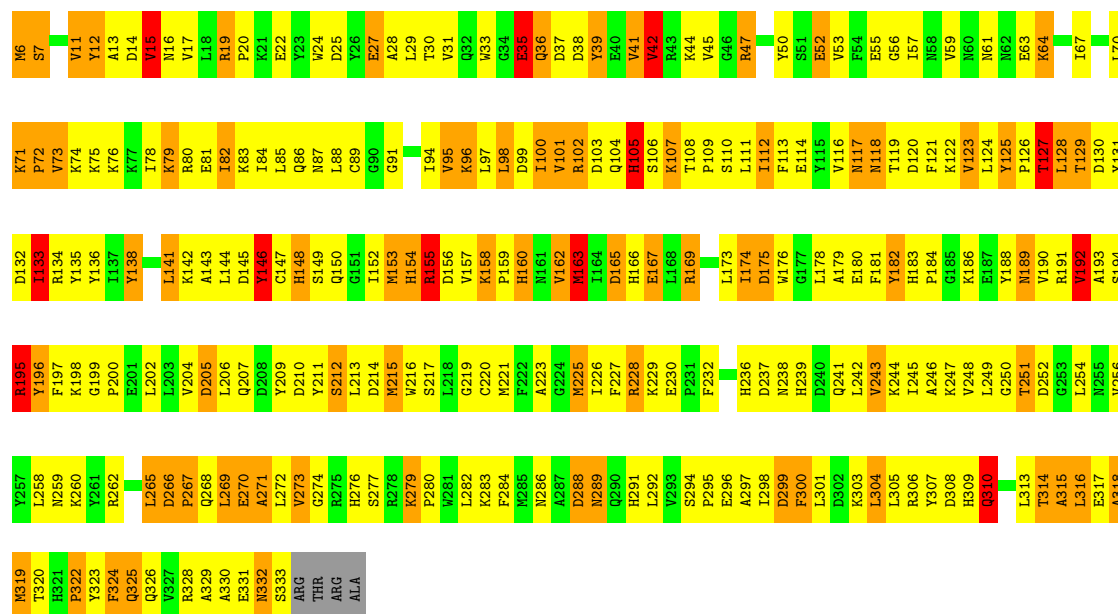
Chain B:  22% 48% 25% . .





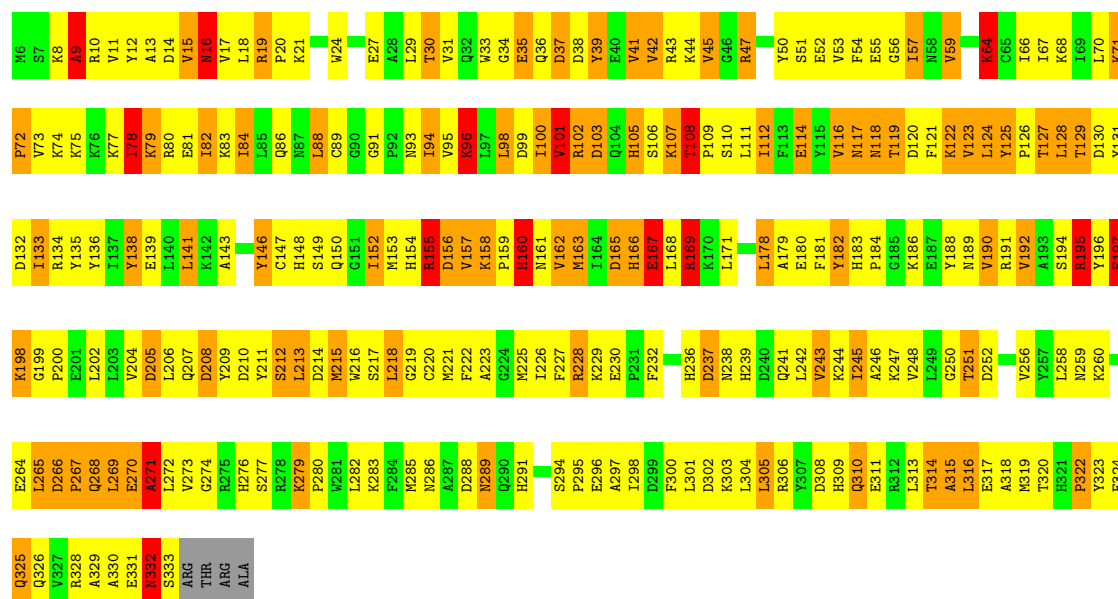
• Molecule 1: CASEIN KINASE, ALPHA CHAIN

Chain C: 21% 51% 23%



• Molecule 1: CASEIN KINASE, ALPHA CHAIN

Chain D: 22% 48% 24% 5%



• Molecule 2: CASEIN KINASE, BETA CHAIN

Chain E:  13% 39% 13% 30%

• Molecule 2: CASEIN KINASE, BETA CHAIN

Chain F:  17% 35% 22% 22%

• Molecule 2: CASEIN KINASE, BETA CHAIN

Chain G:  17% 39% 9% 30%

• Molecule 2: CASEIN KINASE, BETA CHAIN

Chain H:  13% 35% 22% 30%

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.68Å 119.85Å 145.56Å 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	1.70	30/2803 (1.1%)	1.67	65/3788 (1.7%)
1	B	1.63	24/2803 (0.9%)	1.64	49/3788 (1.3%)
1	C	1.68	31/2803 (1.1%)	1.64	45/3788 (1.2%)
1	D	1.58	22/2803 (0.8%)	1.66	59/3788 (1.6%)
2	E	1.76	0/139	2.63	8/185 (4.3%)
2	F	1.75	1/158 (0.6%)	2.97	9/210 (4.3%)
2	G	1.77	1/139 (0.7%)	2.73	8/185 (4.3%)
2	H	2.03	4/139 (2.9%)	2.08	9/185 (4.9%)
All	All	1.65	113/11787 (1.0%)	1.71	252/15917 (1.6%)

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 (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	MET	SD-CE	-15.54	1.40	1.79
1	B	41	VAL	CA-CB	-14.20	1.36	1.54
1	D	157	VAL	CA-C	-10.65	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	VAL	CA-CB	-9.99	1.40	1.54
1	A	41	VAL	CA-CB	9.97	1.67	1.54
2	H	202	GLN	CA-C	9.62	1.64	1.53
1	C	266	ASP	CA-C	-9.02	1.44	1.53
1	D	57	ILE	CA-CB	-8.50	1.46	1.55
1	A	266	ASP	CA-C	-8.48	1.44	1.53
1	A	143	ALA	CA-CB	-8.45	1.39	1.53
1	B	153	MET	SD-CE	-8.43	1.58	1.79
1	B	94	ILE	CA-CB	-8.23	1.44	1.54
1	B	221	MET	SD-CE	-8.15	1.59	1.79
1	B	318	ALA	CA-CB	-8.14	1.39	1.53
1	C	228	ARG	CA-C	-8.03	1.46	1.53
1	D	163	MET	SD-CE	-7.90	1.59	1.79
2	H	197	TYR	CA-C	-7.83	1.42	1.52
1	C	59	VAL	CA-CB	-7.79	1.43	1.54
1	D	228	ARG	CA-C	-7.77	1.46	1.53
1	A	59	VAL	CA-CB	-7.71	1.44	1.54
1	B	53	VAL	CA-CB	-7.69	1.45	1.54
1	B	69	ILE	CA-CB	-7.69	1.44	1.53
1	A	109	PRO	CA-C	7.66	1.61	1.52
2	G	198	GLN	CA-C	7.63	1.59	1.52
1	B	266	ASP	CA-C	-7.49	1.45	1.53
1	B	163	MET	SD-CE	-7.40	1.61	1.79
1	B	228	ARG	CA-C	-7.40	1.46	1.53
1	C	292	LEU	CA-C	7.37	1.62	1.52
1	A	78	ILE	CA-CB	-7.34	1.45	1.54
1	D	53	VAL	CA-CB	-7.19	1.45	1.54
1	A	327	VAL	CA-CB	-7.12	1.46	1.54
1	B	225	MET	SD-CE	7.04	1.97	1.79
1	D	103	ASP	CA-C	-7.04	1.43	1.52
1	A	127	THR	CA-CB	-6.98	1.41	1.53
1	D	59	VAL	CA-CB	-6.96	1.44	1.54
1	C	15	VAL	CA-CB	-6.92	1.45	1.54
1	A	53	VAL	CA-CB	-6.86	1.46	1.54
1	D	298	ILE	CA-CB	-6.83	1.45	1.54
1	D	94	ILE	CA-CB	-6.69	1.46	1.54
1	C	11	VAL	CA-CB	6.66	1.62	1.55
1	D	143	ALA	CA-CB	-6.62	1.43	1.53
1	A	100	ILE	CA-C	6.62	1.61	1.52
1	C	225	MET	SD-CE	6.62	1.96	1.79
1	A	198	LYS	CA-C	-6.55	1.44	1.52
1	D	35	GLU	CA-CB	6.53	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	MET	SD-CE	6.46	1.95	1.79
1	C	192	VAL	CA-CB	-6.42	1.45	1.54
1	C	6	MET	SD-CE	6.42	1.95	1.79
1	C	95	VAL	CA-C	-6.41	1.45	1.52
1	D	166	HIS	CA-C	-6.38	1.44	1.52
1	C	73	VAL	CA-CB	-6.29	1.49	1.55
1	B	112	ILE	CA-CB	6.16	1.61	1.53
1	A	318	ALA	CA-CB	-6.06	1.42	1.53
1	C	163	MET	SD-CE	-6.06	1.64	1.79
1	C	174	ILE	CA-CB	-6.06	1.46	1.54
1	C	319	MET	SD-CE	6.05	1.94	1.79
1	C	154	HIS	C-O	-6.05	1.15	1.24
1	C	206	LEU	CA-C	-6.04	1.45	1.53
1	C	318	ALA	CA-CB	-6.04	1.42	1.53
1	D	271	ALA	CA-CB	-5.94	1.43	1.53
1	B	215	MET	CA-C	-5.87	1.45	1.52
1	A	16	ASN	CA-C	-5.82	1.44	1.52
1	B	255	ASN	CA-C	-5.79	1.45	1.52
2	F	202	GLN	CA-C	5.78	1.60	1.52
1	A	102	ARG	CA-C	-5.77	1.45	1.53
1	A	138	TYR	CA-C	5.73	1.60	1.52
1	B	174	ILE	CA-C	5.72	1.59	1.53
1	A	285	MET	SD-CE	-5.69	1.65	1.79
1	B	285	MET	SD-CE	5.68	1.93	1.79
1	C	129	THR	CA-C	-5.68	1.46	1.52
1	C	300	PHE	C-O	-5.62	1.17	1.24
1	A	66	ILE	CA-CB	-5.53	1.47	1.54
1	B	248	VAL	CA-CB	5.50	1.61	1.54
1	B	133	ILE	CA-CB	-5.50	1.48	1.54
1	D	35	GLU	CB-CG	5.49	1.69	1.52
1	B	215	MET	SD-CE	5.48	1.93	1.79
1	C	97	LEU	C-O	-5.48	1.17	1.24
1	A	95	VAL	CA-C	-5.47	1.44	1.53
1	A	133	ILE	CA-CB	-5.46	1.48	1.54
1	C	36	GLN	CB-CG	-5.44	1.36	1.52
1	C	47	ARG	CA-C	-5.40	1.48	1.53
1	B	190	VAL	CA-CB	-5.39	1.47	1.54
1	D	246	ALA	CA-CB	-5.39	1.45	1.53
2	H	198	GLN	CA-C	-5.39	1.45	1.53
1	D	123	VAL	C-O	-5.38	1.18	1.23
1	A	99	ASP	C-O	-5.36	1.17	1.24
1	D	129	THR	CA-C	-5.36	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	LYS	CA-C	-5.35	1.46	1.52
1	D	64	LYS	C-O	-5.34	1.17	1.23
1	A	228	ARG	CA-C	-5.33	1.48	1.53
1	A	213	LEU	CA-C	-5.33	1.45	1.52
1	A	214	ASP	CA-C	-5.32	1.45	1.52
1	B	42	VAL	N-CA	5.31	1.51	1.46
1	C	85	LEU	CA-C	-5.31	1.46	1.52
1	B	137	ILE	CA-CB	-5.29	1.47	1.54
1	C	133	ILE	CA-C	-5.28	1.46	1.52
1	C	146	TYR	CA-C	-5.28	1.45	1.52
2	H	194	PRO	CB-CG	5.27	1.76	1.49
1	A	139	GLU	CA-C	-5.27	1.46	1.52
1	C	270	GLU	CA-C	-5.24	1.46	1.52
1	A	14	ASP	CA-C	-5.24	1.45	1.52
1	C	162	VAL	CA-C	5.24	1.59	1.52
1	C	238	ASN	C-O	-5.21	1.17	1.24
1	A	10	ARG	CA-C	-5.16	1.46	1.52
1	D	42	VAL	CA-C	5.15	1.58	1.52
1	A	205	ASP	CA-C	-5.13	1.46	1.53
1	D	88	LEU	CA-C	5.13	1.59	1.52
1	C	292	LEU	C-O	5.13	1.30	1.24
1	A	314	THR	CA-CB	-5.10	1.45	1.53
1	A	150	GLN	CA-C	-5.07	1.46	1.52
1	D	156	ASP	N-CA	5.07	1.52	1.46
1	C	113	PHE	CA-C	-5.05	1.46	1.53
1	D	245	ILE	CA-C	5.04	1.59	1.52

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	193	HIS	CA-C-N	-20.01	94.83	119.84
2	F	193	HIS	C-N-CA	-20.01	94.83	119.84
2	G	198	GLN	N-CA-C	16.53	134.78	112.13
2	E	193	HIS	CA-C-N	-15.43	100.56	119.84
2	E	193	HIS	C-N-CA	-15.43	100.56	119.84
2	G	193	HIS	CA-C-N	-14.88	101.23	119.84
2	G	193	HIS	C-N-CA	-14.88	101.23	119.84
1	A	101	VAL	N-CA-C	14.69	127.74	108.35
1	C	158	LYS	N-CA-C	-13.49	95.99	108.13
2	F	198	GLN	N-CA-C	13.04	131.50	111.56
1	D	207	GLN	N-CA-C	11.78	125.26	111.71
1	A	42	VAL	N-CA-C	11.51	121.79	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	200	GLN	N-CA-C	-11.32	94.17	110.59
1	B	267	PRO	N-CA-C	-10.98	95.63	111.33
1	B	269	LEU	N-CA-C	-10.87	99.44	111.28
1	C	207	GLN	N-CA-C	10.77	124.09	111.71
1	A	207	GLN	N-CA-C	10.72	124.03	111.71
1	C	266	ASP	N-CA-C	-10.52	96.28	109.64
1	D	267	PRO	N-CA-C	-10.46	96.38	111.33
1	B	314	THR	N-CA-C	-10.45	97.05	110.53
1	A	266	ASP	N-CA-C	-10.42	96.41	109.64
1	B	207	GLN	N-CA-C	10.33	123.59	111.71
2	F	202	GLN	N-CA-C	10.06	125.79	107.99
1	B	266	ASP	N-CA-C	-10.00	96.94	109.64
1	B	42	VAL	CB-CA-C	-9.61	101.49	110.91
1	D	266	ASP	N-CA-C	-9.58	97.47	109.64
1	C	108	THR	N-CA-C	-9.47	92.31	109.44
1	A	314	THR	N-CA-C	-9.43	98.36	110.53
1	D	45	VAL	CB-CA-C	-9.27	101.91	110.63
1	D	157	VAL	N-CA-C	-9.12	100.11	110.05
1	D	53	VAL	N-CA-C	9.01	121.25	108.36
1	C	269	LEU	N-CA-C	-8.98	101.58	111.36
2	G	196	ALA	N-CA-C	-8.94	99.10	110.19
1	B	236	HIS	N-CA-C	-8.84	102.63	113.50
1	D	269	LEU	N-CA-C	-8.38	102.15	111.28
2	E	200	GLN	CA-C-N	-8.31	108.17	123.05
2	E	200	GLN	C-N-CA	-8.31	108.17	123.05
1	C	79	LYS	N-CA-C	-8.27	102.20	111.71
1	D	16	ASN	N-CA-C	-8.24	102.17	112.72
1	D	315	ALA	N-CA-C	-8.21	102.29	111.07
1	C	55	GLU	N-CA-C	-8.15	95.95	109.24
1	B	116	VAL	CA-C-N	-8.15	110.70	122.19
1	B	116	VAL	C-N-CA	-8.15	110.70	122.19
1	C	236	HIS	N-CA-C	-8.06	103.59	113.50
1	A	79	LYS	N-CA-C	-7.85	102.80	112.38
1	B	108	THR	CB-CA-C	-7.84	101.73	110.98
1	A	102	ARG	N-CA-C	-7.83	98.35	110.17
2	H	198	GLN	N-CA-C	-7.83	100.23	110.33
1	C	314	THR	N-CA-C	-7.81	99.26	110.59
1	B	55	GLU	N-CA-C	-7.79	96.87	109.96
2	F	196	ALA	N-CA-C	-7.75	99.57	110.50
1	A	267	PRO	N-CA-C	-7.74	96.53	112.47
1	B	79	LYS	N-CA-C	-7.68	103.01	112.38
1	D	314	THR	N-CA-C	-7.65	100.66	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	CB-CA-C	-7.42	101.98	111.70
1	D	198	LYS	N-CA-C	-7.38	98.53	110.20
1	A	269	LEU	N-CA-C	-7.38	103.24	111.28
1	D	332	ASN	N-CA-C	-7.37	103.24	111.71
1	A	117	ASN	N-CA-C	-7.34	98.08	109.76
1	A	8	LYS	N-CA-C	-7.33	97.92	109.07
1	A	236	HIS	N-CA-C	-7.33	104.15	113.23
1	D	71	LYS	CA-C-N	7.30	128.97	119.84
1	D	71	LYS	C-N-CA	7.30	128.97	119.84
1	D	128	LEU	N-CA-C	7.24	120.09	110.53
1	C	267	PRO	N-CA-C	-7.24	97.57	112.47
1	B	155	ARG	N-CA-C	7.21	126.17	110.80
1	D	197	PHE	N-CA-C	7.21	121.38	112.59
1	A	15	VAL	N-CA-C	-7.17	104.78	111.45
1	D	165	ASP	N-CA-C	-7.14	95.31	108.24
2	F	199	LEU	N-CA-C	7.14	119.60	108.96
1	C	117	ASN	N-CA-C	-7.13	97.63	109.46
1	A	128	LEU	N-CA-C	7.10	119.91	110.53
1	D	236	HIS	N-CA-C	-7.03	104.70	113.28
2	G	195	MET	N-CA-C	7.03	120.42	110.50
1	B	315	ALA	N-CA-C	-7.03	103.31	110.97
1	D	34	GLY	CA-C-N	-6.99	113.47	122.77
1	D	34	GLY	C-N-CA	-6.99	113.47	122.77
1	C	305	LEU	N-CA-C	6.94	120.03	109.62
2	H	201	LEU	N-CA-C	-6.94	98.92	109.95
1	A	14	ASP	CA-C-N	-6.93	111.39	121.65
1	A	14	ASP	C-N-CA	-6.93	111.39	121.65
1	C	35	GLU	N-CA-C	6.93	119.98	108.96
1	D	84	ILE	CB-CA-C	-6.93	103.01	111.88
1	C	125	TYR	CA-C-N	-6.93	111.18	119.84
1	C	125	TYR	C-N-CA	-6.93	111.18	119.84
1	B	96	LYS	N-CA-C	6.91	119.78	108.52
1	A	55	GLU	N-CA-C	-6.84	98.08	109.24
1	B	173	LEU	N-CA-C	-6.81	98.59	109.76
1	C	110	SER	N-CA-C	6.78	119.53	108.55
1	B	117	ASN	N-CA-C	-6.75	98.26	109.46
1	C	127	THR	CB-CA-C	-6.74	97.01	110.42
1	B	35	GLU	N-CA-C	6.70	119.78	107.99
1	B	53	VAL	N-CA-C	6.70	117.94	108.36
1	D	251	THR	N-CA-C	6.70	119.41	111.71
1	D	270	GLU	N-CA-C	-6.69	103.68	110.97
1	D	205	ASP	N-CA-C	6.68	120.88	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ASN	N-CA-C	-6.67	99.16	109.76
1	B	71	LYS	CA-C-N	6.66	128.17	119.84
1	B	71	LYS	C-N-CA	6.66	128.17	119.84
1	A	35	GLU	N-CA-C	6.58	119.46	108.73
1	C	95	VAL	N-CA-C	-6.58	101.04	109.80
1	C	299	ASP	N-CA-C	-6.56	104.05	111.07
2	H	196	ALA	N-CA-C	-6.54	100.22	110.36
1	A	315	ALA	N-CA-C	-6.53	103.78	111.03
1	D	42	VAL	N-CA-CB	-6.53	106.29	111.64
2	E	196	ALA	N-CA-C	-6.52	102.10	110.19
1	D	311	GLU	N-CA-C	6.50	120.89	113.15
1	D	9	ALA	CA-C-N	-6.49	112.36	122.67
1	D	9	ALA	C-N-CA	-6.49	112.36	122.67
1	C	304	LEU	N-CA-C	-6.47	105.03	113.12
1	B	42	VAL	N-CA-C	6.47	117.56	112.12
2	F	188	TYR	CA-CB-CG	6.47	125.55	113.90
1	A	124	LEU	N-CA-C	6.45	118.19	111.03
2	H	193	HIS	CA-C-N	-6.44	111.79	119.84
2	H	193	HIS	C-N-CA	-6.44	111.79	119.84
1	C	123	VAL	CB-CA-C	-6.43	102.59	111.65
1	B	128	LEU	N-CA-C	6.40	119.19	110.55
1	C	251	THR	N-CA-C	6.38	119.05	111.71
1	D	138	TYR	N-CA-C	-6.37	104.43	111.82
1	C	128	LEU	N-CA-C	6.34	118.90	110.53
1	B	148	HIS	N-CA-C	-6.34	104.45	111.36
1	D	167	GLU	N-CA-C	-6.34	103.06	111.24
1	C	270	GLU	N-CA-C	-6.33	104.07	110.97
1	D	124	LEU	N-CA-C	6.33	119.12	111.40
1	B	68	LYS	N-CA-C	-6.32	98.12	108.41
1	D	305	LEU	N-CA-C	6.30	119.41	109.39
1	D	55	GLU	N-CA-C	-6.30	99.38	109.96
1	C	53	VAL	N-CA-C	6.27	116.95	108.17
1	A	38	ASP	N-CA-C	-6.27	104.90	112.54
1	A	19	ARG	N-CA-C	6.25	118.70	110.08
1	D	178	LEU	N-CA-C	-6.15	106.37	114.31
1	C	42	VAL	CB-CA-C	-6.14	101.22	111.29
1	B	305	LEU	N-CA-C	6.13	119.14	109.39
1	D	19	ARG	N-CA-C	6.10	118.99	110.20
1	B	138	TYR	N-CA-C	-6.09	104.65	111.28
1	C	96	LYS	N-CA-C	6.05	118.38	108.52
1	B	8	LYS	N-CA-C	-5.96	99.34	108.76
1	A	251	THR	N-CA-C	5.96	118.56	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	VAL	N-CA-C	5.95	116.50	108.17
1	A	270	GLU	N-CA-C	-5.92	104.00	111.11
1	A	152	ILE	N-CA-C	5.92	117.89	108.89
1	B	198	LYS	N-CA-C	-5.91	101.73	110.48
1	C	27	GLU	N-CA-C	-5.90	105.35	112.54
1	A	198	LYS	N-CA-C	-5.88	100.92	110.20
1	D	79	LYS	N-CA-C	-5.87	104.96	111.71
1	C	205	ASP	N-CA-C	5.85	119.71	111.52
1	B	174	ILE	N-CA-C	5.82	115.92	108.82
1	D	152	ILE	N-CA-C	5.80	116.94	108.53
2	F	193	HIS	N-CA-C	-5.80	97.00	109.81
1	D	51	SER	N-CA-C	5.79	117.59	108.96
1	C	101	VAL	N-CA-C	5.79	118.51	108.90
1	D	42	VAL	N-CA-C	5.79	116.19	111.62
1	C	155	ARG	N-CA-C	5.78	123.12	110.80
1	A	311	GLU	N-CA-C	5.77	120.01	113.15
2	H	193	HIS	N-CA-C	-5.75	97.10	109.81
1	C	315	ALA	N-CA-C	-5.75	104.92	111.07
1	B	124	LEU	CA-CB-CG	-5.75	96.19	116.30
1	C	138	TYR	N-CA-C	-5.74	105.11	111.71
1	B	297	ALA	N-CA-C	-5.71	104.42	111.33
1	B	102	ARG	N-CA-C	-5.69	98.67	110.80
1	D	67	ILE	N-CA-C	-5.66	99.59	107.80
1	D	110	SER	N-CA-C	5.65	116.99	108.46
1	B	217	SER	N-CA-C	-5.62	105.05	111.07
2	G	193	HIS	N-CA-C	-5.59	97.45	109.81
2	G	191	LYS	N-CA-C	5.59	118.33	109.50
1	A	217	SER	N-CA-C	-5.58	105.11	111.14
1	A	26	TYR	N-CA-C	5.57	119.34	112.54
1	B	251	THR	N-CA-C	5.57	118.11	111.71
1	C	71	LYS	CA-C-N	5.56	126.79	119.84
1	C	71	LYS	C-N-CA	5.56	126.79	119.84
1	A	174	ILE	N-CA-C	5.53	115.57	108.82
1	A	310	GLN	N-CA-C	-5.53	105.17	111.14
1	D	96	LYS	N-CA-C	5.53	117.53	108.52
1	A	155	ARG	N-CA-C	5.53	122.57	110.80
1	B	205	ASP	N-CA-C	5.52	119.25	111.52
1	B	108	THR	CA-C-N	5.51	125.44	119.76
1	B	108	THR	C-N-CA	5.51	125.44	119.76
1	A	205	ASP	N-CA-C	5.50	118.98	111.39
1	D	116	VAL	CB-CA-C	-5.50	102.03	110.50
1	A	77	LYS	N-CA-C	-5.49	106.35	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	195	MET	N-CA-C	5.48	118.85	110.20
1	A	68	LYS	N-CA-C	-5.46	100.28	109.07
1	A	71	LYS	CA-C-N	5.45	126.65	119.84
1	A	71	LYS	C-N-CA	5.45	126.65	119.84
1	D	108	THR	CA-C-N	5.44	126.20	120.11
1	D	108	THR	C-N-CA	5.44	126.20	120.11
1	C	129	THR	CB-CA-C	-5.44	99.92	109.71
1	A	165	ASP	N-CA-C	-5.43	97.95	107.73
1	A	247	LYS	CA-C-N	-5.43	117.40	123.16
1	A	247	LYS	C-N-CA	-5.43	117.40	123.16
1	A	78	ILE	N-CA-C	-5.41	107.52	111.90
1	A	153	MET	CB-CA-C	-5.39	101.35	110.19
1	D	208	ASP	CA-C-O	-5.36	115.94	122.64
1	C	19	ARG	N-CA-C	5.35	117.47	110.08
1	A	42	VAL	CB-CA-C	-5.35	105.67	110.91
1	C	319	MET	N-CA-C	-5.35	107.06	113.21
2	H	192	ILE	N-CA-CB	5.34	118.19	111.46
1	B	114	GLU	N-CA-C	-5.33	102.59	110.48
1	D	125	TYR	CA-C-N	-5.33	113.17	119.84
1	D	125	TYR	C-N-CA	-5.33	113.17	119.84
1	C	310	GLN	N-CA-C	-5.32	105.39	111.14
1	C	284	PHE	N-CA-C	-5.32	105.49	113.89
1	D	78	ILE	N-CA-C	-5.32	107.24	111.81
1	D	190	VAL	N-CA-C	5.30	118.89	112.80
1	A	176	TRP	N-CA-C	-5.28	106.14	112.59
1	A	112	ILE	CB-CA-C	-5.26	104.69	111.53
1	B	290	GLN	N-CA-C	5.26	118.49	111.75
1	D	103	ASP	CB-CA-C	-5.26	102.37	110.26
1	D	248	VAL	N-CA-C	-5.25	107.47	111.62
2	G	189	GLY	N-CA-C	-5.25	100.74	113.18
1	A	9	ALA	CA-C-N	-5.23	114.28	122.49
1	A	9	ALA	C-N-CA	-5.23	114.28	122.49
1	A	116	VAL	CA-C-N	-5.22	114.04	121.50
1	A	116	VAL	C-N-CA	-5.22	114.04	121.50
1	D	114	GLU	N-CA-C	-5.22	103.15	110.50
1	C	148	HIS	N-CA-C	-5.21	105.60	111.28
1	A	319	MET	N-CA-C	-5.21	107.22	113.21
1	D	218	LEU	N-CA-C	-5.19	104.88	111.11
1	C	165	ASP	N-CA-C	-5.19	96.92	107.41
1	C	324	PHE	N-CA-C	5.18	119.58	113.16
1	D	213	LEU	CA-C-N	-5.18	112.82	120.28
1	D	213	LEU	C-N-CA	-5.18	112.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ILE	CB-CA-C	-5.18	105.25	111.88
2	H	200	GLN	CB-CA-C	-5.17	100.84	113.15
1	D	101	VAL	N-CA-C	5.17	116.14	108.65
1	A	134	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	B	78	ILE	N-CA-C	-5.16	107.37	111.81
1	B	27	GLU	N-CA-C	-5.15	106.50	112.89
1	A	123	VAL	CB-CA-C	-5.15	105.45	111.94
1	A	115	TYR	CA-C-N	-5.13	115.85	122.99
1	A	115	TYR	C-N-CA	-5.13	115.85	122.99
1	A	289	ASN	N-CA-C	5.13	118.80	112.54
2	E	191	LYS	N-CA-C	5.13	117.78	109.06
1	B	167	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	305	LEU	N-CA-C	5.12	117.30	109.62
1	B	304	LEU	N-CA-C	-5.11	105.89	112.68
1	A	101	VAL	CB-CA-C	-5.11	101.85	111.30
2	E	193	HIS	N-CA-C	-5.07	98.60	109.81
1	B	91	GLY	CA-C-N	5.07	125.36	119.93
1	B	91	GLY	C-N-CA	5.07	125.36	119.93
1	D	155	ARG	N-CA-C	5.07	121.59	110.80
1	B	99	ASP	N-CA-C	-5.07	100.01	110.80
1	A	95	VAL	N-CA-C	-5.03	101.83	109.78
1	A	197	PHE	N-CA-C	5.03	118.73	112.59
1	C	108	THR	CA-C-N	5.03	125.50	120.52
1	C	108	THR	C-N-CA	5.03	125.50	120.52
1	A	27	GLU	N-CA-C	-5.03	106.41	112.54
1	A	96	LYS	N-CA-C	5.03	116.71	108.52
2	H	189	GLY	N-CA-C	-5.02	101.29	113.18
1	A	33	TRP	N-CA-C	5.01	117.31	110.24
1	A	45	VAL	CB-CA-C	5.00	119.49	111.29
1	B	310	GLN	N-CA-C	-5.00	105.74	111.14

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

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Mol	Chain	Res	Type	Group
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 [i](#)

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	304	0
1	B	2735	0	2721	368	0
1	C	2735	0	2721	327	0
1	D	2735	0	2721	328	0
2	E	135	0	132	53	0
2	F	154	0	156	60	0
2	G	135	0	132	61	0
2	H	135	0	132	50	0
3	A	23	0	11	7	0
3	B	23	0	11	5	0
3	C	23	0	11	4	0
3	D	23	0	11	3	0
4	B	2	0	0	0	0
4	D	2	0	0	0	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
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	1448	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 63.

All (1448) 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:CG	2:H:194:PRO:CB	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:HG2	1:B:43:ARG:HH11	0.93	1.04
1:B:36:GLN:OE1	1:B:103:ASP:HA	1.57	1.04
2:H:197:TYR:N	2:H:197:TYR:HD1	1.52	1.02
1:D:169:ARG:HH21	1:D:169:ARG:HG3	1.24	1.00
1:C:33:TRP:CE3	1:C:100:ILE:HD11	1.95	1.00
1:D:36:GLN:CD	2:H:194:PRO:HB2	1.87	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:C:118:ASN:CG	1:C:163:MET:HE3	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ILE:HD12	1:C:100:ILE:C	1.90	0.96
1:D:124:LEU:O	1:D:127:THR:HG22	1.66	0.96
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:N	2:H:197:TYR:CD1	2.30	0.92
1:D:100:ILE:HD12	1:D:100:ILE:C	1.94	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
1:D:158:LYS:HG2	1:D:161:ASN:HD22	1.36	0.90
2:H:190:PHE:HD1	2:H:190:PHE:O	1.52	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:CD2	1:D:160:HIS:H	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:GLN:C	2:H:199:LEU:HD23	2.00	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:A:136:TYR:OH	1:A:166:HIS:HD2	1.60	0.84
1:D:169:ARG:HH21	1:D:169:ARG:CG	1.90	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:C:36:GLN:NE2	2:G:194:PRO:C	2.37	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:36:GLN:CD	2:E:194:PRO:HB2	2.05	0.82
1:A:314:THR:HB	1:A:317:GLU:HG3	1.62	0.82
1:B:84:ILE:HD12	1:B:152:ILE:HD13	1.61	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:B:35:GLU:HB3	1:B:38:ASP:OD2	1.80	0.81
1:D:124:LEU:CD1	1:D:127:THR:HG21	2.09	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:A:267:PRO:O	1:A:268:GLN:HB3	1.80	0.81
1:B:160:HIS:CD2	1:B:160:HIS:H	1.96	0.81
1:D:119:THR:OG1	1:D:124:LEU:HB2	1.80	0.81
1:D:267:PRO:O	1:D:268:GLN:HB3	1.78	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:C:125:TYR:O	1:C:126:PRO:C	2.20	0.81
1:D:66:ILE:HG13	3: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ASN:CG	1:D:163:MET:HE3	2.05	0.80
1:D:286:ASN:HD21	1:D:288:ASP:HB3	1.46	0.80
1:B:64:LYS:HZ2	1:B:64:LYS:HB2	1.47	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:B:44:LYS:HZ2	1:B:47:ARG:HD3	1.45	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:B:325:GLN:HG3	1:B:326:GLN:H	1.47	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:D:223:ALA:HB2	1:D:301:LEU:HD11	1.62	0.79
1:A:331:GLU:C	1:A:333:SER:H	1.87	0.79
1:C:136:TYR:OH	1:C:166:HIS:HD2	1.66	0.79
1:A:33:TRP:CD1	1:A:33:TRP:H	1.96	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:64:LYS:HB2	1:B:64:LYS:NZ	1.99	0.78
2:E:198:GLN:C	2:E:199:LEU:HD23	2.08	0.78
1:D:242:LEU:HD23	1:D:269:LEU:HD21	1.65	0.78
1:C:169:ARG:HH21	1:C:169:ARG:CG	1.96	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
1:A:100:ILE:HD12	1:A:100:ILE:C	2.08	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:288:ASP:OD2	1:A:289:ASN:N	2.17	0.77
1:A:314:THR:HG22	1:A:315:ALA:N	1.97	0.77
1:A:119:THR:OG1	1:A:124:LEU:HB2	1.84	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:B:325:GLN:HG3	1:B:326:GLN:N	1.98	0.77
1:B:100:ILE:C	1:B:100:ILE:HD12	2.09	0.76
1:B:158:LYS:CE	1:B:161:ASN:HD21	1.98	0.76
1:B:169:ARG:HH21	1:B:169:ARG:CG	1.99	0.76
1:A:72:PRO:O	1:A:73:VAL:HG13	1.84	0.76
1:B:35:GLU:O	1:B:38:ASP:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:TRP:CZ2	1:B:245:ILE:HD13	2.20	0.76
2:G:198:GLN:O	2:G:199:LEU:CD2	2.33	0.76
1:A:41:VAL:CG1	2:F:197:TYR:HB3	2.12	0.76
1:B:158:LYS:HE3	1:B:161:ASN:ND2	1.99	0.76
1:B:212:SER:HB2	1:B:309:HIS:HB2	1.67	0.76
1:C:163:MET:HE2	3:C:601:AMP:N3	2.01	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
1:C:228:ARG:HD2	1:C:288:ASP:OD1	1.86	0.75
2:H:193:HIS:HB3	2:H:194:PRO:HD3	1.65	0.75
1:D:47:ARG:O	1:D:47:ARG:HG2	1.85	0.75
1:A:189:ASN:HD22	1:A:189:ASN:C	1.92	0.75
2:F:190:PHE:C	2:F:191:LYS:HG3	2.11	0.75
1:D:325:GLN:HG3	1:D:326:GLN:H	1.51	0.75
1:C:33:TRP:CD1	1:C:33:TRP:H	2.05	0.75
1:D:89:CYS:SG	1:D:96:LYS:NZ	2.60	0.74
2:F:191:LYS:HG2	2:F:196:ALA:HA	1.69	0.74
2:F:192:ILE:O	2:F:194:PRO:N	2.20	0.74
2:G:192:ILE:O	2:G:194:PRO:N	2.20	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:A:133:ILE:HD13	1:A:225:MET:HE2	1.68	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:314:THR:HG22	1:D:315:ALA:N	2.00	0.74
1:D:36:GLN:HE22	2:H:194:PRO:HB2	1.50	0.74
1:A:331:GLU:C	1:A:333:SER:N	2.40	0.73
2:E:191:LYS:HA	2:E:197:TYR:CE1	2.22	0.73
1:B:300:PHE:HE1	1:B:318:ALA:HB1	1.53	0.73
1:D:325:GLN:HG3	1:D:326:GLN:N	2.04	0.73
1:B:189:ASN:ND2	1:B:191:ARG:H	1.87	0.73
1:B:182:TYR:OH	1:B:184:PRO:HA	1.87	0.73
1:B:215:MET:CE	1:B:315:ALA:HA	2.18	0.73
1:D:163:MET:HE2	3:D:701:AMP:N3	2.03	0.73
1:C:165:ASP:OD1	1:C:167:GLU:HB3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:TRP:H	1:D:33:TRP:CD1	2.05	0.72
1:B:133:ILE:HD13	1:B:225:MET:HE2	1.71	0.72
1:C:189:ASN:ND2	1:C:191:ARG:H	1.87	0.72
2:F:200:GLN:NE2	2:F:202:GLN:NE2	2.37	0.72
1:A:106:SER:OG	1:A:107:LYS:N	2.20	0.72
1:A:286:ASN:ND2	1:A:288:ASP:N	2.38	0.72
1:B:202:LEU:HD11	1:B:213:LEU:HD11	1.71	0.72
1:D:91:GLY:HA3	1:D:146:TYR:CE2	2.25	0.72
1:D:125:TYR:O	1:D:126:PRO:C	2.30	0.72
1:C:215:MET:CE	1:C:315:ALA:HA	2.20	0.71
1:B:98:LEU:O	1:B:99:ASP:HB2	1.89	0.71
1:B:136:TYR:OH	1:B:166:HIS:HD2	1.72	0.71
1:D:70:LEU:HD12	1:D:78:ILE:HD13	1.71	0.71
1:B:125:TYR:O	1:B:126:PRO:C	2.30	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:B:84:ILE:CD1	1:B:152:ILE:HD13	2.20	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:D:124:LEU:C	1:D:126:PRO:HD2	2.16	0.71
1:D:215:MET:HE2	1:D:315:ALA:HA	1.71	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:C:289:ASN:OD1	1:C:289:ASN:C	2.34	0.71
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.26	0.70
1:A:153:MET:HE2	1:A:182:TYR:HD1	1.55	0.70
1:A:19:ARG:HB3	1:A:20:PRO:HD2	1.72	0.70
1:A:125:TYR:O	1:A:126:PRO:C	2.30	0.70
1:A:182:TYR:OH	1:A:184:PRO:HA	1.91	0.70
1:B:124:LEU:O	1:B:127:THR:HB	1.91	0.70
1:B:212:SER:CB	1:B:309:HIS:HB2	2.21	0.70
1:C:314:THR:HG22	1:C:315:ALA:N	2.06	0.70
1:D:121:PHE:HB2	1:D:125:TYR:CD2	2.26	0.70
1:D:166:HIS:CG	1:D:166:HIS:O	2.39	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:B:243:VAL:HG22	1:B:273:VAL:HA	1.73	0.70
1:C:36:GLN:O	1:C:38:ASP:N	2.25	0.70
1:C:243:VAL:HG22	1:C:273:VAL:HA	1.74	0.70
1:A:186:LYS:HD3	1:A:188:TYR:CZ	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:MET:HE2	1:D:182:TYR:HD1	1.57	0.70
1:D:332:ASN:HD22	1:D:332:ASN:N	1.88	0.70
1:A:186:LYS:HD3	1:A:188:TYR:CE1	2.27	0.69
1:D:33:TRP:CE3	1:D:102:ARG:HB3	2.26	0.69
1:B:6:MET:HE2	1:B:6:MET:O	1.91	0.69
1:C:6:MET:N	1:C:262:ARG:NH2	2.41	0.69
1:C:16:ASN:ND2	1:C:182:TYR:O	2.24	0.69
1:C:36:GLN:HE22	2:G:194:PRO:CB	2.04	0.69
1:A:215:MET:CE	1:A:315:ALA:HA	2.22	0.69
1:C:78:ILE:O	1:C:82:ILE:HG13	1.93	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:D:314:THR:CB	1:D:317:GLU:HG3	2.21	0.69
1:C:102:ARG:HD2	1:C:107:LYS:CD	2.23	0.69
2:H:191:LYS:C	2:H:197:TYR:OH	2.36	0.69
1:A:103:ASP:HB2	2:F:194:PRO:CG	2.23	0.68
1:C:33:TRP:CE2	1:C:102:ARG:HD3	2.28	0.68
1:C:212:SER:HB2	1:C:309:HIS:HB2	1.74	0.68
1:D:125:TYR:CD1	1:D:225:MET:HE3	2.29	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:C:36:GLN:HE22	2:G:194:PRO:C	2.00	0.68
1:D:36:GLN:HE22	2:H:194:PRO:CB	2.07	0.68
1:A:103:ASP:HB2	2:F:194:PRO:CB	2.24	0.68
1:D:124:LEU:O	1:D:127:THR:CG2	2.42	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:G:190:PHE:N	2:G:190:PHE:CD1	2.62	0.68
2:H:200:GLN:CG	5:H:208:HOH:O	2.28	0.68
2:G:188:TYR:O	2:G:189:GLY:C	2.35	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:HD1	2:H:197:TYR:H	1.40	0.67
1:B:126:PRO:CB	2:F:197:TYR:OH	2.41	0.67
1:C:189:ASN:HD22	1:C:189:ASN:C	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TRP:H	1:B:33:TRP:CD1	2.12	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:112:ILE:HD12	1:D:112:ILE:N	2.10	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:106:SER:C	1:D:107:LYS:HG3	2.20	0.67
1:D:215:MET:CE	1:D:315:ALA:HA	2.24	0.67
1:C:36:GLN:C	1:C:38:ASP:H	2.02	0.67
1:A:243:VAL:HG12	1:A:244:LYS:N	2.10	0.67
1:B:325:GLN:HA	1:B:328:ARG:HH12	1.60	0.67
1:C:300:PHE:HE1	1:C:318:ALA:HB1	1.59	0.67
1:A:189:ASN:ND2	1:A:189:ASN:C	2.52	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
1:A:198:LYS:HB3	1:A:202:LEU:HD12	1.78	0.66
1:B:40:GLU:OE2	2:E:198:GLN:NE2	2.28	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: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:A:105:HIS:CD2	1:A:105:HIS:C	2.73	0.66
1:A:103:ASP:HB2	2:F:194:PRO:HG3	1.77	0.66
1:A:289:ASN:C	1:A:289:ASN:OD1	2.39	0.65
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:A:101:VAL:O	1:A:109:PRO:HA	1.96	0.65
1:A:272:LEU:HD12	1:A:272:LEU:H	1.61	0.65
1:B:129:THR:O	1:B:130:ASP:C	2.39	0.65
1:D:125:TYR:N	1:D:126:PRO:HD2	2.11	0.65
1:B:288:ASP:OD2	1:B:288:ASP:C	2.40	0.65
1:D:212:SER:HB2	1:D:309:HIS:HB2	1.79	0.65
1:B:192:VAL:O	1:B:198:LYS:HE2	1.96	0.65
1:B:282:LEU:N	1:B:282:LEU:HD22	2.11	0.65
1:A:192:VAL:O	1:A:198:LYS:HE2	1.97	0.65
1:D:125:TYR:CE1	1:D:225:MET:HE3	2.32	0.65
1:B:251:THR:HG21	1:B:274:GLY:O	1.95	0.65
1:B:314:THR:HG22	1:B:315:ALA:N	2.12	0.65
1:C:41:VAL:HB	2:G:197:TYR:HB3	1.79	0.65
1:A:158:LYS:HG3	1:A:160:HIS:CD2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASP:OD1	1:D:44:LYS:HD2	1.96	0.65
1:D:50:TYR:O	1:D:71:LYS:HB2	1.96	0.65
1:D:243:VAL:HG22	1:D:273:VAL:HA	1.77	0.65
2:H:200:GLN:CB	5:H:208:HOH:O	2.45	0.65
1:A:118:ASN:CG	1:A:163:MET:HE3	2.22	0.64
1:B:105:HIS:CD2	1:B:106:SER:N	2.65	0.64
1:C:189:ASN:ND2	1:C:190:VAL:N	2.44	0.64
1:B:279:LYS:HD2	1:B:283:LYS:HD2	1.80	0.64
1:C:41:VAL:HG21	2:G:192:ILE:CG2	2.26	0.64
1:D:154:HIS:O	1:D:154:HIS:ND1	2.31	0.64
1:B:158:LYS:CE	1:B:161:ASN:ND2	2.60	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:C:29:LEU:HD12	1:C:79:LYS:HG2	1.79	0.64
1:D:194:SER:O	1:D:195:ARG:C	2.40	0.64
1:C:73:VAL:HG21	5:C:681:HOH:O	1.97	0.64
1:C:186:LYS:HD3	1:C:188:TYR:CZ	2.32	0.64
1:D:125:TYR:OH	1:D:221:MET:HE3	1.98	0.64
1:A:300:PHE:HE1	1:A:318:ALA:HB1	1.62	0.64
1:C:325:GLN:HA	1:C:328:ARG:HH12	1.61	0.64
2:H:193:HIS:CB	2:H:194:PRO:CD	2.75	0.64
1:A:268:GLN:O	1:A:272:LEU:HD13	1.97	0.64
2:F:192:ILE:O	2:F:193:HIS:C	2.41	0.64
1:B:29:LEU:O	1:B:79:LYS:HE3	1.97	0.63
1:C:286:ASN:ND2	1:C:288:ASP:N	2.47	0.63
1:D:212:SER:CB	1:D:309:HIS:HB2	2.27	0.63
2:E:191:LYS:C	2:E:197:TYR:OH	2.41	0.63
1:B:239:HIS:CG	1:B:269:LEU:HD13	2.32	0.63
1:D:118:ASN:CB	1:D:163:MET:HE3	2.28	0.63
1:A:103:ASP:OD1	2:F:194:PRO:HB3	1.98	0.63
1:A:251:THR:HG21	1:A:274:GLY:O	1.98	0.63
1:D:189:ASN:ND2	1:D:191:ARG:H	1.95	0.63
1:A:36:GLN:O	1:A:38:ASP:N	2.32	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: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
1:A:266:ASP:C	1:A:267:PRO:O	2.33	0.63
1:C:41:VAL:HG12	2:G:197:TYR:HB2	1.80	0.63
1:A:36:GLN:C	1:A:38:ASP:H	2.07	0.63
1:B:286:ASN:HD22	1:B:288:ASP:H	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ASP:O	1:C:134:ARG:HG3	1.97	0.63
1:D:45:VAL:HG12	1:D:45:VAL:O	1.97	0.63
1:A:242:LEU:HD23	1:A:269:LEU:HD21	1.81	0.63
1:B:288:ASP:OD2	1:B:288:ASP:O	2.16	0.63
1:D:169:ARG:HG3	1:D:169:ARG:NH2	2.00	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:A:121:PHE:O	1:A:122:LYS:C	2.39	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:B:153:MET:HE2	1:B:182:TYR:HD1	1.63	0.62
1:B:289:ASN:OD1	1:B:289:ASN:C	2.41	0.62
1:C:72:PRO:O	1:C:73:VAL:HG13	1.99	0.62
1:C:129:THR:H	1:C:132:ASP:HB2	1.64	0.62
1:D:105:HIS:CD2	1:D:106:SER:N	2.68	0.62
2:F:200:GLN:CB	2:F:202:GLN:NE2	2.52	0.62
1:B:67:ILE:CD1	2:E:195:MET:HE2	2.30	0.62
1:D:289:ASN:C	1:D:289:ASN:OD1	2.40	0.62
1:B:196:TYR:HA	1:B:241:GLN:HE22	1.64	0.62
1:C:212:SER:CB	1:C:309:HIS:HB2	2.29	0.62
1:C:325:GLN:HA	1:C:328:ARG:NH1	2.15	0.62
1:D:70:LEU:CD1	1:D:78:ILE:HD13	2.29	0.62
1:D:198:LYS:HB3	1:D:202:LEU:HD12	1.81	0.62
1:B:36:GLN:C	1:B:38:ASP:H	2.08	0.62
1:B:64:LYS:NZ	1:B:64:LYS:CB	2.62	0.62
1:B:72:PRO:O	1:B:73:VAL:HG13	1.98	0.62
1:A:78:ILE:O	1:A:82:ILE:HG13	2.00	0.62
1:A:272:LEU:HD12	1:A:272:LEU:N	2.15	0.62
1:B:36:GLN:CD	2:E:194:PRO:CB	2.73	0.62
1:C:202:LEU:HD11	1:C:213:LEU:HD11	1.82	0.62
2:F:186:ARG:O	2:F:188:TYR:N	2.33	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
1:B:223:ALA:HB2	1:B:301:LEU:HD11	1.82	0.61
1:C:332:ASN:N	1:C:332:ASN:ND2	2.48	0.61
1:D:216:TRP:CZ2	1:D:245:ILE:HD13	2.35	0.61
2:G:193:HIS:CB	2:G:194:PRO:CD	2.75	0.61
1:D:77:LYS:O	1:D:77:LYS:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:O	1:A:73:VAL:CG1	2.48	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:C:100:ILE:C	1:C:100:ILE:CD1	2.63	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:294:SER:O	1:C:295:PRO:C	2.40	0.61
1:C:326:GLN:O	1:C:329:ALA:HB3	2.00	0.61
1:A:212:SER:HB2	1:A:309:HIS:HB2	1.82	0.61
1:B:239:HIS:ND1	1:B:269:LEU:HD13	2.16	0.61
1:B:118:ASN:OD1	1:B:118:ASN:C	2.43	0.61
1:C:64:LYS:HB2	1:C:64:LYS:HZ2	1.65	0.61
1:A:10:ARG:C	1:A:11:VAL:HG23	2.24	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
1:C:19:ARG:HH22	1:C:150:GLN:NE2	1.99	0.60
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:B:19:ARG:HH22	1:B:150:GLN:NE2	1.99	0.60
1:D:180:GLU:OE1	1:D:181:PHE:N	2.31	0.60
1:C:36:GLN:CD	2:G:194:PRO:HB2	2.26	0.60
2:E:191:LYS:CA	2:E:197:TYR:HE1	2.14	0.60
2:H:192:ILE:HG23	2:H:192:ILE:O	2.00	0.60
1:A:44:LYS:O	1:A:45:VAL:HG23	2.01	0.60
1:C:127:THR:HG22	1:C:127:THR:O	2.00	0.60
1:D:17:VAL:HG12	1:D:18:LEU:HD23	1.83	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:A:98:LEU:O	1:A:99:ASP:HB2	2.01	0.60
1:D:112:ILE:N	1:D:112:ILE:CD1	2.65	0.60
1:D:189:ASN:HD22	1:D:189:ASN:C	2.07	0.60
2:E:191:LYS:HA	2:E:197:TYR:HE1	1.66	0.60
1:A:64:LYS:HB2	1:A:64:LYS:NZ	2.17	0.60
1:B:41:VAL:HG12	1:B:42:VAL:N	2.16	0.60
1:C:154:HIS:O	1:C:154:HIS:ND1	2.34	0.60
1:D:158:LYS:HE2	1:D:161:ASN:ND2	2.17	0.60
1:D:294:SER:O	1:D:295:PRO:C	2.43	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:A:314:THR:CG2	1:A:315:ALA:N	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:HG3	1:B:177:GLY:HA2	1.83	0.60
1:B:286:ASN:HD21	1:B:288:ASP:HB3	1.65	0.60
1:C:36:GLN:C	1:C:38:ASP:N	2.56	0.60
1:D:11:VAL:O	1:D:12:TYR:HB2	2.02	0.60
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
1:B:106:SER:O	1:B:107:LYS:O	2.20	0.59
1:C:215:MET:HE2	1:C:315:ALA:HA	1.83	0.59
1:B:189:ASN:HD22	1:B:189:ASN:C	2.09	0.59
1:B:266:ASP:C	1:B:267:PRO:O	2.36	0.59
1:D:186:LYS:HD3	1:D:188:TYR:CZ	2.37	0.59
2:E:191:LYS:CA	2:E:197:TYR:CE1	2.85	0.59
1:A:212:SER:CB	1:A:309:HIS:HB2	2.32	0.59
1:A:325:GLN:HG3	1:A:326:GLN:H	1.67	0.59
1:B:103:ASP:CG	2:E:194:PRO:HB3	2.28	0.59
1:A:331:GLU:O	1:A:333:SER:N	2.36	0.59
1:D:72:PRO:C	1:D:73:VAL:HG13	2.27	0.59
1:D:314:THR:CG2	1:D:315:ALA:N	2.65	0.59
1:A:154:HIS:O	1:A:154:HIS:ND1	2.36	0.59
2:H:192:ILE:O	2:H:194:PRO:N	2.35	0.59
1:B:13:ALA:O	1:B:184:PRO:HG3	2.02	0.59
1:B:189:ASN:HD22	1:B:190:VAL:H	1.47	0.59
1:D:36:GLN:NE2	2:H:194:PRO:C	2.61	0.59
1:D:286:ASN:ND2	1:D:288:ASP:N	2.50	0.59
1:A:199:GLY:HA2	1:A:216:TRP:CD1	2.37	0.59
1:A:294:SER:O	1:A:295:PRO:C	2.41	0.59
1:D:121:PHE:HB2	1:D:125:TYR:CE2	2.37	0.59
2:G:198:GLN:C	2:G:199:LEU:HG	2.28	0.59
1:A:72:PRO:C	1:A:73:VAL:HG13	2.27	0.59
1:B:44:LYS:CE	1:B:47:ARG:HD3	2.33	0.59
1:B:133:ILE:O	1:B:134:ARG:C	2.46	0.59
1:A:215:MET:HE2	1:A:315:ALA:HA	1.83	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
1:A:103:ASP:CG	2:F:194:PRO:HB3	2.28	0.58
1:C:71:LYS:O	1:C:73:VAL:HG22	2.02	0.58
1:C:133:ILE:O	1:C:134:ARG:C	2.45	0.58
1:C:286:ASN:OD1	1:C:289:ASN:ND2	2.37	0.58
1:B:88:LEU:O	1:B:89:CYS:C	2.44	0.58
1:B:199:GLY:HA2	1:B:216:TRP:CD1	2.37	0.58
1:C:44:LYS:HD3	1:D:120:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ARG:HH22	1:D:150:GLN:NE2	2.00	0.58
1:D:182:TYR:HH	1:D:184:PRO:HA	1.68	0.58
1:C:198:LYS:HB3	1:C:202:LEU:HD12	1.84	0.58
1:A:112:ILE:HD12	1:A:112:ILE:N	2.17	0.58
1:C:194:SER:O	1:C:195:ARG:C	2.47	0.58
1:D:36:GLN:NE2	2:H:194:PRO:CB	2.61	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:10:ARG:O	1:A:11:VAL:CG2	2.51	0.58
1:A:35:GLU:OE1	1:A:36:GLN:N	2.36	0.58
1:C:42:VAL:HG23	1:C:56:GLY:HA2	1.85	0.58
1:C:169:ARG:HG3	1:C:169:ARG:NH2	2.15	0.58
1:C:243:VAL:HG12	1:C:244:LYS:N	2.17	0.58
1:D:197:PHE:N	1:D:197:PHE:CD2	2.71	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
1:A:129:THR:H	1:A:132:ASP:HB2	1.67	0.58
1:C:133:ILE:HD13	1:C:225:MET:HE2	1.86	0.58
2:F:188:TYR:CE1	2:F:191:LYS:HD3	2.39	0.58
1:B:200:PRO:O	1:B:204:VAL:HG22	2.03	0.58
1:C:64:LYS:HB2	1:C:64:LYS:NZ	2.19	0.58
2:E:191:LYS:C	2:E:197:TYR:HH	2.11	0.58
2:F:200:GLN:NE2	2:F:202:GLN:HE21	1.83	0.58
1:C:182:TYR:OH	1:C:184:PRO:HA	2.03	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:A:120:ASP:C	1:A:120:ASP:OD2	2.47	0.57
1:C:296:GLU:O	1:C:297:ALA:C	2.47	0.57
1:D:300:PHE:CE1	1:D:318:ALA:HB1	2.36	0.57
2:F:187:LEU:C	2:F:187:LEU:HD12	2.29	0.57
1:B:189:ASN:ND2	1:B:190:VAL:N	2.47	0.57
1:B:194:SER:O	1:B:195:ARG:C	2.48	0.57
1:C:322:PRO:O	1:C:325:GLN:HG2	2.04	0.57
1:D:153:MET:HE2	1:D:182:TYR:CD1	2.38	0.57
1:D:196:TYR:HB2	1:D:197:PHE:CD2	2.40	0.57
1:B:156:ASP:CG	1:B:158:LYS:HE2	2.30	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
2:H:188:TYR:HD2	2:H:188:TYR:N	2.02	0.57
1:C:91:GLY:HA3	1:C:146:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLN:O	1:C:272:LEU:HD13	2.05	0.56
2:H:188:TYR:N	2:H:188:TYR:CD2	2.73	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:A:124:LEU:O	1:A:127:THR:HB	2.04	0.56
1:A:105:HIS:HD2	1:A:106:SER:HA	1.69	0.56
1:A:314:THR:HG22	1:A:315:ALA:H	1.67	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:C:50:TYR:O	1:C:71:LYS:HB2	2.06	0.56
1:C:314:THR:CG2	1:C:315:ALA:N	2.69	0.56
1:D:120:ASP:O	1:D:123:VAL:HG12	2.05	0.56
1:D:300:PHE:CZ	1:D:304:LEU:HD11	2.40	0.56
1:A:258:LEU:HD11	1:A:265:LEU:HD13	1.87	0.56
1:B:103:ASP:O	1:B:104:GLN:C	2.49	0.56
1:C:33:TRP:CE3	1:C:100:ILE:CD1	2.81	0.56
2:E:197:TYR:N	2:E:197:TYR:CD1	2.73	0.56
1:B:286:ASN:OD1	1:B:289:ASN:ND2	2.38	0.56
1:C:123:VAL:HG13	2:H:197:TYR:HD2	1.70	0.56
1:C:155:ARG:NH1	1:C:209:TYR:OH	2.38	0.56
2:F:202:GLN:O	2:F:203:ALA:CB	2.53	0.56
1:A:272:LEU:H	1:A:272:LEU:CD1	2.19	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
1:C:47:ARG:CG	1:C:47:ARG:O	2.53	0.56
1:D:286:ASN:OD1	1:D:289:ASN:ND2	2.39	0.56
2:F:202:GLN:O	2:F:203:ALA:HB2	2.06	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:C:118:ASN:CB	1:C:163:MET:HE3	2.35	0.56
1:C:118:ASN:ND2	1:C:163:MET:HE3	2.21	0.56
1:D:47:ARG:O	1:D:47:ARG:CG	2.54	0.56
1:A:296:GLU:O	1:A:297:ALA:C	2.49	0.55
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:C:118:ASN:CG	1:C:163:MET:CE	2.72	0.55
1:D:272:LEU:HD12	1:D:272:LEU:H	1.71	0.55
1:B:108:THR:HG22	1:B:108:THR:O	2.07	0.55
1:C:189:ASN:ND2	1:C:189:ASN:C	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:LEU:N	1:C:282:LEU:HD22	2.21	0.55
1:D:106:SER:C	1:D:107:LYS:CG	2.79	0.55
1:D:215:MET:HE2	1:D:315:ALA:CA	2.35	0.55
1:D:269:LEU:O	1:D:273:VAL:HG23	2.06	0.55
1:A:105:HIS:O	1:A:106:SER:C	2.48	0.55
1:A:131:TYR:O	1:A:132:ASP:C	2.47	0.55
1:A:211:TYR:O	1:A:213:LEU:N	2.40	0.55
1:C:47:ARG:O	1:C:47:ARG:HG3	2.07	0.55
1:C:266:ASP:C	1:C:267:PRO:O	2.41	0.55
1:B:282:LEU:N	1:B:282:LEU:CD2	2.69	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:A:116:VAL:HG12	1:A:117:ASN:O	2.06	0.55
1:A:197:PHE:CD2	1:A:197:PHE:N	2.74	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:189:ASN:ND2	1:A:190:VAL:N	2.46	0.55
1:A:194:SER:O	1:A:195:ARG:C	2.47	0.55
1:A:282:LEU:N	1:A:282:LEU:HD22	2.22	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:D:318:ALA:C	1:D:320:THR:H	2.14	0.55
2:H:197:TYR:C	2:H:198:GLN:O	2.47	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: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
2:F:193:HIS:HB3	2:F:194:PRO:HD3	1.89	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
1:C:314:THR:HG22	1:C:316:LEU:H	1.72	0.55
1:C:125:TYR:O	1:C:126:PRO:O	2.23	0.54
1:C:142:LYS:NZ	1:C:331:GLU:OE1	2.37	0.54
1:D:186:LYS:O	1:D:208:ASP:HA	2.07	0.54
2:G:202:GLN:O	2:G:203:ALA:CB	2.55	0.54
1:A:211:TYR:O	1:A:212:SER:C	2.48	0.54
1:B:77:LYS:O	1:B:77:LYS:HD3	2.08	0.54
1:B:186:LYS:HD3	1:B:188:TYR:CE1	2.42	0.54
1:D:37:ASP:OD2	1:D:37:ASP:N	2.38	0.54
1:D:84:ILE:HD12	1:D:152:ILE:HD13	1.88	0.54
1:D:303:LYS:HB3	1:D:313:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:ILE:O	2:E:194:PRO:N	2.41	0.54
1:A:31:VAL:HG12	1:A:33:TRP:CE2	2.42	0.54
1:A:128:LEU:HB3	1:A:132:ASP:CB	2.36	0.54
1:C:215:MET:HE1	1:C:315:ALA:HA	1.88	0.54
1:D:106:SER:C	1:D:108:THR:H	2.15	0.54
1:D:136:TYR:OH	1:D:166:HIS:HD2	1.90	0.54
1:A:157:VAL:O	1:A:217:SER:HB3	2.07	0.54
1:B:158:LYS:HD3	1:B:194:SER:CB	2.37	0.54
2:F:188:TYR:HD1	2:F:191:LYS:HD2	1.71	0.54
1:A:66:ILE:HG13	3:A:501:AMP:N6	2.23	0.54
1:A:69:ILE:HG12	1:A:110:SER:OG	2.07	0.54
1:A:112:ILE:N	1:A:112:ILE:CD1	2.71	0.54
1:A:160:HIS:O	3:A:501:AMP:O3P	2.25	0.54
1:B:12:TYR:HB3	1:B:15:VAL:CG2	2.38	0.54
1:C:102:ARG:HD2	1:C:107:LYS:HD3	1.89	0.54
1:D:267:PRO:O	1:D:268:GLN:CB	2.52	0.54
1:B:198:LYS:HB3	1:B:202:LEU:HD12	1.89	0.54
1:D:163:MET:HE2	3:D:701:AMP:C2	2.42	0.54
1:A:153:MET:O	1:A:179:ALA:HA	2.08	0.54
1:B:82:ILE:O	1:B:86:GLN:HG3	2.08	0.54
1:C:82:ILE:O	1:C:86:GLN:HG3	2.08	0.54
1:D:29:LEU:O	1:D:79:LYS:HE3	2.08	0.54
1:D:153:MET:CE	1:D:182:TYR:HD1	2.20	0.54
1:D:308:ASP:OD1	1:D:310:GLN:HB2	2.08	0.54
1:A:286:ASN:OD1	1:A:289:ASN:CG	2.51	0.54
1:B:35:GLU:O	1:B:36:GLN:C	2.51	0.54
1:C:258:LEU:HD11	1:C:265:LEU:HD13	1.89	0.54
1:C:325:GLN:HG3	1:C:326:GLN:N	2.23	0.54
1:D:272:LEU:HD12	1:D:272:LEU:N	2.23	0.54
1:A:153:MET:HE2	1:A:182:TYR:CD1	2.42	0.54
1:B:14:ASP:O	1:B:15:VAL:C	2.46	0.54
1:B:127:THR:HA	2:F:190:PHE:CZ	2.40	0.54
1:B:155:ARG:NH1	1:B:209:TYR:OH	2.40	0.54
1:D:160:HIS:CD2	1:D:160:HIS:N	2.71	0.54
1:A:103:ASP:HB2	2:F:194:PRO:HB3	1.89	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: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:B:67:ILE:HD11	2:E:195:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:HB2	1:B:125:TYR:CD2	2.42	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:A:118:ASN:CB	1:A:163:MET:HE3	2.38	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:A:215:MET:HE2	1:A:315:ALA:CA	2.39	0.53
1:C:98:LEU:O	1:C:99:ASP:HB2	2.08	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:C:138:TYR:CE2	1:C:331:GLU:OE2	2.61	0.53
1:D:21:LYS:HG3	1:D:24:TRP:CH2	2.44	0.53
1:B:189:ASN:ND2	1:B:189:ASN:C	2.64	0.53
1:D:107:LYS:O	1:D:109:PRO:HD3	2.09	0.53
1:D:266:ASP:C	1:D:267:PRO:O	2.40	0.53
1:A:158:LYS:HE2	1:A:160:HIS:HB2	1.90	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:10:ARG:O	1:A:11:VAL:HG23	2.09	0.53
1:A:52:GLU:HG2	1:A:54:PHE:CE1	2.44	0.53
1:B:42:VAL:CB	1:B:43:ARG:HH12	2.21	0.53
1:B:66:ILE:HG13	3:B:801:AMP:C6	2.44	0.53
1:C:116:VAL:HG12	1:C:117:ASN:O	2.09	0.53
1:D:237:ASP:OD1	1:D:238:ASN:N	2.42	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:D:129:THR:O	1:D:130:ASP:C	2.51	0.53
1:C:44:LYS:CE	1:C:52:GLU:OE2	2.56	0.53
1:C:131:TYR:O	1:C:132:ASP:C	2.52	0.53
1:C:153:MET:HE2	1:C:182:TYR:HD1	1.74	0.53
1:D:251:THR:HG21	1:D:274:GLY:O	2.09	0.53
2:F:193:HIS:CB	2:F:194:PRO:HD3	2.39	0.53
1:A:129:THR:O	1:A:130:ASP:C	2.51	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
1:C:200:PRO:HD3	1:C:216:TRP:CE2	2.44	0.52
1:A:33:TRP:CE3	1:A:102:ARG:HG3	2.45	0.52
1:B:130:ASP:O	1:B:134:ARG:HG3	2.10	0.52
1:B:175:ASP:HB2	3:B:801:AMP:O2P	2.09	0.52
1:C:192:VAL:O	1:C:198:LYS:HE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:PHE:O	1:D:223:ALA:C	2.53	0.52
1:A:44:LYS:HD3	1:A:47:ARG:CZ	2.40	0.52
1:A:82:ILE:O	1:A:86:GLN:HG3	2.09	0.52
1:B:175:ASP:C	1:B:177:GLY:H	2.18	0.52
1:D:128:LEU:HB3	1:D:132:ASP:CB	2.39	0.52
1:D:192:VAL:O	1:D:198:LYS:HE2	2.08	0.52
1:D:300:PHE:O	1:D:301:LEU:C	2.52	0.52
2:E:192:ILE:HB	2:E:197:TYR:CE2	2.45	0.52
2:E:198:GLN:HE21	2:E:198:GLN:CA	2.21	0.52
1:A:44:LYS:HD2	1:B:120:ASP:OD2	2.09	0.52
1:C:36:GLN:NE2	2:G:194:PRO:O	2.42	0.52
1:B:100:ILE:C	1:B:100:ILE:CD1	2.77	0.52
1:B:121:PHE:CD2	1:B:122:LYS:HG2	2.44	0.52
2:G:191:LYS:HG2	2:G:196:ALA:HA	1.90	0.52
2:G:197:TYR:CD1	2:G:197:TYR:C	2.87	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:D:258:LEU:HD11	1:D:265:LEU:HD13	1.90	0.52
2:F:190:PHE:O	2:F:196:ALA:HA	2.10	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:A:215:MET:HG3	1:A:313:LEU:O	2.09	0.52
1:C:103:ASP:HB2	2:G:194:PRO:CG	2.39	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:A:215:MET:HE1	1:A:315:ALA:HA	1.91	0.52
1:B:29:LEU:HD12	1:B:79:LYS:HG2	1.91	0.52
1:D:126:PRO:HG2	1:D:127:THR:H	1.74	0.52
1:D:134:ARG:HG2	1:D:323:TYR:CZ	2.45	0.52
1:A:36:GLN:O	1:A:39:TYR:N	2.37	0.52
1:B:215:MET:HE2	1:B:315:ALA:HA	1.91	0.52
1:C:41:VAL:O	2:G:197:TYR:HB2	2.09	0.52
1:C:112:ILE:N	1:C:112:ILE:HD12	2.25	0.52
1:C:129:THR:O	1:C:130:ASP:C	2.53	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:D:50:TYR:C	1:D:71:LYS:HB2	2.35	0.51
1:D:189:ASN:ND2	1:D:189:ASN:C	2.68	0.51
1:A:127:THR:O	1:A:127:THR:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:HB2	1:A:324:PHE:CD1	2.46	0.51
1:B:286:ASN:HD21	1:B:288:ASP:CA	2.23	0.51
1:C:102:ARG:HH11	1:C:107:LYS:CD	2.16	0.51
1:C:154:HIS:O	1:C:156:ASP:N	2.43	0.51
1:D:10:ARG:C	1:D:11:VAL:HG23	2.35	0.51
1:D:33:TRP:CZ3	1:D:102:ARG:CB	2.93	0.51
1:D:157:VAL:HB	1:D:217:SER:HB2	1.93	0.51
2:H:190:PHE:O	2:H:197:TYR:HE1	1.93	0.51
1:A:35:GLU:OE1	1:A:35:GLU:C	2.53	0.51
1:B:215:MET:HE2	1:B:315:ALA:CA	2.41	0.51
1:C:29:LEU:O	1:C:79:LYS:HE3	2.10	0.51
1:C:158:LYS:HD2	1:C:160:HIS:CD2	2.46	0.51
1:D:133:ILE:O	1:D:134:ARG:C	2.53	0.51
2:G:188:TYR:HE2	5:G:246:HOH:O	1.93	0.51
1:B:196:TYR:HA	1:B:241:GLN:NE2	2.25	0.51
1:B:105:HIS:CD2	1:B:105:HIS:C	2.89	0.51
1:B:106:SER:O	1:B:107:LYS:C	2.53	0.51
1:B:157:VAL:HB	1:B:217:SER:CB	2.41	0.51
1:C:41:VAL:HG21	2:G:192:ILE:HG21	1.91	0.51
1:C:300:PHE:CZ	1:C:304:LEU:HD11	2.45	0.51
1:D:82:ILE:O	1:D:86:GLN:HG3	2.09	0.51
1:D:154:HIS:O	1:D:156:ASP:N	2.44	0.51
1:A:44:LYS:HZ3	1:A:47:ARG:HE	1.59	0.51
1:A:263:ILE:HD11	5:A:536:HOH:O	2.11	0.51
1:B:19:ARG:HB3	1:B:20:PRO:HD2	1.93	0.51
1:D:33:TRP:CZ3	1:D:102:ARG:HB2	2.46	0.51
1:D:119:THR:HG1	1:D:124:LEU:HB2	1.73	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:29:LEU:O	1:A:79:LYS:HE3	2.11	0.51
1:A:44:LYS:HE2	1:A:47:ARG:HG3	1.86	0.51
1:A:308:ASP:OD1	1:A:310:GLN:HB2	2.11	0.51
1:B:12:TYR:HB3	1:B:15:VAL:HG21	1.92	0.51
1:B:129:THR:H	1:B:132:ASP:HB2	1.76	0.51
1:A:88:LEU:O	1:A:89:CYS:C	2.54	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:B:31:VAL:CG1	1:B:33:TRP:CE2	2.94	0.51
1:B:117:ASN:ND2	2:F:202:GLN:HB2	2.26	0.51
1:B:272:LEU:H	1:B:272:LEU:HD12	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
2:F:191:LYS:HA	2:F:195:MET:O	2.11	0.51
2:H:190:PHE:O	2:H:197:TYR:CE1	2.63	0.51
1:C:84:ILE:O	1:C:87:ASN:HB2	2.09	0.50
1:C:124:LEU:HD12	1:C:124:LEU:O	2.11	0.50
1:D:103:ASP:HA	2:H:194:PRO:HB3	1.92	0.50
2:H:198:GLN:HG3	2:H:199:LEU:N	2.25	0.50
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.74	0.50
1:C:300:PHE:O	1:C:301:LEU:C	2.51	0.50
2:H:196:ALA:C	2:H:197:TYR:CD1	2.90	0.50
1:A:50:TYR:O	1:A:71:LYS:HB2	2.11	0.50
1:B:158:LYS:NZ	1:B:194:SER:OG	2.39	0.50
1:C:45:VAL:HG22	1:C:45:VAL:O	2.11	0.50
1:D:94:ILE:HG22	1:D:95:VAL:O	2.11	0.50
1:D:223:ALA:HB2	1:D:301:LEU:CD1	2.38	0.50
2:F:198:GLN:C	2:F:199:LEU:HD23	2.36	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:71:LYS:O	1:D:73:VAL:HG22	2.12	0.50
2:F:191:LYS:CG	2:F:196:ALA:HA	2.40	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
1:C:215:MET:HE2	1:C:315:ALA:CA	2.41	0.50
1:A:29:LEU:HD12	1:A:79:LYS:HG2	1.93	0.50
2:F:191:LYS:HG2	2:F:196:ALA:CA	2.39	0.50
1:D:129:THR:N	1:D:132:ASP:HB2	2.25	0.50
1:D:237:ASP:OD1	1:D:237:ASP:C	2.54	0.50
2:E:192:ILE:N	2:E:197:TYR:CZ	2.80	0.50
2:E:194:PRO:HD2	2:E:195:MET:SD	2.52	0.50
2:H:191:LYS:CA	2:H:197:TYR:HE1	2.23	0.50
1:C:223:ALA:HB2	1:C:301:LEU:HD11	1.93	0.50
1:D:268:GLN:O	1:D:271:ALA:HB3	2.11	0.50
1:A:332:ASN:ND2	1:A:332:ASN:C	2.67	0.50
1:B:84:ILE:CD1	1:B:152:ILE:CD1	2.89	0.50
1:B:211:TYR:O	1:B:212:SER:C	2.55	0.50
1:B:294:SER:O	1:B:295:PRO:C	2.55	0.50
2:E:190:PHE:C	2:E:197:TYR:HE1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:PHE:O	1:D:122:LYS:C	2.51	0.49
1:D:279:LYS:HD3	1:D:280:PRO:HD2	1.94	0.49
1:A:77:LYS:O	1:A:77:LYS:HD3	2.12	0.49
1:A:81:GLU:O	1:A:82:ILE:C	2.52	0.49
1:A:163:MET:HE2	3:A:501:AMP:N3	2.27	0.49
1:B:169:ARG:HG3	1:B:169:ARG:NH2	2.13	0.49
1:B:169:ARG:CG	1:B:169:ARG:NH2	2.68	0.49
1:C:81:GLU:O	1:C:82:ILE:C	2.55	0.49
1:C:148:HIS:HA	1:C:152:ILE:O	2.12	0.49
1:D:291:HIS:H	1:D:291:HIS:CD2	2.29	0.49
1:B:131:TYR:O	1:B:132:ASP:C	2.54	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: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:B:266:ASP:O	1:B:267:PRO:C	2.53	0.49
1:C:41:VAL:CG1	2:G:197:TYR:HB3	2.42	0.49
1:C:154:HIS:CE1	1:C:156:ASP:C	2.90	0.49
1:D:119:THR:O	1:D:120:ASP:C	2.53	0.49
1:B:33:TRP:CZ2	1:B:102:ARG:HD3	2.47	0.49
1:D:165:ASP:C	1:D:167:GLU:H	2.21	0.49
1:D:211:TYR:O	1:D:212:SER:C	2.55	0.49
1:D:216:TRP:HZ2	1:D:245:ILE:HD13	1.76	0.49
1:A:154:HIS:CE1	1:A:156:ASP:HB3	2.47	0.49
1:A:326:GLN:O	1:A:329:ALA:HB3	2.13	0.49
1:B:265:LEU:O	1:B:266:ASP:C	2.55	0.49
1:D:98:LEU:HB2	1:D:112:ILE:O	2.12	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: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:C:121:PHE:CD1	1:C:159:PRO:HB2	2.48	0.49
1:C:211:TYR:O	1:C:212:SER:C	2.55	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:B:300:PHE:O	1:B:301:LEU:C	2.56	0.49
1:A:204:VAL:HG12	1:A:265:LEU:HD11	1.94	0.49
1:D:123:VAL:HG13	1:D:124:LEU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:VAL:HB	1:D:217:SER:CB	2.43	0.49
2:E:193:HIS:HB2	2:E:194:PRO:HD3	1.88	0.49
1:B:195:ARG:HG3	1:B:195:ARG:HH11	1.78	0.48
1:B:262:ARG:HA	5:B:1070:HOH:O	2.12	0.48
1:D:36:GLN:OE1	2:H:194:PRO:CB	2.48	0.48
1:A:266:ASP:O	1:A:267:PRO:C	2.53	0.48
1:C:33:TRP:CH2	1:C:102:ARG:HD3	2.47	0.48
1:D:226:ILE:CG1	1:D:227:PHE:N	2.76	0.48
2:H:200:GLN:NE2	2:H:201:LEU:O	2.46	0.48
1:A:288:ASP:O	1:A:291:HIS:HD2	1.97	0.48
1:B:10:ARG:HG3	1:B:11:VAL:HG23	1.95	0.48
1:B:300:PHE:CE1	1:B:318:ALA:HB1	2.40	0.48
1:C:163:MET:HE1	3:C:601:AMP:H2'	1.95	0.48
1:D:158:LYS:HD2	1:D:160:HIS:CD2	2.48	0.48
1:D:279:LYS:HD2	1:D:283:LYS:HD2	1.94	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:B:180:GLU:OE1	1:B:181:PHE:N	2.36	0.48
1:D:196:TYR:HA	1:D:241:GLN:NE2	2.27	0.48
2:H:192:ILE:O	2:H:192:ILE:CG2	2.61	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:A:94:ILE:HG22	1:A:95:VAL:O	2.14	0.48
1:A:259:ASN:O	1:A:260:LYS:C	2.55	0.48
1:B:33:TRP:CD1	1:B:102:ARG:HE	2.32	0.48
1:B:44:LYS:NZ	1:B:47:ARG:CD	2.71	0.48
1:B:153:MET:HE2	1:B:182:TYR:CD1	2.48	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:CG	2:E:202:GLN:O	2.62	0.48
1:A:10:ARG:C	1:A:11:VAL:CG2	2.84	0.48
1:D:134:ARG:HG2	1:D:323:TYR:CE2	2.48	0.48
1:B:270:GLU:O	1:B:271:ALA:C	2.56	0.48
1:D:129:THR:O	1:D:132:ASP:N	2.47	0.48
1:A:242:LEU:CD2	1:A:269:LEU:HD21	2.44	0.48
1:B:52:GLU:HG2	1:B:54:PHE:CE1	2.48	0.48
1:B:78:ILE:O	1:B:82:ILE:HG13	2.13	0.48
1:C:153:MET:O	1:C:179:ALA:HA	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:286:ASN:ND2	1:A:289:ASN:H	2.12	0.48
1:B:138:TYR:HB2	1:B:324:PHE:CD1	2.49	0.48
1:B:215:MET:HE1	1:B:315:ALA:HA	1.93	0.48
1:C:88:LEU:O	1:C:89:CYS:C	2.57	0.48
1:D:98:LEU:O	1:D:99:ASP:HB2	2.14	0.48
1:D:119:THR:CA	2:G:202:GLN:NE2	2.77	0.48
2:E:197:TYR:C	2:E:198:GLN:O	2.54	0.48
1:A:33:TRP:HE3	1:A:101:VAL:HA	1.79	0.47
1:A:200:PRO:O	1:A:204:VAL:HG22	2.14	0.47
1:A:222:PHE:O	1:A:223:ALA:C	2.56	0.47
1:B:96:LYS:CG	1:B:98:LEU:HD13	2.44	0.47
1:B:279:LYS:HD3	1:B:280:PRO:HD2	1.96	0.47
1:C:123:VAL:O	1:C:123:VAL:CG1	2.60	0.47
2:H:191:LYS:HA	2:H:197:TYR:CE1	2.45	0.47
1:B:249:LEU:N	1:B:249:LEU:HD12	2.29	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:D:314:THR:HG22	1:D:315:ALA:H	1.77	0.47
2:F:194:PRO:HD2	2:F:195:MET:CG	2.37	0.47
1:A:265:LEU:O	1:A:266:ASP:C	2.54	0.47
1:B:132:ASP:OD1	1:B:169:ARG:NH1	2.46	0.47
1:B:158:LYS:O	1:B:159:PRO:C	2.57	0.47
1:B:259:ASN:O	1:B:260:LYS:C	2.57	0.47
1:C:124:LEU:HD12	1:C:124:LEU:C	2.39	0.47
1:D:100:ILE:C	1:D:100:ILE:CD1	2.65	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
1:B:14:ASP:C	1:B:16:ASN:N	2.73	0.47
1:B:186:LYS:HD3	1:B:188:TYR:CZ	2.50	0.47
1:B:258:LEU:HD11	1:B:265:LEU:HD13	1.97	0.47
1:D:266:ASP:O	1:D:267:PRO:C	2.57	0.47
2:E:197:TYR:O	2:E:198:GLN:O	2.32	0.47
2:F:188:TYR:HE1	2:F:191:LYS:HD3	1.77	0.47
1:A:74:LYS:HD3	1:D:264:GLU:HB2	1.97	0.47
1:B:254:LEU:O	1:B:258:LEU:HG	2.15	0.47
1:C:36:GLN:HE21	2:G:195:MET:HA	1.78	0.47
1:C:166:HIS:O	1:C:169:ARG:HD2	2.14	0.47
1:D:129:THR:HG23	1:D:132:ASP:OD2	2.14	0.47
1:D:296:GLU:O	1:D:297:ALA:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HG2	1:A:323:TYR:CE2	2.49	0.47
1:A:196:TYR:HB2	1:A:197:PHE:CD2	2.50	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:C:98:LEU:HD22	1:C:114:GLU:N	2.29	0.47
1:A:129:THR:N	1:A:132:ASP:HB2	2.30	0.47
1:A:288:ASP:O	1:A:291:HIS:CD2	2.68	0.47
1:C:11:VAL:HG12	1:C:12:TYR:CD2	2.50	0.47
1:C:219:GLY:O	1:C:220:CYS:C	2.56	0.47
1:C:229:LYS:HD3	1:C:232:PHE:HD1	1.78	0.47
1:D:196:TYR:HB2	1:D:197:PHE:HD2	1.79	0.47
1:B:121:PHE:HB2	1:B:125:TYR:CE2	2.49	0.47
1:C:121:PHE:O	1:C:122:LYS:C	2.56	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: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: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:33:TRP:CZ3	1:D:102:ARG:HB3	2.50	0.47
1:A:229:LYS:HD3	1:A:232:PHE:HD1	1.80	0.47
1:B:50:TYR:O	1:B:71:LYS:HB2	2.14	0.47
1:C:41:VAL:HG21	2:G:192:ILE:HG22	1.95	0.47
1:D:116:VAL:HG12	1:D:117:ASN:O	2.15	0.47
1:A:83:LYS:HD2	1:A:83:LYS:HA	1.71	0.46
1:B:154:HIS:O	1:B:154:HIS:ND1	2.48	0.46
1:C:128:LEU:HB3	1:C:132:ASP:HB3	1.97	0.46
1:C:291:HIS:CD2	1:C:291:HIS:H	2.33	0.46
1:A:102:ARG:HD2	1:A:107:LYS:CD	2.45	0.46
1:A:268:GLN:O	1:A:272:LEU:CD1	2.63	0.46
1:B:36:GLN:C	1:B:38:ASP:N	2.63	0.46
1:C:157:VAL:HB	1:C:217:SER:CB	2.43	0.46
1:D:88:LEU:O	1:D:89:CYS:C	2.57	0.46
1:D:237:ASP:O	1:D:238:ASN:C	2.55	0.46
2:E:191:LYS:N	2:E:197:TYR:HE1	2.13	0.46
1:A:33:TRP:CE3	1:A:100:ILE:CD1	2.91	0.46
1:A:130:ASP:O	1:A:134:ARG:HG3	2.15	0.46
1:B:160:HIS:CD2	1:B:160:HIS:N	2.75	0.46
1:D:131:TYR:O	1:D:132:ASP:C	2.58	0.46
1:D:148:HIS:HE1	1:D:214:ASP:OD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:LEU:HD12	1:D:285:MET:HE2	1.98	0.46
1:A:39:TYR:CE1	1:A:112:ILE:HG21	2.50	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:D:36:GLN:NE2	2:H:194:PRO:O	2.48	0.46
1:D:296:GLU:OE2	1:D:296:GLU:N	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:163:MET:HE1	3:B:801:AMP:H2'	1.97	0.46
1:B:246:ALA:O	1:B:250:GLY:N	2.47	0.46
1:B:6:MET:HB3	1:B:261:TYR:CD2	2.51	0.46
1:B:33:TRP:CZ3	1:B:100:ILE:CD1	2.92	0.46
1:B:68:LYS:NZ	1:B:81:GLU:OE2	2.47	0.46
1:C:119:THR:O	1:C:120:ASP:C	2.59	0.46
1:C:226:ILE:CG1	1:C:227:PHE:N	2.79	0.46
1:C:288:ASP:O	1:C:291:HIS:CD2	2.68	0.46
1:D:119:THR:CG2	2:G:202:GLN:HE21	2.29	0.46
1:D:168:LEU:O	1:D:169:ARG:C	2.58	0.46
2:G:190:PHE:N	2:G:190:PHE:HD1	2.13	0.46
1:A:25:ASP:O	1:A:28:ALA:HB3	2.16	0.46
1:B:163:MET:CE	3:B:801:AMP:H2'	2.46	0.46
1:B:314:THR:CG2	1:B:315:ALA:N	2.77	0.46
1:C:210:ASP:OD1	1:C:212:SER:OG	2.34	0.46
1:B:36:GLN:NE2	2:E:194:PRO:HB3	2.30	0.46
1:B:83:LYS:HD2	1:B:83:LYS:HA	1.63	0.46
1:C:44:LYS:HZ3	1:C:47:ARG:HE	1.63	0.46
1:D:74:LYS:O	1:D:75:LYS:C	2.58	0.46
1:D:272:LEU:H	1:D:272:LEU:CD1	2.28	0.46
1:D:332:ASN:N	1:D:332:ASN:ND2	2.58	0.46
1:A:189:ASN:HD22	1:A:190:VAL:H	1.58	0.46
1:B:173:LEU:HD23	1:B:176:TRP:CZ2	2.50	0.46
1:C:72:PRO:C	1:C:73:VAL:HG13	2.39	0.46
1:C:268:GLN:O	1:C:271:ALA:HB3	2.15	0.46
2:F:200:GLN:H	2:F:200:GLN:HG3	1.24	0.46
1:C:145:ASP:HB2	1:C:315:ALA:HB3	1.98	0.45
1:D:84:ILE:CD1	1:D:152:ILE:HD13	2.46	0.45
2:E:192:ILE:N	2:E:197:TYR:OH	2.48	0.45
1:B:72:PRO:O	1:B:73:VAL:CG1	2.63	0.45
1:B:192:VAL:HG23	1:B:202:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:OD1	1:B:289:ASN:CG	2.60	0.45
1:C:14:ASP:O	1:C:15:VAL:C	2.56	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: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:A:103:ASP:OD2	1:A:106:SER:OG	2.19	0.45
1:B:25:ASP:O	1:B:28:ALA:HB3	2.16	0.45
1:B:33:TRP:CG	1:B:102:ARG:HE	2.34	0.45
1:B:136:TYR:OH	1:B:166:HIS:CD2	2.62	0.45
1:B:296:GLU:O	1:B:297:ALA:C	2.58	0.45
1:C:70:LEU:CD1	1:C:78:ILE:HD13	2.46	0.45
1:D:24:TRP:HA	1:D:181:PHE:CZ	2.50	0.45
1:B:103:ASP:HB2	2:E:194:PRO:CG	2.47	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:70:LEU:HD12	1:C:78:ILE:HD13	1.98	0.45
1:C:121:PHE:CD1	1:C:159:PRO:CB	2.98	0.45
1:C:136:TYR:HH	1:C:166:HIS:HD2	1.63	0.45
1:C:158:LYS:HA	1:C:197:PHE:CE1	2.51	0.45
1:C:296:GLU:OE2	1:C:296:GLU:N	2.47	0.45
1:D:211:TYR:O	1:D:213:LEU:N	2.48	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:B:148:HIS:HA	1:B:152:ILE:O	2.16	0.45
1:B:264:GLU:CG	1:C:76:LYS:HD3	2.46	0.45
1:B:299:ASP:OD1	1:B:303:LYS:NZ	2.50	0.45
1:C:15:VAL:O	1:C:19:ARG:HG3	2.17	0.45
1:C:25:ASP:O	1:C:28:ALA:HB3	2.15	0.45
1:C:265:LEU:O	1:C:266:ASP:C	2.57	0.45
1:D:126:PRO:HG2	2:G:197:TYR:OH	2.16	0.45
1:D:210:ASP:OD1	1:D:212:SER:N	2.40	0.45
1:D:229:LYS:HD3	1:D:232:PHE:CD1	2.52	0.45
1:A:101:VAL:O	1:A:110:SER:N	2.48	0.45
1:A:325:GLN:HA	1:A:328:ARG:NH1	2.32	0.45
1:D:228:ARG:HD2	1:D:288:ASP:OD2	2.17	0.45
1:A:76:LYS:N	1:D:264:GLU:OE2	2.46	0.45
1:A:100:ILE:HD12	1:A:101:VAL:H	1.70	0.45
1:A:329:ALA:C	1:A:331:GLU:N	2.75	0.45
1:A:331:GLU:O	1:A:332:ASN:C	2.55	0.45
1:B:74:LYS:O	1:B:75:LYS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LYS:HG2	1:B:276:HIS:CE1	2.51	0.45
1:D:124:LEU:HD21	1:D:166:HIS:HB2	1.98	0.45
1:D:322:PRO:O	1:D:325:GLN:HG2	2.17	0.45
1:A:74:LYS:O	1:A:75:LYS:C	2.58	0.45
1:B:103:ASP:OD1	1:B:103:ASP:C	2.58	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:A:163:MET:HE2	3:A:501:AMP:C4	2.52	0.45
1:D:36:GLN:C	1:D:38:ASP:H	2.24	0.45
1:D:125:TYR:N	1:D:126:PRO:CD	2.80	0.45
1:D:154:HIS:O	1:D:154:HIS:CG	2.70	0.45
1:D:178:LEU:HD23	1:D:178:LEU:HA	1.75	0.45
1:A:44:LYS:HE2	1:A:52:GLU:OE2	2.14	0.45
1:A:98:LEU:HD22	1:A:114:GLU:N	2.32	0.45
1:B:186:LYS:O	1:B:208:ASP:HA	2.16	0.45
1:C:163:MET:HE2	3:C:601:AMP:C2	2.52	0.45
1:D:43:ARG:NH1	2:G:203:ALA:O	2.41	0.45
1:D:153:MET:O	1:D:179:ALA:HA	2.17	0.45
1:D:265:LEU:O	1:D:266:ASP:C	2.60	0.45
1:D:269:LEU:O	1:D:270:GLU:C	2.60	0.45
2:G:198:GLN:C	2:G:199:LEU:CG	2.90	0.45
1:A:15:VAL:HG22	1:A:16:ASN:N	2.32	0.44
1:A:44:LYS:HG2	1:A:45:VAL:N	2.32	0.44
1:A:163:MET:HE2	3:A:501:AMP:C2	2.52	0.44
1:A:324:PHE:O	1:A:325:GLN:C	2.60	0.44
1:B:33:TRP:CD2	1:B:102:ARG:HB2	2.52	0.44
1:B:95:VAL:HA	1:B:172:ARG:HD2	2.00	0.44
1:B:112:ILE:N	1:B:112:ILE:HD12	2.32	0.44
1:A:75:LYS:N	1:D:264:GLU:OE1	2.50	0.44
1:A:120:ASP:OD2	1:A:121:PHE:N	2.50	0.44
1:A:217:SER:O	1:A:218:LEU:C	2.61	0.44
1:B:33:TRP:CD1	1:B:33:TRP:N	2.82	0.44
1:C:129:THR:O	1:C:132:ASP:N	2.50	0.44
1:D:158:LYS:CE	1:D:161:ASN:ND2	2.80	0.44
1:D:165:ASP:C	1:D:167:GLU:N	2.74	0.44
1:D:332:ASN:H	1:D:332:ASN:ND2	1.99	0.44
2:E:199:LEU:HD23	2:E:199:LEU:N	2.31	0.44
1:A:11:VAL:O	1:A:12:TYR:HB2	2.18	0.44
1:A:325:GLN:HA	1:A:328:ARG:HH12	1.82	0.44
1:B:11:VAL:O	1:B:12:TYR:HB2	2.15	0.44
1:B:44:LYS:HE3	1:B:47:ARG:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HD21	1:B:176:TRP:CD1	2.52	0.44
1:B:288:ASP:HB2	5:F:206:HOH:O	2.18	0.44
1:B:324:PHE:O	1:B:325:GLN:C	2.61	0.44
1:C:303:LYS:HB3	1:C:313:LEU:HD21	1.98	0.44
1:D:10:ARG:O	1:D:11:VAL:CG2	2.66	0.44
1:D:259:ASN:O	1:D:260:LYS:C	2.60	0.44
2:H:190:PHE:CD1	2:H:190:PHE:N	2.83	0.44
2:H:195:MET:HE3	2:H:195:MET:HB3	1.91	0.44
1:A:10:ARG:HH22	1:A:317:GLU:CD	2.25	0.44
1:A:96:LYS:O	1:A:96:LYS:HG2	2.17	0.44
1:B:70:LEU:CD1	1:B:78:ILE:HD13	2.47	0.44
1:B:126:PRO:CG	2:F:197:TYR:OH	2.65	0.44
1:C:80:ARG:O	1:C:81:GLU:C	2.60	0.44
1:D:111:LEU:C	1:D:112:ILE:HD12	2.41	0.44
2:E:198:GLN:NE2	2:E:198:GLN:HA	2.33	0.44
2:G:195:MET:C	2:G:196:ALA:O	2.54	0.44
1:B:21:LYS:HG3	1:B:24:TRP:CH2	2.53	0.44
1:C:20:PRO:HB2	1:C:22:GLU:CD	2.42	0.44
1:C:145:ASP:HB2	1:C:315:ALA:CB	2.47	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:19:ARG:CB	1:B:20:PRO:HD2	2.47	0.44
1:B:286:ASN:OD1	1:B:289:ASN:HB3	2.16	0.44
1:A:288:ASP:OD2	1:A:288:ASP:C	2.61	0.44
1:B:246:ALA:C	1:B:248:VAL:H	2.25	0.44
1:B:299:ASP:HB3	1:B:321:HIS:HE2	1.83	0.44
1:C:16:ASN:HB3	1:C:24:TRP:CD1	2.53	0.44
1:C:36:GLN:O	1:C:39:TYR:N	2.38	0.44
1:C:127:THR:O	1:C:127:THR:CG2	2.64	0.44
1:C:197:PHE:CD2	1:C:197:PHE:N	2.86	0.44
1:C:279:LYS:HD3	1:C:280:PRO:HD2	1.98	0.44
1:C:282:LEU:N	1:C:282:LEU:CD2	2.81	0.44
1:C:298:ILE:O	1:C:299:ASP:C	2.54	0.44
1:D:10:ARG:HH22	1:D:317:GLU:CD	2.26	0.44
1:D:216:TRP:CE3	1:D:305:LEU:HD23	2.53	0.44
1:A:241:GLN:O	1:A:245:ILE:HG13	2.17	0.44
1:B:217:SER:O	1:B:218:LEU:C	2.60	0.44
1:C:12:TYR:O	1:C:211:TYR:OH	2.29	0.44
1:C:72:PRO:O	1:C:73:VAL:CG1	2.63	0.44
1:C:96:LYS:HG2	1:C:98:LEU:HD13	1.98	0.44
1:C:318:ALA:C	1:C:320:THR:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LYS:O	1:D:9:ALA:O	2.36	0.44
1:D:159:PRO:O	1:D:162:VAL:HG13	2.18	0.44
1:D:324:PHE:O	1:D:325:GLN:C	2.60	0.44
2:H:199:LEU:N	2:H:199:LEU:CD2	2.68	0.44
1:A:216:TRP:HZ2	1:A:245:ILE:HD13	1.80	0.44
1:B:91:GLY:HA3	1:B:146:TYR:CD2	2.53	0.44
1:B:156:ASP:HA	1:B:193:ALA:HA	1.99	0.44
1:B:229:LYS:O	1:B:229:LYS:HG2	2.17	0.44
1:C:19:ARG:CB	1:C:20:PRO:HD2	2.40	0.44
1:C:111:LEU:C	1:C:112:ILE:HD12	2.42	0.44
1:C:153:MET:HE2	1:C:182:TYR:CD1	2.51	0.44
1:D:36:GLN:C	1:D:38:ASP:N	2.75	0.44
1:D:211:TYR:O	1:D:214:ASP:N	2.51	0.44
1:D:305:LEU:HD23	1:D:305:LEU:HA	1.82	0.44
2:E:189:GLY:O	2:E:190:PHE:C	2.59	0.44
2:F:190:PHE:O	2:F:191:LYS:HG3	2.18	0.44
1:B:210:ASP:OD1	1:B:212:SER:OG	2.33	0.43
1:C:330:ALA:C	1:C:332:ASN:N	2.76	0.43
1:D:96:LYS:CG	1:D:98:LEU:HD13	2.48	0.43
1:A:279:LYS:HD3	1:A:280:PRO:HD2	1.98	0.43
1:A:300:PHE:O	1:A:301:LEU:C	2.62	0.43
1:B:196:TYR:HB2	1:B:197:PHE:CD2	2.53	0.43
1:B:265:LEU:HG	1:B:269:LEU:HD23	2.00	0.43
1:D:14:ASP:O	1:D:18:LEU:HG	2.18	0.43
1:D:158:LYS:O	1:D:159:PRO:C	2.61	0.43
1:D:169:ARG:CG	1:D:169:ARG:NH2	2.61	0.43
1:D:258:LEU:CD1	1:D:265:LEU:HD13	2.48	0.43
1:B:10:ARG:C	1:B:11:VAL:HG23	2.43	0.43
1:D:186:LYS:HB3	1:D:188:TYR:CE2	2.54	0.43
1:D:198:LYS:CB	1:D:202:LEU:HD12	2.48	0.43
1:D:328:ARG:CZ	1:D:328:ARG:CB	2.97	0.43
2:H:202:GLN:O	2:H:203:ALA:HB2	2.18	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: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:A:148:HIS:C	1:A:150:GLN:N	2.75	0.43
1:C:19:ARG:HH22	1:C:150:GLN:HE22	1.65	0.43
1:C:41:VAL:CG1	2:G:197:TYR:CB	2.96	0.43
1:C:125:TYR:OH	1:C:221:MET:HE3	2.19	0.43
1:C:239:HIS:CG	1:C:269:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:GLU:O	1:D:271:ALA:C	2.60	0.43
2:H:200:GLN:HB3	5:H:208:HOH:O	2.16	0.43
1:A:310:GLN:HA	1:A:310:GLN:OE1	2.19	0.43
1:A:314:THR:CB	1:A:317:GLU:HG3	2.39	0.43
1:B:6:MET:HB3	1:B:261:TYR:HD2	1.84	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:B:126:PRO:CB	2:F:197:TYR:HH	2.31	0.43
1:C:146:TYR:O	1:C:149:SER:N	2.51	0.43
1:D:64:LYS:NZ	1:D:64:LYS:HB2	2.33	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:98:LEU:CD2	1:C:114:GLU:HA	2.48	0.43
1:C:105:HIS:HB3	1:C:106:SER:H	1.38	0.43
1:C:175:ASP:OD1	3:C:601:AMP:O1P	2.36	0.43
1:C:195:ARG:HG3	1:C:195:ARG:HH11	1.84	0.43
1:C:200:PRO:O	1:C:204:VAL:HG22	2.18	0.43
1:C:269:LEU:O	1:C:270:GLU:C	2.61	0.43
2:E:192:ILE:O	2:E:193:HIS:C	2.61	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:B:36:GLN:O	1:B:39:TYR:N	2.47	0.43
1:B:112:ILE:N	1:B:112:ILE:CD1	2.82	0.43
1:B:226:ILE:CG1	1:B:227:PHE:N	2.82	0.43
1:C:67:ILE:HD13	2:G:195:MET:HE2	2.00	0.43
1:C:98:LEU:HB2	1:C:112: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
2:E:192:ILE:O	2:E:192:ILE:HG23	2.19	0.43
1:A:227:PHE:O	1:A:228:ARG:HB2	2.18	0.43
1:B:96:LYS:HG2	1:B:98:LEU:HD13	2.00	0.43
1:C:61:ASN:OD1	1:C:63:GLU:HG3	2.18	0.43
1:A:282:LEU:N	1:A:282:LEU:CD2	2.82	0.43
1:B:33:TRP:CE3	1:B:100:ILE:CD1	2.92	0.43
1:B:125:TYR:HA	1:B:128:LEU:HG	2.00	0.43
1:B:157:VAL:C	1:B:158:LYS:CG	2.92	0.43
1:B:237:ASP:O	1:B:238:ASN:C	2.60	0.43
1:B:279:LYS:HD3	1:B:279:LYS:HA	1.45	0.43
1:C:50:TYR:C	1:C:71:LYS:HB2	2.44	0.43
1:C:190:VAL:CG1	1:C:202:LEU:HA	2.49	0.43
1:D:135:TYR:HE2	1:D:169:ARG:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:THR:O	1:A:132:ASP:N	2.52	0.42
1:A:268:GLN:HE21	1:A:268:GLN:HB2	1.51	0.42
1:A:329:ALA:O	1:A:333:SER:HA	2.18	0.42
1:B:94:ILE:HG22	1:B:95:VAL:O	2.19	0.42
1:B:223:ALA:HB2	1:B:301:LEU:CD1	2.49	0.42
1:C:156:ASP:O	1:C:156:ASP:CG	2.58	0.42
1:C:294:SER:O	1:C:296:GLU:N	2.52	0.42
1:A:249:LEU:N	1:A:249:LEU:HD12	2.34	0.42
1:A:279:LYS:HD2	1:A:283:LYS:HD2	2.01	0.42
1:B:237:ASP:OD1	1:B:238:ASN:N	2.52	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:11:VAL:HG12	1:D:12:TYR:CD2	2.54	0.42
1:D:125:TYR:HD1	1:D:128:LEU:HD11	1.83	0.42
1:B:70:LEU:HD12	1:B:78:ILE:HD13	2.01	0.42
1:B:316:LEU:O	1:B:316:LEU:HD12	2.19	0.42
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.71	0.42
1:C:210:ASP:OD1	1:C:212:SER:N	2.44	0.42
1:C:213:LEU:O	1:C:214:ASP:C	2.56	0.42
1:C:252:ASP:O	1:C:256:VAL:HG23	2.19	0.42
1:D:108:THR:O	1:D:108:THR:HG22	2.19	0.42
2:F:200:GLN:C	2:F:202:GLN:HG2	2.43	0.42
2:H:193:HIS:HB3	2:H:194:PRO:CD	2.43	0.42
1:A:279:LYS:HD3	1:A:279:LYS:HA	1.26	0.42
1:B:116:VAL:HG23	3:B:801:AMP:HN62	1.83	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:C:259:ASN:O	1:C:260:LYS:C	2.60	0.42
1:B:10:ARG:O	1:B:11:VAL:CG2	2.68	0.42
1:B:31:VAL:HG12	1:B:33:TRP:CE2	2.55	0.42
1:B:36:GLN:CD	1:B:103:ASP:HA	2.36	0.42
1:C:135:TYR:O	1:C:138:TYR:N	2.53	0.42
1:C:215:MET:HE2	1:C:315:ALA:N	2.34	0.42
1:D:206:LEU:HD23	1:D:208:ASP:OD2	2.19	0.42
1:D:217:SER:O	1:D:218:LEU:C	2.63	0.42
2:F:200:GLN:HB2	2:F:200:GLN:HE21	1.47	0.42
1:A:106:SER:O	1:A:107:LYS:HB2	2.20	0.42
1:A:215:MET:HE2	1:A:315:ALA:N	2.34	0.42
1:B:58:ASN:HB3	1:B:61:ASN:OD1	2.19	0.42
1:B:122:LYS:O	2:F:192:ILE:HD12	2.20	0.42
1:B:197:PHE:CD2	1:B:197:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:CG1	1:C:33:TRP:CE2	3.03	0.42
1:D:12:TYR:CD1	1:D:149:SER:HA	2.55	0.42
1:D:239:HIS:CG	1:D:269:LEU:HD13	2.54	0.42
2:F:198:GLN:OE1	2:F:201:LEU:HD11	2.19	0.42
1:B:12:TYR:CD1	1:B:149:SER:HA	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:B:318:ALA:C	1:B:320:THR:H	2.28	0.42
1:B:325:GLN:O	1:B:326:GLN:C	2.62	0.42
1:C:64:LYS:NZ	1:C:64:LYS:CB	2.83	0.42
1:C:83:LYS:HD2	1:C:83:LYS:HA	1.75	0.42
1:C:103:ASP:O	1:C:104:GLN:C	2.62	0.42
1:C:173:LEU:HD23	1:C:176:TRP:CZ2	2.54	0.42
1:C:269:LEU:HA	1:C:269:LEU:HD12	1.76	0.42
1:C:288:ASP:O	1:C:291:HIS:HD2	2.02	0.42
1:D:116:VAL:HG12	1:D:117:ASN:N	2.34	0.42
1:D:121:PHE:CG	1:D:159:PRO:HB3	2.55	0.42
1:D:213:LEU:O	1:D:214:ASP:C	2.58	0.42
1:D:226:ILE:HD11	1:D:227:PHE:CE2	2.54	0.42
1:D:282:LEU:HD13	1:D:282:LEU:HA	1.87	0.42
2:H:196:ALA:C	2:H:197:TYR:HD1	2.18	0.42
1:B:200:PRO:O	1:B:201:GLU:C	2.60	0.42
1:B:245:ILE:HD13	1:B:245:ILE:HG21	1.82	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:D:78:ILE:O	1:D:82:ILE:HG13	2.20	0.42
1:D:301:LEU:O	1:D:302:ASP:C	2.62	0.42
2:G:192:ILE:O	2:G:193:HIS:C	2.63	0.42
2:G:202:GLN:H	2:G:202:GLN:HG2	1.45	0.42
1:A:24:TRP:HA	1:A:181:PHE:CZ	2.55	0.42
1:A:66:ILE:HG13	3:A:501:AMP:C6	2.55	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:C:249:LEU:N	1:C:249:LEU:HD12	2.35	0.42
1:C:265:LEU:HG	1:C:269:LEU:HD23	2.02	0.42
1:C:272:LEU:H	1:C:272:LEU:CD1	2.32	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
2:G:188:TYR:N	2:G:190:PHE:CD1	2.87	0.42
1:B:40:GLU:HA	2:E:196:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:CG	1:B:163:MET:HE3	2.45	0.42
1:B:137:ILE:HG22	1:B:141:LEU:HD13	2.02	0.42
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:A:107:LYS:HE2	1:A:107:LYS:HB3	1.90	0.41
1:A:286:ASN:HD21	1:A:289:ASN:H	1.66	0.41
1:C:39:TYR:HA	1:C:57:ILE:O	2.20	0.41
1:C:129:THR:N	1:C:132:ASP:HB2	2.33	0.41
1:C:239:HIS:ND1	1:C:269:LEU:HD13	2.35	0.41
1:D:80:ARG:O	1:D:81:GLU:C	2.63	0.41
2:F:186:ARG:O	2:F:187:LEU:C	2.63	0.41
1:A:148:HIS:C	1:A:150:GLN:H	2.27	0.41
1:A:252:ASP:O	1:A:256:VAL:HG23	2.20	0.41
1:A:318:ALA:C	1:A:320:THR:H	2.28	0.41
1:B:69:ILE:HD13	2:E:193:HIS:CD2	2.56	0.41
1:B:153:MET:CE	1:B:182:TYR:HD1	2.32	0.41
1:C:74:LYS:O	1:C:75:LYS:C	2.60	0.41
1:D:294:SER:O	1:D:296:GLU:N	2.53	0.41
1:B:216:TRP:O	1:B:217:SER:C	2.58	0.41
1:B:226:ILE:HD11	1:B:227:PHE:CE2	2.55	0.41
1:C:67:ILE:HD13	1:C:67:ILE:HG21	1.85	0.41
1:C:134:ARG:HG2	1:C:323:TYR:CE2	2.54	0.41
1:C:246:ALA:C	1:C:248:VAL:H	2.29	0.41
1:D:31:VAL:CG1	1:D:33:TRP:CE2	3.03	0.41
1:D:219:GLY:O	1:D:220:CYS:C	2.64	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.84	0.41
1:A:157:VAL:HB	1:A:217:SER:HB2	2.02	0.41
1:B:29:LEU:HD22	1:B:30:THR:H	1.85	0.41
1:B:111:LEU:C	1:B:112:ILE:HD12	2.45	0.41
1:B:222:PHE:O	1:B:223:ALA:C	2.63	0.41
1:B:286:ASN:ND2	1:B:288:ASP:CB	2.77	0.41
1:C:157:VAL:O	1:C:217:SER:HB3	2.19	0.41
1:C:220:CYS:O	1:C:221:MET:C	2.60	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: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
2:E:188:TYR:O	2:E:189:GLY:O	2.38	0.41
1:A:13:ALA:O	1:A:184:PRO:HG3	2.21	0.41
1:A:200:PRO:HD3	1:A:216:TRP:CE2	2.56	0.41
1:B:84:ILE:O	1:B:88:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:189:ASN:HD22	1:D:190:VAL:H	1.62	0.41
1:A:73:VAL:O	1:A:74:LYS:C	2.62	0.41
1:A:156:ASP:OD2	1:A:161:ASN:ND2	2.53	0.41
1:A:299:ASP:OD1	1:A:303:LYS:NZ	2.54	0.41
1:A:301:LEU:HD11	1:A:305:LEU:HD12	2.02	0.41
1:B:33:TRP:CE2	1:B:102:ARG:NE	2.86	0.41
1:C:143:ALA:O	1:C:144:LEU:C	2.63	0.41
1:C:169:ARG:HH21	1:C:169:ARG:CB	2.34	0.41
2:G:190:PHE:HB2	2:G:197:TYR:OH	2.21	0.41
1:A:14:ASP:N	1:A:14:ASP:OD2	2.39	0.41
1:A:165:ASP:OD1	1:A:167:GLU:HB3	2.21	0.41
1:A:195:ARG:HG3	1:A:195:ARG:NH1	2.35	0.41
1:A:237:ASP:O	1:A:238:ASN:C	2.62	0.41
1:B:84:ILE:HG23	1:B:152:ILE:CD1	2.32	0.41
1:B:269:LEU:O	1:B:270:GLU:C	2.61	0.41
1:C:282:LEU:HA	1:C:282:LEU:HD13	1.78	0.41
1:D:35:GLU:O	1:D:38:ASP:HB2	2.21	0.41
1:D:39:TYR:HA	1:D:57:ILE:O	2.21	0.41
1:D:195:ARG:HG3	1:D:195:ARG:HH11	1.84	0.41
1:D:247:LYS:HG2	1:D:276:HIS:CE1	2.56	0.41
2:E:188:TYR:CG	2:E:189:GLY:N	2.88	0.41
1:A:31:VAL:CG1	1:A:33:TRP:CD2	3.03	0.41
1:A:36:GLN:OE1	2:F:194:PRO:HB2	2.20	0.41
1:A:251:THR:HG23	1:A:276:HIS:HB2	2.03	0.41
1:A:289:ASN:OD1	1:A:290:GLN:N	2.54	0.41
1:B:11:VAL:HG12	1:B:12:TYR:CD2	2.56	0.41
1:B:58:ASN:ND2	1:B:61:ASN:HD21	2.18	0.41
1:B:125:TYR:O	1:B:128:LEU:HG	2.21	0.41
1:D:189:ASN:ND2	1:D:190:VAL:N	2.57	0.41
2:G:188:TYR:C	2:G:190:PHE:HD1	2.29	0.41
1:A:120:ASP:OD2	1:A:122:LYS:N	2.51	0.41
1:A:122:LYS:HE3	1:B:44:LYS:CD	2.51	0.41
1:A:127:THR:HG22	1:A:128:LEU:N	2.34	0.41
1:A:180:GLU:OE1	1:A:181:PHE:N	2.39	0.41
1:A:286:ASN:OD1	1:A:289:ASN:HB3	2.21	0.41
1:A:294:SER:O	1:A:296:GLU:N	2.54	0.41
1:B:103:ASP:O	1:B:105:HIS:N	2.54	0.41
1:B:119:THR:O	1:B:120:ASP:C	2.62	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:HIS:CE1	1:B:211:TYR:HB3	2.56	0.41
1:B:195:ARG:O	1:B:196:TYR:C	2.64	0.41
1:B:204:VAL:HG12	1:B:265:LEU:HD11	2.03	0.41
1:B:279:LYS:CD	1:B:283:LYS:HD2	2.49	0.41
1:B:316:LEU:HD13	1:B:316:LEU:HA	1.79	0.41
1:C:112:ILE:N	1:C:112:ILE:CD1	2.83	0.41
1:C:183:HIS:O	1:C:184:PRO:C	2.63	0.41
1:C:200:PRO:HD3	1:C:216:TRP:CD2	2.56	0.41
1:D:38:ASP:O	1:D:59:VAL:HG22	2.20	0.41
1:D:268:GLN:HE21	1:D:268:GLN:HB2	1.71	0.41
1:A:44:LYS:HD3	1:A:47:ARG:NE	2.36	0.41
1:A:74:LYS:HE2	1:D:264:GLU:O	2.21	0.41
1:A:128:LEU:HB3	1:A:132:ASP:HB2	2.03	0.41
1:A:272:LEU:N	1:A:272:LEU:CD1	2.79	0.41
1:B:175:ASP:C	1:B:177:GLY:N	2.79	0.41
1:C:332:ASN:O	1:C:333:SER:HB2	2.21	0.41
1:D:158:LYS:CE	1:D:161:ASN:HD21	2.34	0.41
1:D:199:GLY:O	1:D:200:PRO:C	2.63	0.41
1:D:252:ASP:O	1:D:256:VAL:HG23	2.21	0.41
1:D:318:ALA:C	1:D:320:THR:N	2.74	0.41
2:E:200:GLN:CG	2:E:201:LEU:N	2.84	0.41
1:A:10:ARG:O	1:A:11:VAL:HG22	2.21	0.40
1:A:84:ILE:O	1:A:88:LEU:HG	2.21	0.40
1:A:100:ILE:C	1:A:101:VAL:HG13	2.46	0.40
1:B:71:LYS:O	1:B:73:VAL:HG22	2.20	0.40
1:B:332:ASN:CG	1:B:333:SER:N	2.79	0.40
1:C:120:ASP:OD2	1:C:122:LYS:N	2.53	0.40
1:C:135:TYR:HE2	1:C:169:ARG:HB3	1.86	0.40
1:D:45:VAL:O	1:D:45:VAL:CG1	2.67	0.40
1:D:93:ASN:ND2	1:D:139:GLU:O	2.52	0.40
1:A:72:PRO:C	1:A:73:VAL:CG1	2.94	0.40
1:A:111:LEU:C	1:A:112:ILE:HD12	2.46	0.40
1:A:133:ILE:O	1:A:134:ARG:C	2.60	0.40
3:A:501:AMP:H5'2	1:B:47:ARG:NH2	2.36	0.40
1:B:196:TYR:O	1:B:241:GLN:NE2	2.54	0.40
1:B:264:GLU:H	1:C:76:LYS:HZ2	1.69	0.40
1:B:269:LEU:O	1:B:273:VAL:HG23	2.21	0.40
1:C:31:VAL:CG2	1:C:82:ILE:HD12	2.52	0.40
1:D:160:HIS:H	1:D:160:HIS:HD2	1.61	0.40
1:A:84:ILE:CD1	1:A:152:ILE:HD13	2.51	0.40
1:A:282:LEU:HA	1:A:282:LEU:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG13	1:B:100:ILE:HG12	2.03	0.40
1:B:195:ARG:HG3	1:B:195:ARG:NH1	2.36	0.40
1:C:39:TYR:CD2	1:C:112:ILE:HG12	2.57	0.40
1:C:78:ILE:C	1:C:80:ARG:N	2.75	0.40
1:C:196:TYR:HB2	1:C:197:PHE:CD2	2.56	0.40
1:D:105:HIS:CD2	1:D:105:HIS:C	2.97	0.40
2:H:195:MET:H	2:H:195:MET:HG2	1.59	0.40
1:A:121:PHE:CG	1:A:122:LYS:N	2.89	0.40
1:A:153:MET:CE	1:A:182:TYR:HD1	2.27	0.40
1:A:329:ALA:C	1:A:331:GLU:H	2.30	0.40
1:B:101:VAL:O	1:B:109:PRO:HA	2.21	0.40
1:B:267:PRO:O	1:B:268:GLN:CB	2.54	0.40
1:A:226:ILE:CG1	1:A:227:PHE:N	2.84	0.40
1:A:247:LYS:HG2	1:A:276:HIS:CE1	2.57	0.40
1:A:332:ASN:ND2	1:A:333:SER:N	2.70	0.40
1:B:121:PHE:O	1:B:122:LYS:C	2.62	0.40
1:D:279:LYS:HD3	1:D:279:LYS:HA	1.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/332 (98%)	271 (83%)	41 (13%)	14 (4%)	2	13
1	B	326/332 (98%)	270 (83%)	40 (12%)	16 (5%)	1	11
1	C	326/332 (98%)	268 (82%)	44 (14%)	14 (4%)	2	13
1	D	326/332 (98%)	268 (82%)	44 (14%)	14 (4%)	2	13
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	14/23 (61%)	10 (71%)	2 (14%)	2 (14%)	0	1
All	All	1362/1420 (96%)	1117 (82%)	176 (13%)	69 (5%)	1	10

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
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

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Mol	Chain	Res	Type
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
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%)	239 (80%)	58 (20%)	1	7
1	B	297/300 (99%)	251 (84%)	46 (16%)	2	12
1	C	297/300 (99%)	253 (85%)	44 (15%)	3	13
1	D	297/300 (99%)	249 (84%)	48 (16%)	2	11
2	E	13/20 (65%)	6 (46%)	7 (54%)	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%)	6 (46%)	7 (54%)	0	0
All	All	1242/1280 (97%)	1020 (82%)	222 (18%)	2	8

All (222) 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	17	VAL
1	A	27	GLU
1	A	30	THR
1	A	35	GLU
1	A	38	ASP
1	A	41	VAL
1	A	45	VAL
1	A	52	GLU
1	A	64	LYS
1	A	72	PRO
1	A	78	ILE
1	A	82	ILE
1	A	96	LYS
1	A	98	LEU
1	A	100	ILE
1	A	101	VAL
1	A	103	ASP
1	A	105	HIS
1	A	107	LYS
1	A	108	THR
1	A	112	ILE
1	A	118	ASN
1	A	119	THR

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Mol	Chain	Res	Type
1	A	122	LYS
1	A	123	VAL
1	A	127	THR
1	A	128	LEU
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
1	A	237	ASP
1	A	243	VAL
1	A	262	ARG
1	A	265	LEU
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	6	MET
1	B	27	GLU
1	B	30	THR
1	B	36	GLN
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	82	ILE

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Mol	Chain	Res	Type
1	B	96	LYS
1	B	98	LEU
1	B	100	ILE
1	B	112	ILE
1	B	118	ASN
1	B	119	THR
1	B	129	THR
1	B	133	ILE
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	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
1	B	262	ARG
1	B	265	LEU
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	35	GLU
1	C	41	VAL
1	C	42	VAL
1	C	52	GLU
1	C	64	LYS

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Mol	Chain	Res	Type
1	C	72	PRO
1	C	82	ILE
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	112	ILE
1	C	118	ASN
1	C	133	ILE
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	243	VAL
1	C	265	LEU
1	C	277	SER
1	C	279	LYS
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	332	ASN
1	D	15	VAL
1	D	16	ASN
1	D	27	GLU
1	D	30	THR
1	D	41	VAL

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Mol	Chain	Res	Type
1	D	47	ARG
1	D	64	LYS
1	D	72	PRO
1	D	78	ILE
1	D	82	ILE
1	D	96	LYS
1	D	98	LEU
1	D	100	ILE
1	D	101	VAL
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	122	LYS
1	D	127	THR
1	D	133	ILE
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	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	243	VAL
1	D	265	LEU
1	D	277	SER
1	D	279	LYS
1	D	289	ASN
1	D	306	ARG
1	D	310	GLN
1	D	316	LEU
1	D	322	PRO
1	D	325	GLN
1	D	332	ASN

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Mol	Chain	Res	Type
1	D	333	SER
2	E	191	LYS
2	E	192	ILE
2	E	195	MET
2	E	197	TYR
2	E	199	LEU
2	E	200	GLN
2	E	202	GLN
2	F	187	LEU
2	F	190	PHE
2	F	191	LYS
2	F	199	LEU
2	F	200	GLN
2	F	201	LEU
2	F	202	GLN
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	202	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	86	GLN
1	A	105	HIS
1	A	148	HIS
1	A	160	HIS
1	A	166	HIS
1	A	189	ASN
1	A	238	ASN
1	A	276	HIS
1	A	291	HIS
1	A	325	GLN

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	332	ASN
1	B	105	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	286	ASN
1	B	289	ASN
1	B	291	HIS
1	B	325	GLN
1	B	326	GLN
1	C	36	GLN
1	C	86	GLN
1	C	117	ASN
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	241	GLN
1	C	276	HIS
1	C	291	HIS
1	C	325	GLN
1	C	326	GLN
1	C	332	ASN
1	D	36	GLN
1	D	86	GLN
1	D	105	HIS
1	D	148	HIS
1	D	160	HIS
1	D	161	ASN
1	D	166	HIS
1	D	183	HIS
1	D	189	ASN
1	D	238	ASN

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Mol	Chain	Res	Type
1	D	259	ASN
1	D	268	GLN
1	D	286	ASN
1	D	289	ASN
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	E	202	GLN
2	F	193	HIS
2	F	200	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 oligosaccharides 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
3	AMP	D	701	-	25,25,25	1.83	6 (24%)	37,38,38	1.93	7 (18%)
3	AMP	A	501	-	25,25,25	1.83	9 (36%)	37,38,38	2.13	10 (27%)
3	AMP	B	801	-	25,25,25	1.63	7 (28%)	37,38,38	2.22	10 (27%)
3	AMP	C	601	-	25,25,25	1.51	6 (24%)	37,38,38	1.95	8 (21%)

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	AMP	D	701	-	1/1/5/5	7/10/26/26	0/3/3/3
3	AMP	A	501	-	1/1/5/5	5/10/26/26	0/3/3/3
3	AMP	B	801	-	1/1/5/5	4/10/26/26	0/3/3/3
3	AMP	C	601	-	1/1/5/5	6/10/26/26	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	AMP	C4-N3	4.85	1.43	1.34
3	D	701	AMP	O5'-C5'	4.00	1.59	1.44
3	D	701	AMP	C5-C4	3.92	1.46	1.39
3	B	801	AMP	C5-C4	3.61	1.45	1.39
3	D	701	AMP	C3'-C4'	3.47	1.61	1.53
3	B	801	AMP	O5'-C5'	3.24	1.56	1.44
3	D	701	AMP	C5'-C4'	3.14	1.61	1.51
3	C	601	AMP	P-O3P	3.05	1.66	1.54
3	C	601	AMP	O5'-C5'	2.93	1.55	1.44
3	C	601	AMP	C5-C4	2.77	1.44	1.39
3	A	501	AMP	C3'-C4'	2.68	1.59	1.53
3	D	701	AMP	P-O3P	2.68	1.64	1.54
3	B	801	AMP	C6-N6	2.64	1.41	1.34
3	C	601	AMP	P-O5'	-2.63	1.52	1.60
3	A	501	AMP	P-O5'	-2.56	1.52	1.60
3	A	501	AMP	C5-C6	2.39	1.47	1.41
3	A	501	AMP	C2'-C3'	-2.36	1.47	1.53
3	A	501	AMP	C5-C4	2.34	1.43	1.39
3	C	601	AMP	O4'-C1'	-2.27	1.36	1.42
3	B	801	AMP	C3'-C4'	2.26	1.58	1.53
3	C	601	AMP	C4-N3	2.23	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	AMP	P-O3P	2.15	1.62	1.54
3	B	801	AMP	P-O2P	-2.15	1.46	1.54
3	A	501	AMP	C5-N7	2.13	1.43	1.39
3	A	501	AMP	P-O3P	2.08	1.62	1.54
3	D	701	AMP	P-O2P	-2.08	1.47	1.54
3	A	501	AMP	O5'-C5'	2.02	1.52	1.44
3	B	801	AMP	C5'-C4'	2.02	1.57	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	AMP	O4'-C1'-N9	8.22	123.88	108.09
3	A	501	AMP	O4'-C1'-N9	7.47	122.44	108.09
3	D	701	AMP	O4'-C1'-N9	6.36	120.30	108.09
3	C	601	AMP	C2'-C1'-N9	5.99	128.19	113.30
3	C	601	AMP	O4'-C1'-N9	5.18	118.05	108.09
3	D	701	AMP	C2'-C1'-N9	5.16	126.13	113.30
3	A	501	AMP	C2'-C1'-N9	4.48	124.44	113.30
3	B	801	AMP	C2'-C1'-N9	4.23	123.80	113.30
3	B	801	AMP	C3'-C2'-C1'	-3.79	94.30	101.46
3	C	601	AMP	O4'-C1'-C2'	3.32	113.72	106.62
3	C	601	AMP	O3P-P-O2P	-3.14	96.04	107.80
3	D	701	AMP	O3P-P-O2P	-3.11	96.15	107.80
3	D	701	AMP	O4'-C1'-C2'	3.05	113.14	106.62
3	B	801	AMP	O5'-C5'-C4'	3.01	119.24	108.99
3	B	801	AMP	C4-C5-N7	-3.01	107.15	110.58
3	A	501	AMP	O4'-C1'-C2'	2.97	112.97	106.62
3	B	801	AMP	C4'-O4'-C1'	-2.96	102.93	109.47
3	D	701	AMP	O3P-P-O1P	2.95	122.35	110.83
3	A	501	AMP	C4-C5-N7	-2.95	107.21	110.58
3	A	501	AMP	O3P-P-O5'	-2.72	99.57	106.67
3	A	501	AMP	C4'-O4'-C1'	-2.67	103.56	109.47
3	A	501	AMP	O3P-P-O1P	2.65	121.16	110.83
3	C	601	AMP	C4-C5-N7	-2.63	107.58	110.58
3	C	601	AMP	O2P-P-O1P	2.55	120.78	110.83
3	C	601	AMP	O3P-P-O1P	2.54	120.71	110.83
3	A	501	AMP	C6-C5-N7	2.45	136.81	132.09
3	A	501	AMP	C5-N7-C8	2.43	107.28	103.45
3	D	701	AMP	O5'-C5'-C4'	2.42	117.22	108.99
3	D	701	AMP	O2P-P-O5'	2.38	112.88	106.67
3	B	801	AMP	O3'-C3'-C4'	2.37	117.89	111.08
3	B	801	AMP	O3P-P-O2P	-2.36	98.94	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	AMP	O2'-C2'-C1'	2.26	117.88	110.10
3	B	801	AMP	C5'-C4'-N3	-2.21	123.67	126.72
3	C	601	AMP	C3'-C2'-C1'	-2.17	97.36	101.46
3	A	501	AMP	O3P-P-O2P	-2.03	100.20	107.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	AMP	C1'
3	B	801	AMP	C1'
3	C	601	AMP	C1'
3	D	701	AMP	C1'

All (22) torsion outliers are listed below:

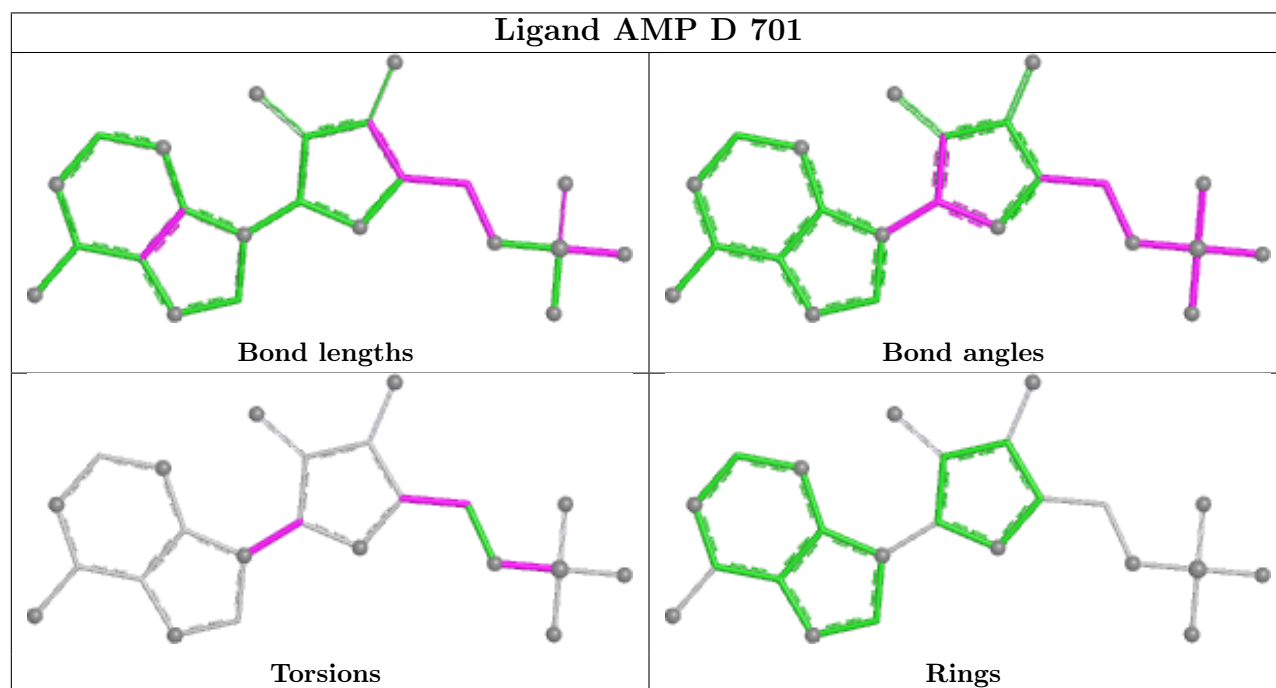
Mol	Chain	Res	Type	Atoms
3	B	801	AMP	C5'-O5'-P-O2P
3	B	801	AMP	O4'-C4'-C5'-O5'
3	C	601	AMP	C5'-O5'-P-O2P
3	D	701	AMP	C5'-O5'-P-O1P
3	D	701	AMP	C5'-O5'-P-O2P
3	D	701	AMP	C5'-O5'-P-O3P
3	A	501	AMP	O4'-C4'-C5'-O5'
3	B	801	AMP	C3'-C4'-C5'-O5'
3	D	701	AMP	O4'-C4'-C5'-O5'
3	D	701	AMP	C3'-C4'-C5'-O5'
3	C	601	AMP	O4'-C4'-C5'-O5'
3	C	601	AMP	C3'-C4'-C5'-O5'
3	A	501	AMP	C3'-C4'-C5'-O5'
3	C	601	AMP	C2'-C1'-N9-C4
3	C	601	AMP	C5'-O5'-P-O1P
3	C	601	AMP	C2'-C1'-N9-C8
3	D	701	AMP	C2'-C1'-N9-C4
3	B	801	AMP	C5'-O5'-P-O1P
3	A	501	AMP	C2'-C1'-N9-C4
3	D	701	AMP	C2'-C1'-N9-C8
3	A	501	AMP	C2'-C1'-N9-C8
3	A	501	AMP	C4'-C5'-O5'-P

There are no ring outliers.

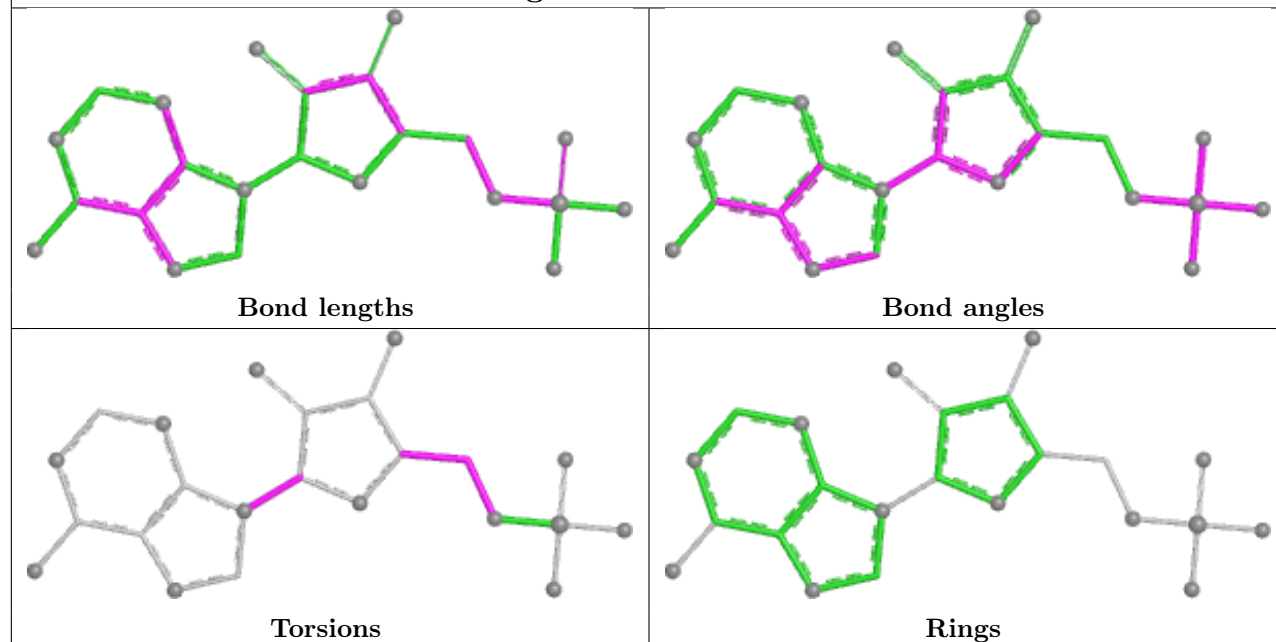
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	AMP	3	0
3	A	501	AMP	7	0
3	B	801	AMP	5	0
3	C	601	AMP	4	0

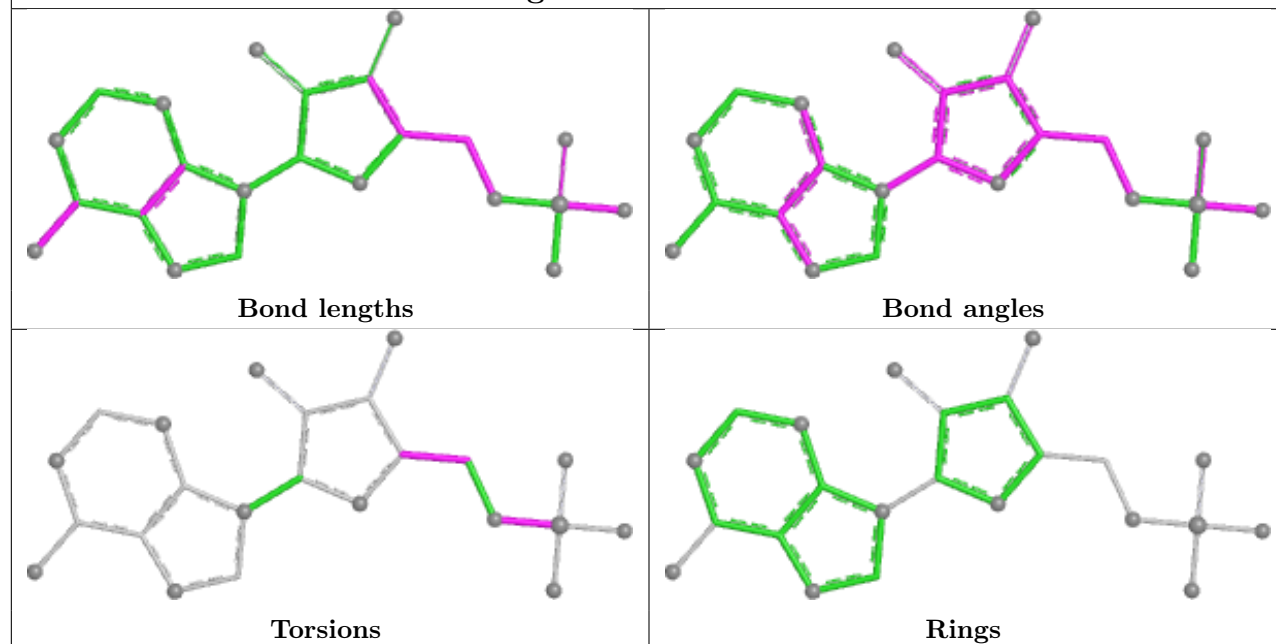
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

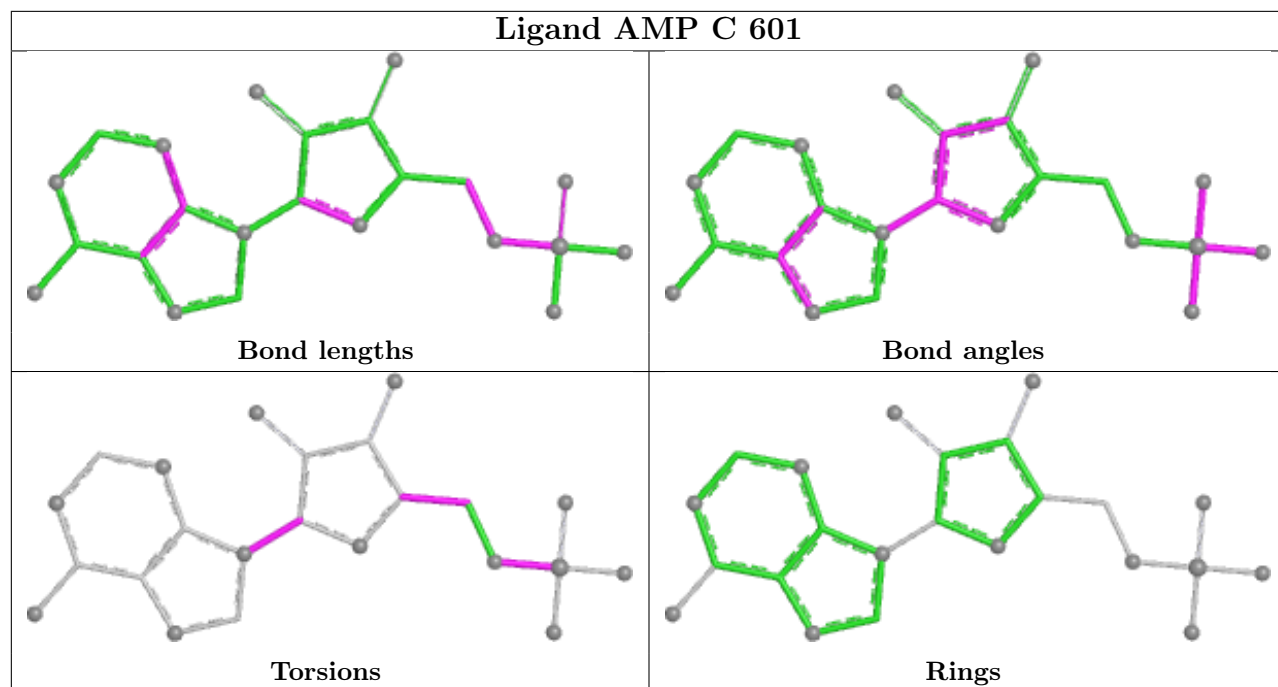


Ligand AMP A 501



Ligand AMP B 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.