



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jun 30, 2019 – 07:56 PM EDT

PDB ID : 6QB8  
EMDB ID: : EMD-4489  
Title : Human CCT:mLST8 complex  
Authors : Cuellar, J.; Santiago, C.; Ludlam, W.G.; Bueno-Carrasco, M.T.; Valpuesta, J.M.; Willardson, B.M.  
Deposited on : 2018-12-20  
Resolution : 3.97 Å(reported)  
Based on PDB ID : 5GW5

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

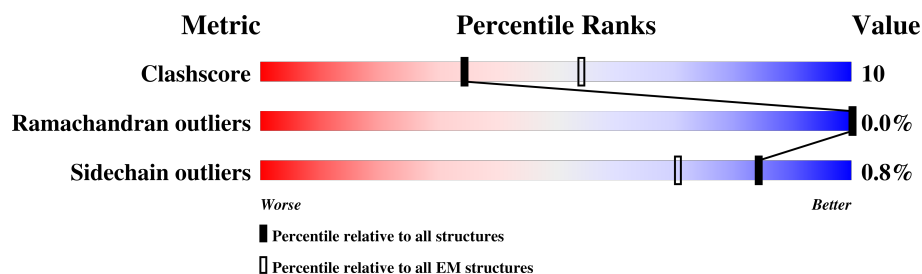
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.97 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	556	50% 38% 11%
1	a	556	87% 12%
2	B	535	54% 37% 8%
2	b	535	89% 11%
3	D	539	54% 36% 10%
3	d	539	90% 9%
4	E	541	52% 40% 7%
4	e	541	93% 7%
5	G	544	53% 36% 11%

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Mol	Chain	Length	Quality of chain
5	g	544	<div><div style="width: 87%;"></div>87%<div style="width: 12%; background-color: #cccccc;"></div>12%</div>
6	H	543	<div><div style="width: 69%;"></div>69%<div style="width: 23%; background-color: #ffff00;"></div>23%<div style="width: 8%; background-color: #cccccc;"></div>8%</div>
6	h	543	<div><div style="width: 91%;"></div>91%<div style="width: 8%; background-color: #cccccc;"></div>8%</div>
7	Q	548	<div><div style="width: 61%;"></div>61%<div style="width: 26%; background-color: #ffff00;"></div>26%<div style="width: 12%; background-color: #cccccc;"></div>12%</div>
7	q	548	<div><div style="width: 84%;"></div>84%<div style="width: 12%; background-color: #cccccc;"></div>12%</div>
8	Z	531	<div><div style="width: 52%;"></div>52%<div style="width: 41%; background-color: #ffff00;"></div>41%<div style="width: 6%; background-color: #cccccc;"></div>6%</div>
8	z	531	<div><div style="width: 95%;"></div>95%<div style="width: 2%; background-color: #cccccc;"></div>2%</div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60035 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	490	Total	C	N	O	S	0	0
			3709	2323	651	713	22		
1	A	494	Total	C	N	O	S	0	0
			3742	2345	656	719	22		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	478	Total	C	N	O	S	0	0
			3590	2248	630	694	18		
2	B	492	Total	C	N	O	S	0	0
			3698	2311	648	720	19		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	489	Total	C	N	O	S	0	0
			3673	2302	636	714	21		
3	D	487	Total	C	N	O	S	0	0
			3655	2292	634	708	21		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	505	Total	C	N	O	S	0	0
			3882	2422	678	752	30		
4	E	503	Total	C	N	O	S	0	0
			3863	2412	672	749	30		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	477	Total	C	N	O	S	0	0
			3678	2295	654	700	29		
5	G	485	Total	C	N	O	S	0	0
			3741	2335	664	713	29		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	500	Total	C	N	O	S	0	0
			3834	2422	662	727	23		
6	H	499	Total	C	N	O	S	0	0
			3825	2417	661	724	23		

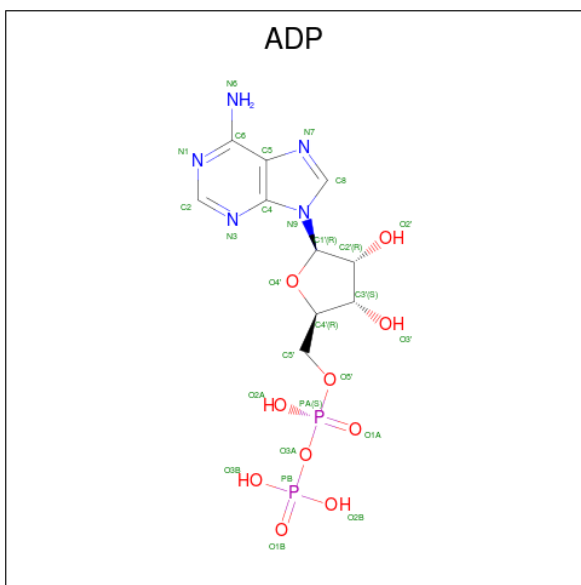
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	483	Total	C	N	O	S	0	0
			3692	2327	628	712	25		
7	Q	483	Total	C	N	O	S	0	0
			3692	2327	628	712	25		

- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	508	Total	C	N	O	S	0	0
			3894	2447	680	747	20		
8	Z	497	Total	C	N	O	S	0	0
			3813	2395	670	728	20		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



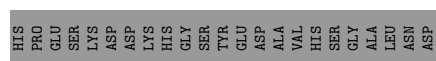
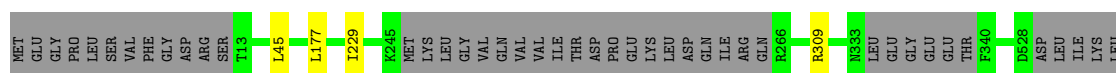
Mol	Chain	Residues	Atoms					AltConf
9	q	1	Total 27	C 10	N 5	O 10	P 2	0
9	Q	1	Total 27	C 10	N 5	O 10	P 2	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

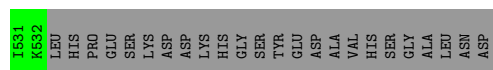
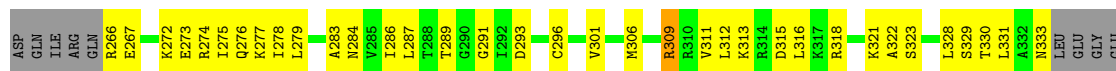
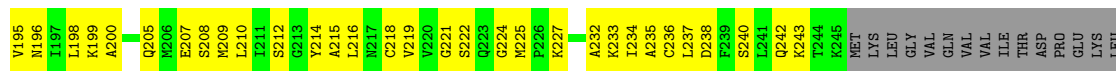
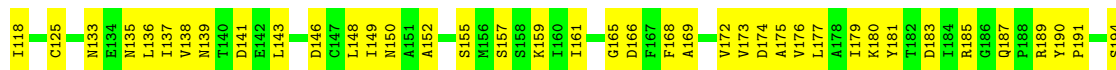
- Molecule 1: T-complex protein 1 subunit alpha

Chain a: 



- Molecule 1: T-complex protein 1 subunit alpha

Chain A: 



- Molecule 2: T-complex protein 1 subunit beta

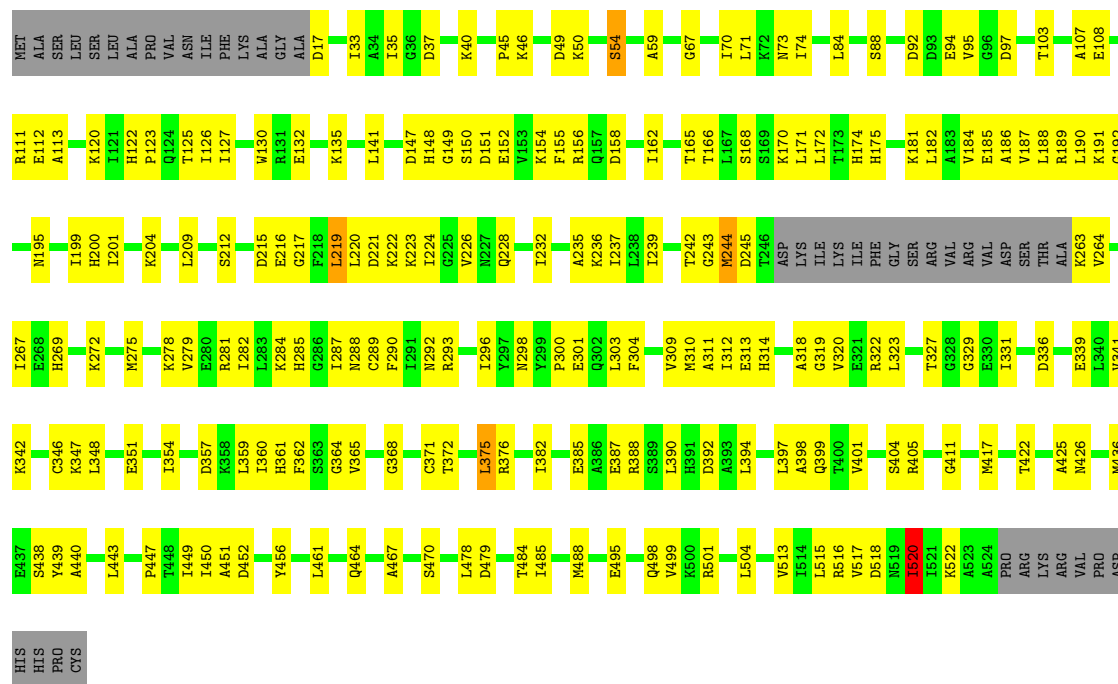
Chain b: 



LYS  
ARG  
VAL  
PRO  
SER  
ASP  
HIS  
HIS  
PRO  
CYS

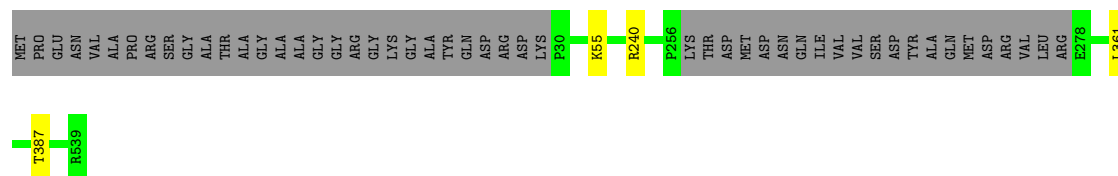
• Molecule 2: T-complex protein 1 subunit beta

Chain B: 54% 37% 8%



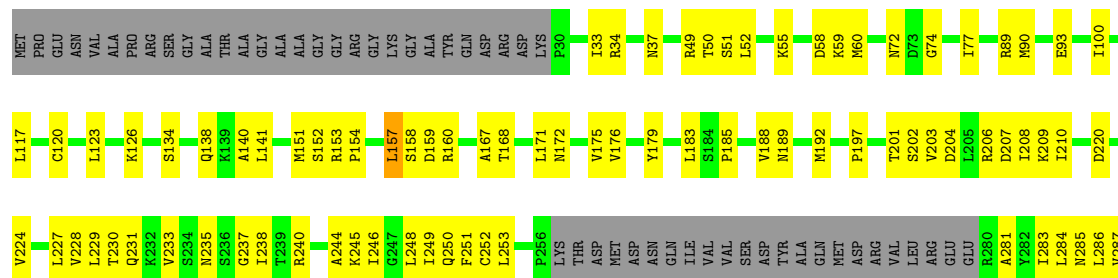
• Molecule 3: T-complex protein 1 subunit delta

Chain d: 90% 9%



• Molecule 3: T-complex protein 1 subunit delta

Chain D: 54% 36% 10%

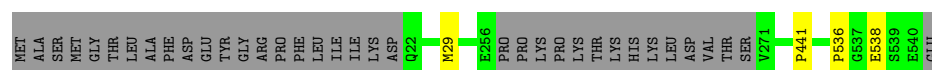






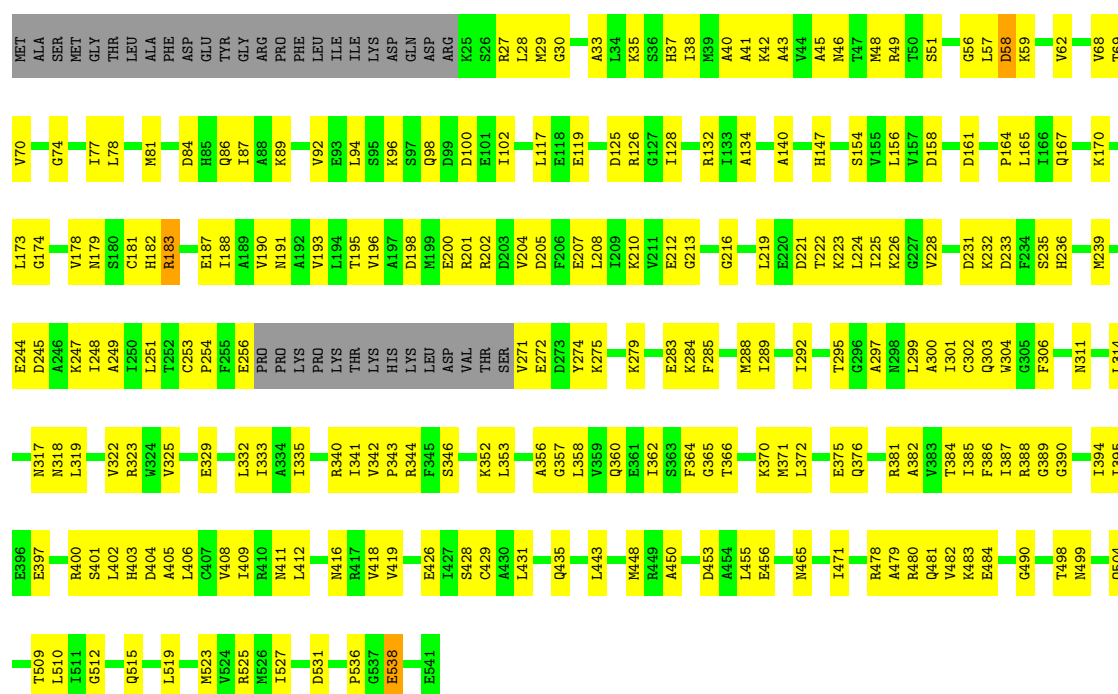
- Molecule 4: T-complex protein 1 subunit epsilon

Chain e: 93% 7%



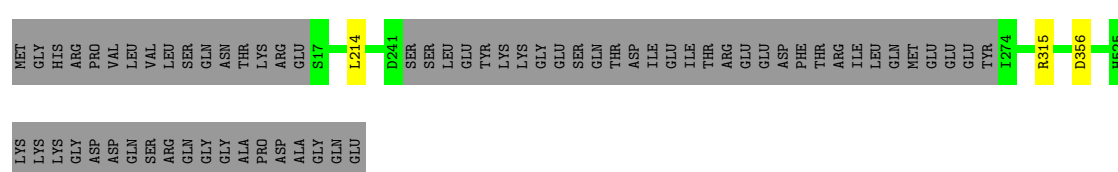
- Molecule 4: T-complex protein 1 subunit epsilon

Chain E: 52% 40% 7%



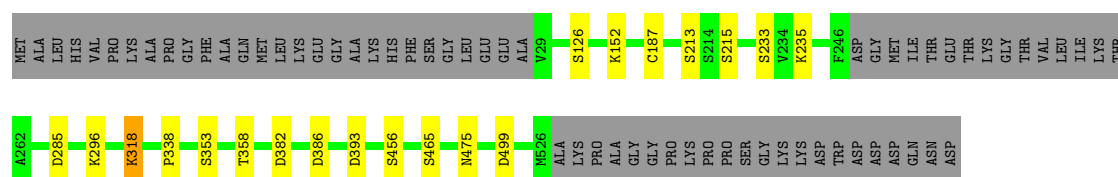
- Molecule 5: T-complex protein 1 subunit gamma

Chain g: 87% 12%



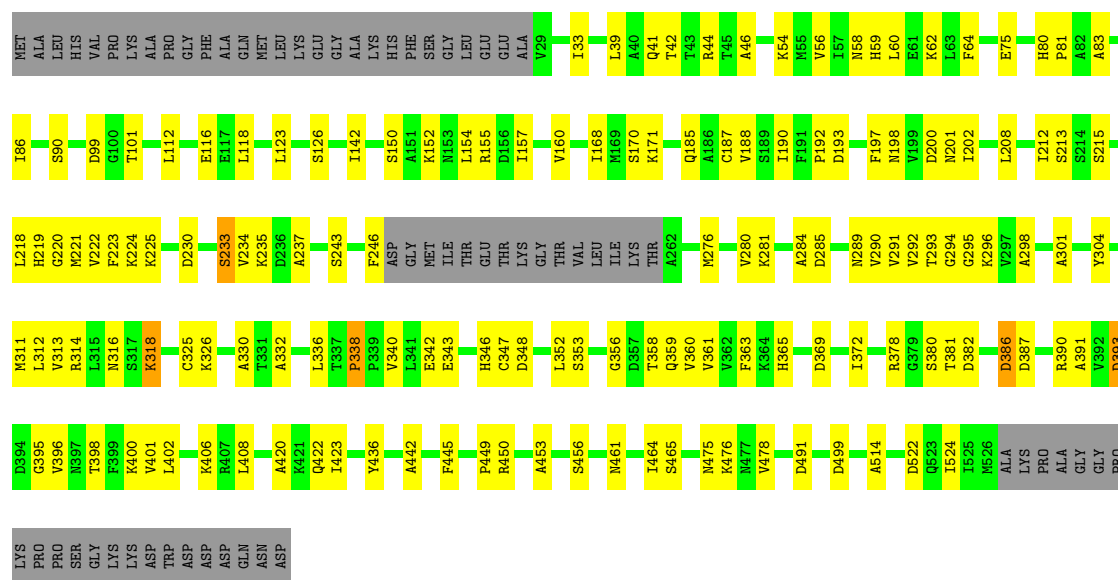
- Molecule 5: T-complex protein 1 subunit gamma





- Molecule 7: T-complex protein 1 subunit theta

Chain Q:  61% 26% 12%



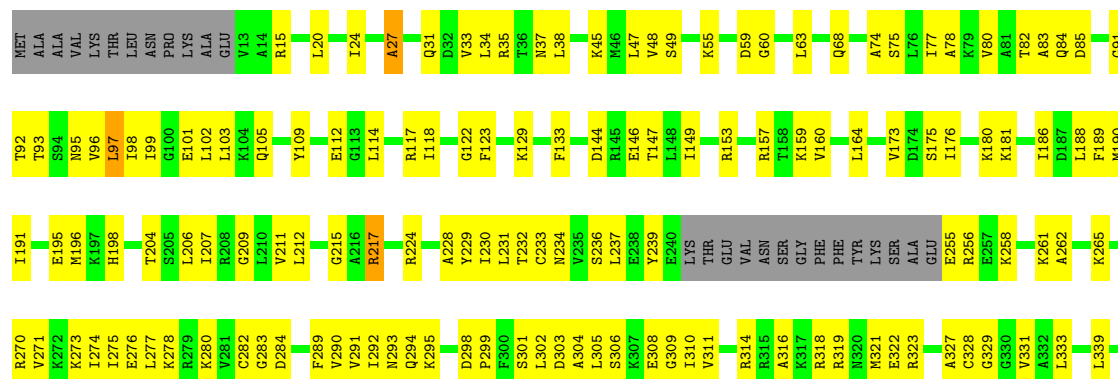
- Molecule 8: T-complex protein 1 subunit zeta

Chain z:  95% . .



- Molecule 8: T-complex protein 1 subunit zeta

Chain Z:  52% 41% • 6%



I521	D442	C343
M522	D442	L344
M523	I446	G345
ALA	I447	H346
GLY	I447	A347
MET	P448	G348
SER	K449	L349
SER	V450	V350
LEU	Q453	Y351
LYS	M454	E352
GLY	M454	Y353
	D458	K359
	L459	F360
	Q460	T361
	E461	F362
	T462	T363
	L463	E364
	V464	K365
	K465	C366
	I466	N367
	Q467	
	A468	R370
	E469	S371
	H470	V372
	S471	T373
	Q474	L374
	Q475	L375
		L376
	D480	K377
	T483	G378
	P486	L384
		L387
	V492	L395
	G493	
	V494	V398
	M497	I402
	V498	
	C499	V408
	V500	
	K501	V414
	K502	E415
	Q503	V416
	L504	A417
	S507	
	C508	A421
	T509	L422
	V510	
		H425
	T513	K426
	L517	
	V518	K430
	D519	R432
	F520	
		G435

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	452000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	36	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.28	0/3775	0.53	1/5093 (0.0%)
1	a	0.28	0/3742	0.55	2/5049 (0.0%)
2	B	0.29	0/3736	0.58	3/5036 (0.1%)
2	b	0.28	0/3628	0.57	1/4891 (0.0%)
3	D	0.28	0/3684	0.57	3/4972 (0.1%)
3	d	0.29	0/3702	0.55	1/4996 (0.0%)
4	E	0.29	0/3904	0.56	0/5256
4	e	0.28	0/3923	0.55	0/5281
5	G	0.29	0/3783	0.54	1/5104 (0.0%)
5	g	0.29	0/3719	0.56	2/5020 (0.0%)
6	H	0.29	0/3878	0.53	0/5232
6	h	0.29	0/3887	0.54	1/5244 (0.0%)
7	Q	0.29	0/3742	0.54	1/5059 (0.0%)
7	q	0.29	0/3742	0.55	1/5059 (0.0%)
8	Z	0.29	0/3855	0.54	3/5197 (0.1%)
8	z	0.30	0/3938	0.57	3/5309 (0.1%)
All	All	0.29	0/60638	0.55	23/81798 (0.0%)

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	1
2	B	0	3
2	b	0	1
3	d	0	1
4	E	0	2
4	e	0	5
6	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	h	0	3
7	Q	0	2
7	q	0	2
8	Z	0	2
8	z	0	1
All	All	0	24

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	356	ASP	CB-CG-OD2	8.33	125.79	118.30
8	z	34	LEU	CA-CB-CG	-7.70	97.59	115.30
3	D	157	LEU	CA-CB-CG	7.05	131.52	115.30
2	B	219	LEU	CA-CB-CG	7.00	131.40	115.30
7	Q	318	LYS	CD-CE-NZ	6.18	125.92	111.70
7	q	318	LYS	CD-CE-NZ	6.17	125.90	111.70
8	Z	504	LEU	CA-CB-CG	6.04	129.18	115.30
8	Z	395	LEU	CA-CB-CG	5.99	129.09	115.30
2	B	520	ILE	CG1-CB-CG2	-5.92	98.38	111.40
5	g	214	LEU	CA-CB-CG	5.91	128.89	115.30
3	d	361	LEU	CA-CB-CG	5.88	128.83	115.30
6	h	378	LEU	CA-CB-CG	5.72	128.45	115.30
8	z	97	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	357	CYS	CA-CB-SG	5.67	124.20	114.00
2	B	375	LEU	CA-CB-CG	5.63	128.25	115.30
5	G	356	ASP	CB-CG-OD2	5.62	123.36	118.30
3	D	361	LEU	CA-CB-CG	5.55	128.06	115.30
1	a	45	LEU	CA-CB-CG	5.43	127.80	115.30
2	b	238	LEU	CA-CB-CG	5.43	127.78	115.30
8	Z	97	LEU	CA-CB-CG	5.26	127.39	115.30
8	z	282	CYS	CA-CB-SG	5.13	123.24	114.00
3	D	299	LEU	CA-CB-CG	5.02	126.84	115.30
1	a	177	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	MET	Peptide
2	B	520	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	B	54	SER	Peptide
4	E	538	GLU	Peptide
4	E	58	ASP	Peptide
6	H	303	PHE	Peptide
7	Q	338	PRO	Peptide
7	Q	475	ASN	Peptide
8	Z	198	HIS	Peptide
8	Z	27	ALA	Mainchain
1	a	229	ILE	Peptide
2	b	59	ALA	Peptide
3	d	387	THR	Peptide
4	e	29	MET	Peptide
4	e	441	PRO	Peptide
4	e	536	PRO	Peptide
4	e	538	GLU	Mainchain,Peptide
6	h	318	VAL	Peptide
6	h	527	PRO	Mainchain,Peptide
7	q	338	PRO	Peptide
7	q	475	ASN	Peptide
8	z	27	ALA	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3742	0	3898	174	0
1	a	3709	0	3859	0	0
2	B	3698	0	3792	155	0
2	b	3590	0	3691	0	0
3	D	3655	0	3874	148	0
3	d	3673	0	3886	0	0
4	E	3863	0	3960	176	0
4	e	3882	0	3979	0	0
5	G	3741	0	3880	142	0
5	g	3678	0	3815	0	0
6	H	3825	0	3914	81	0
6	h	3834	0	3920	0	0
7	Q	3692	0	3746	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	q	3692	0	3746	0	0
8	Z	3813	0	3951	169	0
8	z	3894	0	4021	0	0
9	Q	27	0	12	5	0
9	q	27	0	12	0	0
All	All	60035	0	61956	1095	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 10.

All (1095) 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)
8:Z:204:THR:HA	8:Z:375:LEU:O	1.74	0.88
5:G:352:LYS:O	5:G:359:PHE:HB2	1.86	0.85
1:A:275:ILE:O	1:A:279:LEU:HB2	3.14	0.80
1:A:355:ARG:HA	1:A:359:ASP:O	1.84	0.76
3:D:210:ILE:H	3:D:385:THR:HG23	2.09	0.75
1:A:233:LYS:H	1:A:284:ASN:HB3	1.84	0.73
2:B:244:MET:HG2	2:B:279:VAL:HB	1.71	0.72
3:D:210:ILE:HG13	3:D:388:ILE:H	1.59	0.72
5:G:437:ARG:O	5:G:440:ALA:HB3	1.94	0.71
8:Z:329:GLY:HA3	8:Z:367:ASN:HD21	1.56	0.69
1:A:240:SER:HB3	1:A:242:GLN:HE21	1.58	0.68
3:D:183:LEU:HB3	3:D:405:ILE:HD11	1.89	0.67
4:E:86:GLN:HG2	6:H:50:VAL:HG21	2.64	0.67
8:Z:181:LYS:HZ2	8:Z:370:ARG:HH21	2.68	0.67
2:B:45:PRO:HB3	2:B:168:SER:HB3	2.24	0.67
3:D:207:ASP:HB2	3:D:386:VAL:HG22	1.77	0.67
1:A:215:ALA:HA	1:A:362:ILE:O	2.34	0.66
2:B:244:MET:HG3	2:B:275:MET:HG3	1.77	0.66
2:B:267:ILE:HG13	4:E:271:VAL:HG12	1.77	0.66
4:E:509:THR:HG23	4:E:512:GLY:H	1.61	0.66
4:E:428:SER:HB3	4:E:481:GLN:HE22	1.62	0.65
7:Q:347:CYS:SG	7:Q:348:ASP:N	2.70	0.65
7:Q:150:SER:HB3	7:Q:406:LYS:HG2	1.79	0.65
7:Q:90:SER:HB2	7:Q:101:THR:HG23	1.79	0.65
8:Z:278:LYS:NZ	8:Z:304:ALA:O	2.30	0.65
6:H:518:GLU:HB3	7:Q:54:LYS:HD2	1.79	0.64
5:G:216:GLY:H	5:G:371:CYS:HA	1.61	0.64
2:B:461:LEU:HB2	2:B:485:ILE:HD11	9.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ILE:HG23	2:B:300:PRO:HB2	1.79	0.63
5:G:75:ALA:HB1	5:G:515:LEU:HD11	1.80	0.63
2:B:220:LEU:HD22	2:B:312:ILE:HG23	1.80	0.63
1:A:266:ARG:HG3	1:A:273:GLU:HB3	3.06	0.63
4:E:357:GLY:H	4:E:375:GLU:HA	1.64	0.63
2:B:217:GLY:HA3	2:B:362:PHE:HB2	1.80	0.63
5:G:288:VAL:HA	5:G:309:THR:H	1.64	0.63
8:Z:282:CYS:SG	8:Z:283:GLY:N	2.72	0.63
7:Q:41:GLN:HE22	7:Q:44:ARG:HH11	1.47	0.63
1:A:232:ALA:HB3	1:A:348:ALA:H	1.63	0.62
1:A:278:ILE:HB	1:A:331:LEU:HD21	1.80	0.62
2:B:292:ASN:ND2	2:B:313:GLU:OE1	7.83	0.62
4:E:279:LYS:O	4:E:283:GLU:HB2	1.99	0.62
6:H:26:ILE:HG22	6:H:105:LEU:HD23	1.80	0.62
7:Q:325:CYS:HA	7:Q:330:ALA:HB3	1.81	0.62
8:Z:350:VAL:HG22	8:Z:363:ILE:HG12	1.84	0.62
2:B:219:LEU:HA	2:B:360:ILE:HB	1.81	0.62
2:B:245:ASP:HB2	2:B:272:LYS:HD2	1.81	0.62
2:B:112:GLU:HB3	2:B:438:SER:HB2	1.82	0.62
4:E:244:GLU:HA	4:E:376:GLN:HG2	1.82	0.62
4:E:213:GLY:HA2	4:E:387:ILE:HB	1.81	0.61
5:G:62:GLY:HA2	5:G:65:ILE:HD12	1.81	0.61
4:E:236:HIS:HB3	4:E:239:MET:HB2	1.80	0.61
1:A:274:ARG:HH11	1:A:331:LEU:H	2.63	0.61
3:D:168:THR:HA	3:D:172:ASN:HD22	1.76	0.61
3:D:252:CYS:HB2	3:D:308:ALA:HA	1.93	0.61
3:D:229:LEU:HB2	3:D:374:LEU:HB3	1.82	0.61
8:Z:378:GLY:HA3	8:Z:384:LEU:HD11	1.82	0.61
1:A:15:GLU:HG2	1:A:16:THR:HG22	5.47	0.61
8:Z:195:GLU:HG2	8:Z:384:LEU:HD13	7.01	0.61
2:B:290:PHE:H	2:B:310:MET:HB3	1.66	0.60
4:E:306:PHE:HB3	4:E:323:ARG:HE	2.75	0.60
5:G:445:VAL:HA	5:G:448:ARG:HB3	1.83	0.60
1:A:45:LEU:HB3	1:A:53:THR:HB	1.83	0.60
8:Z:215:GLY:HA2	8:Z:361:THR:HG23	4.30	0.60
1:A:199:LYS:HA	1:A:377:LEU:HB2	1.83	0.60
5:G:90:VAL:HA	5:G:395:GLN:HG3	1.83	0.60
3:D:208:ILE:HA	3:D:383:GLY:HA2	1.83	0.60
8:Z:497:ASN:ND2	8:Z:499:CYS:SG	2.74	0.60
4:E:314:LEU:HD22	4:E:319:LEU:HB2	4.62	0.60
1:A:161:ILE:O	1:A:165:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:225:ILE:HB	4:E:386:PHE:HB2	1.83	0.59
2:B:436:MET:O	2:B:439:TYR:HB3	2.01	0.59
4:E:248:ILE:HA	4:E:299:LEU:HB3	2.08	0.59
1:A:472:ASN:HD21	6:H:425:ARG:HB2	133.83	0.59
5:G:433:GLN:HE21	5:G:437:ARG:HH22	1.71	0.59
6:H:48:LEU:HD13	6:H:58:ILE:HG13	1.83	0.59
3:D:208:ILE:N	3:D:385:THR:O	4.48	0.59
2:B:201:ILE:HD11	2:B:390:LEU:HD22	2.72	0.59
6:H:17:GLN:O	6:H:21:GLN:N	2.35	0.59
8:Z:112:GLU:HG2	8:Z:460:GLN:HE21	21.31	0.59
3:D:227:LEU:HB2	3:D:339:THR:HG21	1.98	0.59
2:B:382:ILE:HA	2:B:385:GLU:HB3	1.85	0.59
8:Z:290:VAL:HG13	8:Z:311:VAL:HB	3.63	0.59
2:B:242:THR:OG1	2:B:275:MET:SD	2.60	0.58
3:D:248:LEU:HD22	3:D:344:PRO:HA	3.89	0.58
3:D:503:ILE:HD12	3:D:506:GLU:HB2	6.56	0.58
4:E:98:GLN:HG2	4:E:519:LEU:HD13	3.45	0.58
5:G:199:ARG:HD2	5:G:321:ARG:HD3	1.84	0.58
2:B:127:ILE:HG13	2:B:515:LEU:HD23	1.94	0.58
4:E:235:SER:HB2	4:E:239:MET:HG3	4.12	0.58
4:E:271:VAL:O	4:E:275:LYS:N	2.34	0.58
8:Z:352:GLU:HA	8:Z:361:THR:HA	2.25	0.58
1:A:45:LEU:HD21	1:A:64:LEU:HB2	1.95	0.58
3:D:330:ARG:HA	3:D:333:ILE:HD12	1.84	0.58
4:E:216:GLY:H	4:E:390:GLY:HA2	1.68	0.58
6:H:157:LYS:O	6:H:160:MET:HB2	2.02	0.58
8:Z:464:VAL:HA	8:Z:467:GLN:HB2	1.86	0.58
1:A:348:ALA:HA	1:A:367:THR:HA	2.17	0.58
7:Q:393:ASP:N	7:Q:393:ASP:OD1	2.36	0.58
5:G:136:LEU:HD23	5:G:139:ILE:HD11	2.03	0.58
5:G:67:ARG:HA	5:G:84:ARG:HH22	1.70	0.58
5:G:71:VAL:HG22	5:G:73:HIS:H	1.67	0.58
8:Z:212:LEU:HB2	8:Z:361:THR:HB	1.84	0.58
8:Z:122:GLY:HA3	8:Z:436:GLY:HA3	2.62	0.58
1:A:210:LEU:HD11	1:A:373:ALA:HB1	1.85	0.58
4:E:167:GLN:HA	4:E:170:LYS:HB2	2.61	0.58
5:G:46:MET:HE1	8:Z:517:LEU:HB2	1.86	0.58
6:H:326:CYS:HA	6:H:365:PRO:HD2	1.86	0.58
7:Q:243:SER:HB3	7:Q:332:ALA:HB1	1.86	0.58
8:Z:322:GLU:OE2	8:Z:323:ARG:NH1	2.36	0.58
4:E:405:ALA:HA	4:E:408:VAL:HG22	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:360:PHE:HB3	6:H:362:THR:HG23	1.85	0.57
2:B:204:LYS:HB3	2:B:376:ARG:HG3	3.94	0.57
2:B:94:GLU:HG3	2:B:95:VAL:HG13	1.85	0.57
3:D:240:ARG:NH1	3:D:364:GLU:OE2	3.16	0.57
4:E:205:ASP:H	4:E:208:LEU:HB2	2.66	0.57
8:Z:123:PHE:HB3	8:Z:509:THR:HG23	1.86	0.57
2:B:516:ARG:NH1	4:E:58:ASP:OD2	2.37	0.57
4:E:128:ILE:HD12	4:E:443:LEU:HD12	1.87	0.57
8:Z:236:SER:HA	8:Z:293:ASN:HD21	1.69	0.57
1:A:137:ILE:HD12	1:A:410:PRO:HD3	1.87	0.57
4:E:400:ARG:NH2	4:E:404:ASP:OD2	2.47	0.57
5:G:329:ARG:NH1	5:G:342:VAL:O	2.37	0.57
7:Q:478:VAL:HA	7:Q:491:ASP:HA	1.87	0.57
8:Z:24:ILE:HD12	8:Z:103:LEU:HB3	1.87	0.57
2:B:174:HIS:H	2:B:209:LEU:HD23	6.25	0.57
3:D:441:ARG:HH22	4:E:435:GLN:HG3	97.05	0.57
5:G:346:ALA:HA	5:G:365:CYS:HA	1.90	0.57
6:H:237:ILE:HB	6:H:328:GLY:HA3	1.87	0.57
8:Z:33:VAL:HG13	8:Z:45:LYS:HE2	3.32	0.57
2:B:17:ASP:OD1	2:B:17:ASP:N	2.38	0.57
2:B:185:GLU:OE1	2:B:189:ARG:NH2	3.60	0.57
4:E:134:ALA:HB1	4:E:525:ARG:HG3	1.87	0.57
2:B:346:CYS:SG	2:B:347:LYS:N	2.78	0.56
3:D:360:GLU:HB2	3:D:378:GLY:HA3	2.21	0.56
4:E:27:ARG:NH1	4:E:28:LEU:O	2.38	0.56
4:E:366:THR:H	4:E:388:ARG:HH22	5.14	0.56
8:Z:280:LYS:NZ	8:Z:339:LEU:O	2.38	0.56
8:Z:38:LEU:O	8:Z:454:ASN:ND2	2.43	0.56
1:A:137:ILE:HG22	1:A:139:ASN:H	2.33	0.56
1:A:183:ASP:OD2	1:A:185:ARG:NH2	4.68	0.56
2:B:293:ARG:O	2:B:314:HIS:ND1	6.09	0.56
5:G:109:GLU:HA	5:G:112:LEU:HB2	1.87	0.56
5:G:137:LYS:HG2	5:G:498:LEU:HD21	1.87	0.56
2:B:221:ASP:OD1	2:B:222:LYS:NZ	2.96	0.56
6:H:240:LEU:HG	6:H:242:VAL:H	1.71	0.56
2:B:149:GLY:HA2	2:B:152:GLU:HB2	2.42	0.56
2:B:292:ASN:HD22	2:B:304:PHE:HZ	1.54	0.56
3:D:248:LEU:HG	3:D:299:LEU:HD21	4.49	0.56
4:E:292:ILE:HG12	4:E:297:ALA:HB3	1.86	0.56
1:A:196:ASN:ND2	1:A:315:ASP:OD1	2.52	0.56
3:D:158:SER:O	3:D:160:ARG:NH1	6.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD21	1:A:306:MET:HE3	1.86	0.56
3:D:33:ILE:O	3:D:37:ASN:ND2	2.52	0.56
2:B:348:LEU:HB3	2:B:364:GLY:HA3	1.88	0.56
4:E:119:GLU:HB3	4:E:450:ALA:HB1	1.88	0.56
2:B:440:ALA:HA	2:B:443:LEU:HD12	1.86	0.56
2:B:132:GLU:HA	2:B:135:LYS:HD2	1.87	0.55
4:E:412:LEU:O	4:E:416:ASN:ND2	2.39	0.55
1:A:267:GLU:HB3	1:A:273:GLU:HB2	1.96	0.55
3:D:311:ASP:HA	3:D:314:LEU:HB3	1.88	0.55
3:D:235:ASN:ND2	3:D:322:ILE:O	2.39	0.55
3:D:246:ILE:HG21	3:D:340:ILE:HD13	1.94	0.55
1:A:277:LYS:NZ	1:A:331:LEU:O	2.86	0.55
2:B:279:VAL:HA	2:B:282:ILE:HG12	1.89	0.55
4:E:78:LEU:HB2	4:E:92:VAL:HG12	1.88	0.55
5:G:179:VAL:HG12	5:G:394:MET:HG3	1.87	0.55
7:Q:33:ILE:HG22	7:Q:112:LEU:HD13	1.88	0.55
8:Z:328:CYS:HA	8:Z:366:CYS:HB3	1.88	0.55
2:B:162:ILE:HD13	2:B:495:GLU:HA	2.65	0.55
2:B:285:HIS:NE2	2:B:339:GLU:O	2.39	0.55
3:D:385:THR:OG1	3:D:386:VAL:N	3.18	0.55
7:Q:423:ILE:HB	7:Q:442:ALA:HB2	1.88	0.55
1:A:135:ASN:ND2	1:A:422:TYR:OH	2.74	0.55
2:B:189:ARG:NH2	2:B:371:CYS:SG	2.79	0.55
4:E:365:GLY:H	4:E:370:LYS:HA	1.71	0.55
2:B:239:ILE:HG13	2:B:331:ILE:HD12	1.88	0.55
5:G:133:ILE:O	5:G:137:LYS:NZ	2.39	0.55
5:G:231:TYR:HA	5:G:349:LEU:HB3	1.96	0.55
8:Z:109:TYR:HB3	8:Z:114:LEU:HD12	1.88	0.55
8:Z:196:MET:HG3	8:Z:375:LEU:HD11	1.95	0.55
2:B:422:THR:O	2:B:426:ASN:ND2	2.44	0.55
3:D:503:ILE:O	3:D:507:LEU:N	2.39	0.55
8:Z:318:ARG:HA	8:Z:321:MET:HG2	1.89	0.55
8:Z:349:LEU:HD22	8:Z:365:LYS:HE3	2.67	0.55
4:E:179:ASN:HA	4:E:182:HIS:HB3	1.89	0.55
7:Q:171:LYS:NZ	9:Q:5000:ADP:O1B	2.38	0.55
1:A:225:MET:SD	1:A:353:GLN:NE2	6.79	0.55
3:D:89:ARG:NH1	3:D:93:GLU:OE2	3.37	0.55
4:E:498:THR:O	4:E:504:GLN:NE2	2.58	0.55
2:B:411:GLY:HA3	2:B:447:PRO:HB3	1.90	0.54
2:B:40:LYS:HG2	2:B:449:ILE:HG21	1.89	0.54
4:E:456:GLU:OE2	4:E:478:ARG:NH2	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:209:LYS:HA	3:D:385:THR:H	1.73	0.54
4:E:132:ARG:HH12	6:H:455:PHE:HD1	1.53	0.54
8:Z:153:ARG:HH21	8:Z:157:ARG:HH11	1.54	0.54
5:G:133:ILE:HG13	5:G:502:LEU:HD22	1.91	0.54
5:G:47:LYS:HD2	5:G:65:ILE:HD13	1.90	0.54
8:Z:258:LYS:HA	8:Z:261:LYS:HB3	2.30	0.54
2:B:150:SER:HB2	2:B:158:ASP:HB3	1.90	0.54
2:B:172:LEU:HD13	2:B:209:LEU:HG	5.68	0.54
3:D:141:LEU:HB2	3:D:523:THR:HG21	1.95	0.54
3:D:449:TYR:O	3:D:453:ALA:N	2.37	0.54
4:E:411:ASN:HD22	4:E:509:THR:HG21	1.73	0.54
5:G:408:PRO:HB3	5:G:489:MET:HB3	1.90	0.54
1:A:219:VAL:HG11	1:A:309:ARG:HE	2.29	0.54
2:B:88:SER:HG	2:B:103:THR:HG1	4.04	0.54
2:B:484:THR:OG1	2:B:485:ILE:N	2.68	0.54
3:D:245:LYS:HB2	3:D:295:CYS:HA	1.90	0.54
5:G:399:ASN:O	5:G:403:ASP:N	2.41	0.54
1:A:207:GLU:O	1:A:378:ARG:NH1	2.51	0.54
3:D:339:THR:HG23	3:D:383:GLY:H	3.91	0.54
1:A:433:ARG:HH22	3:D:472:ASN:H	1.90	0.54
6:H:62:GLY:HA2	6:H:65:ILE:HD12	3.71	0.54
5:G:114:GLN:HE21	7:Q:461:ASN:HD21	90.77	0.54
1:A:227:LYS:NZ	1:A:353:GLN:O	2.41	0.54
1:A:235:ALA:HA	1:A:345:LEU:HD22	1.93	0.54
4:E:140:ALA:HB2	4:E:448:MET:HG2	2.02	0.54
4:E:187:GLU:HA	4:E:190:VAL:HG12	1.89	0.53
8:Z:262:ALA:HA	8:Z:265:LYS:HD2	5.61	0.53
8:Z:96:VAL:HA	8:Z:99:ILE:HD12	2.59	0.53
4:E:254:PRO:HG2	4:E:256:GLU:HB3	1.90	0.53
4:E:62:VAL:HG22	4:E:68:VAL:HG22	1.90	0.53
8:Z:233:CYS:SG	8:Z:234:ASN:N	2.98	0.53
1:A:150:ASN:ND2	1:A:500:GLN:O	2.72	0.53
1:A:138:VAL:O	1:A:406:LYS:NZ	2.78	0.53
3:D:248:LEU:HD12	3:D:342:THR:HG23	6.34	0.53
4:E:292:ILE:HD12	4:E:295:THR:HB	6.45	0.53
4:E:37:HIS:O	4:E:40:ALA:HB3	2.08	0.53
7:Q:292:VAL:HA	7:Q:313:VAL:HB	1.91	0.53
8:Z:92:THR:HA	8:Z:95:ASN:HB2	2.34	0.53
5:G:22:GLN:NE2	5:G:518:ILE:O	2.41	0.53
6:H:158:CYS:O	6:H:161:THR:OG1	2.24	0.53
1:A:208:SER:HA	1:A:378:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD23	1:A:81:LEU:HD12	2.03	0.53
2:B:236:LYS:HB2	2:B:287:ILE:HG22	1.91	0.53
4:E:41:ALA:O	4:E:45:ALA:N	3.07	0.53
7:Q:46:ALA:HB2	7:Q:54:LYS:HE3	1.90	0.53
8:Z:421:ALA:O	8:Z:425:HIS:N	2.42	0.53
3:D:134:SER:HB2	3:D:527:ARG:HG3	1.90	0.53
4:E:198:ASP:OD1	4:E:198:ASP:N	2.42	0.53
7:Q:171:LYS:NZ	9:Q:5000:ADP:O2B	4.81	0.53
8:Z:303:ASP:HA	8:Z:306:SER:HB2	2.22	0.53
1:A:16:THR:HG22	1:A:18:ARG:H	1.74	0.53
2:B:518:ASP:N	2:B:518:ASP:OD1	2.41	0.53
6:H:194:MET:O	6:H:321:ARG:NH2	2.42	0.53
7:Q:386:ASP:HB2	7:Q:390:ARG:HH21	1.73	0.53
8:Z:230:ILE:HD11	8:Z:292:ILE:HG12	2.86	0.53
8:Z:217:ARG:HA	8:Z:359:LYS:HE2	5.14	0.53
1:A:312:LEU:O	1:A:316:LEU:N	2.40	0.53
2:B:95:VAL:HG21	2:B:499:VAL:HG23	2.64	0.53
4:E:179:ASN:O	4:E:182:HIS:ND1	2.42	0.53
5:G:238:VAL:HB	5:G:289:VAL:HG22	1.91	0.53
8:Z:190:MET:HB2	8:Z:371:SER:HA	2.04	0.53
1:A:272:LYS:O	1:A:276:GLN:N	2.75	0.53
3:D:450:CYS:O	3:D:454:PHE:N	2.52	0.53
4:E:251:LEU:HD11	4:E:300:ALA:HB1	1.91	0.53
5:G:51:ASP:N	5:G:51:ASP:OD1	2.40	0.53
7:Q:237:ALA:O	7:Q:346:HIS:ND1	2.42	0.53
7:Q:393:ASP:HA	7:Q:396:VAL:HG22	1.91	0.53
1:A:70:PRO:HA	1:A:73:LYS:HD2	2.01	0.52
3:D:459:GLU:OE2	3:D:481:ARG:NH2	2.52	0.52
5:G:184:PHE:HB2	5:G:192:ILE:HB	1.91	0.52
7:Q:281:LYS:HA	7:Q:284:ALA:HB3	1.91	0.52
1:A:174:ASP:N	1:A:174:ASP:OD1	2.40	0.52
1:A:432:SER:OG	1:A:433:ARG:N	2.83	0.52
2:B:284:LYS:NZ	2:B:339:GLU:O	2.42	0.52
6:H:48:LEU:HD11	6:H:56:ALA:HB1	2.51	0.52
1:A:200:ALA:HB3	1:A:378:ARG:HA	1.93	0.52
2:B:263:LYS:O	4:E:271:VAL:N	6.69	0.52
5:G:195:LYS:O	5:G:391:GLN:NE2	2.42	0.52
7:Q:42:THR:O	7:Q:54:LYS:NZ	2.38	0.52
1:A:468:ARG:O	1:A:472:ASN:ND2	2.43	0.52
2:B:449:ILE:HA	2:B:452:ASP:HB2	1.91	0.52
3:D:204:ASP:OD1	3:D:206:ARG:NH1	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:230:THR:HA	3:D:373:LEU:HG	1.90	0.52
4:E:362:ILE:O	4:E:370:LYS:NZ	2.37	0.52
4:E:364:PHE:HB2	4:E:371:MET:H	1.79	0.52
5:G:38:THR:O	5:G:453:ASN:ND2	2.42	0.52
6:H:299:ALA:HB1	6:H:302:TYR:HB3	1.91	0.52
7:Q:39:LEU:HD22	7:Q:83:ALA:HB1	1.91	0.52
2:B:318:ALA:O	2:B:322:ARG:NH1	3.36	0.52
3:D:157:LEU:HD23	3:D:159:ASP:H	1.74	0.52
4:E:156:LEU:HD13	4:E:416:ASN:HB3	1.90	0.52
4:E:247:LYS:HA	4:E:353:LEU:HD22	1.91	0.52
6:H:156:GLU:O	6:H:159:ALA:HB3	2.10	0.52
6:H:325:ALA:HA	6:H:366:LYS:HB2	1.92	0.52
7:Q:56:VAL:HB	7:Q:64:PHE:HB2	1.91	0.52
2:B:73:ASN:HB3	3:D:539:ARG:HE	1.93	0.52
3:D:117:LEU:HG	3:D:526:VAL:HG22	1.93	0.52
4:E:102:ILE:HD11	4:E:515:GLN:HB3	1.91	0.52
4:E:342:VAL:HG11	4:E:352:LYS:HB3	1.92	0.52
5:G:175:ALA:HB2	5:G:390:LEU:HD22	2.00	0.52
6:H:310:CYS:SG	6:H:311:ALA:N	2.83	0.52
8:Z:209:GLY:HA3	8:Z:364:GLU:HG3	3.60	0.52
2:B:269:HIS:HA	2:B:272:LYS:HD2	4.68	0.52
2:B:351:GLU:HA	2:B:360:ILE:HG23	1.90	0.52
2:B:215:ASP:HB3	2:B:372:THR:HB	1.92	0.52
2:B:513:VAL:HG22	2:B:516:ARG:HH21	1.74	0.52
4:E:341:ILE:HG12	4:E:343:PRO:HD3	2.14	0.52
4:E:483:LYS:HG3	4:E:484:GLU:HG3	1.91	0.52
5:G:515:LEU:HA	5:G:518:ILE:HD12	1.98	0.52
7:Q:225:LYS:HE3	7:Q:352:LEU:HD12	1.92	0.52
7:Q:290:VAL:HG12	7:Q:311:MET:HB3	1.92	0.52
8:Z:175:SER:HB2	8:Z:206:LEU:HD13	3.29	0.52
2:B:278:LYS:HA	2:B:281:ARG:HD3	1.92	0.52
2:B:341:VAL:HG13	2:B:342:LYS:HG3	5.50	0.52
2:B:479:ASP:HB2	2:B:488:MET:HE1	1.91	0.52
4:E:231:ASP:HA	4:E:371:MET:HG2	1.91	0.52
5:G:490:LYS:HA	5:G:495:TRP:HE1	1.78	0.52
5:G:49:LEU:HB3	5:G:57:VAL:HB	1.90	0.52
3:D:152:SER:OG	3:D:153:ARG:N	2.45	0.52
3:D:472:ASN:ND2	3:D:475:SER:OG	2.42	0.52
4:E:181:CYS:HB3	4:E:219:LEU:HD12	1.92	0.52
4:E:253:CYS:SG	4:E:284:LYS:NZ	2.83	0.52
4:E:86:GLN:HA	4:E:89:LYS:HB2	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:186:ILE:HG23	8:Z:189:PHE:HB2	3.43	0.52
8:Z:237:LEU:HD11	8:Z:270:ARG:HG2	3.60	0.52
1:A:137:ILE:HD11	1:A:485:TRP:HE1	6.52	0.51
1:A:148:LEU:HD11	1:A:399:VAL:HG13	2.32	0.51
1:A:322:ALA:HB2	1:A:371:THR:HB	1.92	0.51
1:A:350:GLU:OE2	1:A:366:ASN:ND2	5.38	0.51
7:Q:170:SER:HB2	9:Q:5000:ADP:H8	1.76	0.51
7:Q:291:VAL:HG23	7:Q:312:LEU:HA	1.92	0.51
8:Z:318:ARG:NH1	8:Z:321:MET:SD	2.82	0.51
3:D:388:ILE:HG21	3:D:405:ILE:HG13	1.95	0.51
4:E:195:THR:HG21	4:E:226:LYS:HE3	1.93	0.51
4:E:74:GLY:HA2	4:E:77:ILE:HD12	1.92	0.51
5:G:179:VAL:HG11	5:G:397:CYS:HB2	2.03	0.51
8:Z:463:LEU:O	8:Z:467:GLN:N	2.49	0.51
8:Z:60:GLY:HA2	8:Z:63:LEU:HB2	1.91	0.51
1:A:26:ALA:O	1:A:30:ASN:ND2	2.44	0.51
1:A:363:LEU:HD12	1:A:365:LYS:HD3	1.93	0.51
1:A:86:VAL:HG21	1:A:509:VAL:HG13	1.92	0.51
2:B:154:LYS:HB3	2:B:156:ARG:HH12	1.75	0.51
2:B:390:LEU:HG	2:B:394:LEU:HD13	1.97	0.51
5:G:224:THR:OG1	5:G:312:ARG:NH1	3.26	0.51
6:H:207:ASP:O	6:H:375:ARG:NE	2.43	0.51
1:A:347:GLN:HB3	1:A:368:LYS:HB2	2.01	0.51
3:D:253:LEU:HD22	3:D:283:ILE:HG12	5.76	0.51
8:Z:316:ALA:O	8:Z:318:ARG:NH2	2.38	0.51
7:Q:524:ILE:HG12	8:Z:48:VAL:HB	1.92	0.51
8:Z:224:ARG:HH12	8:Z:349:LEU:HD12	2.82	0.51
1:A:267:GLU:OE1	1:A:272:LYS:N	2.55	0.51
3:D:126:LYS:HB3	4:E:471:ILE:HD11	58.02	0.51
8:Z:153:ARG:HG2	8:Z:157:ARG:HE	1.76	0.51
1:A:183:ASP:OD1	1:A:187:GLN:N	2.42	0.51
1:A:291:GLY:HA2	1:A:309:ARG:HD2	2.11	0.51
4:E:303:GLN:HA	4:E:325:VAL:H	1.74	0.51
5:G:236:ARG:HA	5:G:345:GLY:H	2.08	0.51
1:A:237:LEU:HD11	1:A:275:ILE:HD13	3.10	0.51
4:E:38:ILE:HG23	4:E:117:LEU:HB3	1.92	0.51
7:Q:294:GLY:HA2	7:Q:316:ASN:H	1.76	0.51
3:D:176:VAL:HG12	3:D:179:TYR:HD2	1.80	0.51
3:D:339:THR:HG23	3:D:382:PRO:HA	2.41	0.51
5:G:333:ARG:O	5:G:337:LEU:N	2.43	0.51
5:G:35:ILE:HG22	5:G:36:ILE:HG23	2.06	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:202:LYS:HA	5:G:375:LEU:HB2	2.00	0.51
6:H:277:LYS:HE3	6:H:334:VAL:HA	1.92	0.51
1:A:166:ASP:OD1	1:A:166:ASP:N	2.93	0.51
2:B:394:LEU:HA	2:B:397:LEU:HB2	2.20	0.51
3:D:227:LEU:O	3:D:376:ILE:N	2.41	0.51
4:E:224:LEU:HD11	4:E:226:LYS:HE2	2.11	0.51
5:G:445:VAL:HG12	5:G:448:ARG:HE	1.87	0.51
6:H:16:SER:O	6:H:21:GLN:NE2	2.32	0.51
6:H:172:LYS:HA	6:H:175:PHE:HB2	1.93	0.51
6:H:462:ASN:OD1	6:H:465:ARG:NH2	2.41	0.51
4:E:249:ALA:HB3	4:E:300:ALA:HA	1.93	0.50
6:H:276:ASP:OD1	6:H:277:LYS:NZ	2.40	0.50
6:H:292:LYS:O	6:H:313:ARG:NH1	2.44	0.50
7:Q:356:GLY:O	7:Q:378:ARG:NH1	2.44	0.50
8:Z:118:ILE:HG13	8:Z:432:ARG:HE	2.87	0.50
8:Z:230:ILE:HD11	8:Z:292:ILE:HG23	1.93	0.50
5:G:47:LYS:HG2	8:Z:519:ASP:HB2	1.92	0.50
1:A:13:THR:OG1	1:A:14:GLY:N	4.37	0.50
1:A:275:ILE:O	1:A:279:LEU:CB	3.22	0.50
3:D:281:ALA:O	3:D:285:ASN:ND2	2.45	0.50
8:Z:31:GLN:HE22	8:Z:35:ARG:HH11	1.87	0.50
8:Z:98:ILE:HA	8:Z:446:ILE:HD11	6.13	0.50
1:A:209:MET:H	1:A:376:ILE:HG22	1.75	0.50
3:D:248:LEU:HD13	3:D:299:LEU:HG	1.94	0.50
3:D:423:ALA:HA	3:D:509:VAL:HG12	1.94	0.50
5:G:202:LYS:HG2	5:G:380:LYS:HD3	1.93	0.50
6:H:66:LEU:HD12	6:H:69:LEU:HD12	5.91	0.50
8:Z:465:LYS:HB3	8:Z:486:PRO:HG3	1.94	0.50
1:A:469:ALA:HA	1:A:472:ASN:HD22	1.75	0.50
2:B:189:ARG:HG2	2:B:190:LEU:HD23	1.92	0.50
1:A:472:ASN:ND2	6:H:425:ARG:O	135.62	0.50
8:Z:37:ASN:HD21	8:Z:45:LYS:HE2	1.76	0.50
1:A:411:GLY:O	1:A:498:ASN:ND2	2.44	0.50
1:A:54:ILE:HD13	5:G:514:LEU:HD11	1.93	0.50
4:E:222:THR:HG22	4:E:388:ARG:H	1.76	0.50
4:E:302:CYS:SG	4:E:303:GLN:N	3.12	0.50
4:E:254:PRO:HA	4:E:304:TRP:HB2	2.04	0.50
7:Q:338:PRO:HB3	8:Z:256:ARG:HE	1.76	0.50
8:Z:422:LEU:HA	8:Z:425:HIS:HB2	1.92	0.50
1:A:157:SER:O	1:A:159:LYS:NZ	3.07	0.50
3:D:220:ASP:HB3	3:D:391:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:36:ILE:HD13	5:G:66:LEU:HD21	2.26	0.50
7:Q:233:SER:OG	7:Q:233:SER:O	2.30	0.50
8:Z:284:ASP:N	8:Z:284:ASP:OD1	2.41	0.50
8:Z:353:TYR:N	8:Z:360:PHE:O	2.87	0.50
2:B:461:LEU:HA	2:B:464:GLN:HB3	2.67	0.50
3:D:307:ASP:N	3:D:307:ASP:OD1	2.44	0.50
5:G:25:ASN:HD21	5:G:521:ILE:HD11	1.76	0.50
6:H:379:GLU:OE1	6:H:380:GLN:NE2	2.44	0.50
8:Z:27:ALA:O	8:Z:31:GLN:HB2	2.48	0.50
8:Z:298:ASP:OD2	8:Z:301:SER:N	2.71	0.50
8:Z:298:ASP:O	8:Z:302:LEU:N	2.44	0.50
2:B:517:VAL:O	2:B:522:LYS:NZ	2.44	0.50
3:D:302:LYS:HZ2	3:D:326:LYS:HB3	2.50	0.50
4:E:233:ASP:N	4:E:233:ASP:OD1	2.50	0.50
5:G:140:SER:HB2	5:G:405:GLN:HB3	1.94	0.50
5:G:163:ALA:O	5:G:166:ARG:NH2	2.45	0.50
3:D:352:THR:HG22	3:D:355:MET:HG3	5.31	0.50
3:D:228:VAL:HG13	3:D:373:LEU:HD13	6.23	0.50
6:H:154:LEU:O	6:H:157:LYS:HB3	2.12	0.50
6:H:289:VAL:O	6:H:311:ALA:N	2.45	0.50
1:A:181:TYR:OH	1:A:371:THR:OG1	2.30	0.49
2:B:158:ASP:N	2:B:158:ASP:OD1	4.12	0.49
2:B:189:ARG:NH1	2:B:368:GLY:O	2.45	0.49
4:E:38:ILE:HG12	4:E:117:LEU:HB3	2.46	0.49
4:E:228:VAL:HG21	4:E:333:ILE:HA	1.94	0.49
4:E:42:LYS:O	4:E:46:ASN:N	2.43	0.49
5:G:215:ARG:HE	5:G:368:PRO:HB3	1.81	0.49
8:Z:191:ILE:HD13	8:Z:395:LEU:HD22	5.63	0.49
7:Q:524:ILE:HD13	8:Z:47:LEU:HA	2.59	0.49
4:E:453:ASP:O	4:E:456:GLU:HB2	2.11	0.49
2:B:237:ILE:HG23	2:B:329:GLY:HA3	3.15	0.49
2:B:92:ASP:O	2:B:388:ARG:NH2	2.45	0.49
3:D:230:THR:OG1	3:D:231:GLN:NE2	2.45	0.49
3:D:317:LEU:HB3	3:D:322:ILE:HG12	5.33	0.49
5:G:282:ILE:O	5:G:285:LYS:NZ	2.43	0.49
7:Q:420:ALA:HA	7:Q:442:ALA:HB1	1.95	0.49
8:Z:395:LEU:HA	8:Z:398:VAL:HG12	1.93	0.49
3:D:310:SER:O	3:D:314:LEU:N	2.42	0.49
4:E:58:ASP:OD1	4:E:58:ASP:N	2.46	0.49
8:Z:34:LEU:HD13	8:Z:93:THR:HG22	1.94	0.49
1:A:478:PRO:HA	1:A:481:LYS:HE2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:240:LEU:N	5:G:290:ILE:O	2.78	0.49
7:Q:220:GLY:HA2	7:Q:372:ILE:HG23	1.94	0.49
8:Z:105:GLN:NE2	8:Z:442:ASP:OD2	3.35	0.49
1:A:141:ASP:HB2	1:A:143:LEU:HG	1.94	0.49
2:B:215:ASP:OD1	2:B:216:GLU:N	2.46	0.49
2:B:242:THR:OG1	2:B:243:GLY:N	3.70	0.49
3:D:224:VAL:H	3:D:387:THR:HG21	2.29	0.49
3:D:462:PRO:O	3:D:466:ALA:N	2.44	0.49
4:E:335:ILE:HG21	4:E:382:ALA:HB3	1.94	0.49
8:Z:49:SER:OG	8:Z:68:GLN:NE2	6.98	0.49
1:A:125:CYS:HB3	1:A:518:THR:HG21	2.89	0.49
1:A:528:ASP:OD1	1:A:528:ASP:N	2.64	0.49
4:E:515:GLN:HG3	4:E:519:LEU:HD12	1.94	0.49
5:G:297:ASP:OD1	5:G:300:GLN:NE2	2.46	0.49
7:Q:340:VAL:H	7:Q:343:GLU:HB2	1.78	0.49
8:Z:255:GLU:HG2	8:Z:256:ARG:HG3	1.95	0.49
1:A:146:ASP:N	1:A:146:ASP:OD1	2.47	0.49
3:D:167:ALA:O	3:D:171:LEU:N	2.46	0.49
3:D:345:VAL:HG11	3:D:350:GLN:HB3	2.68	0.49
5:G:381:GLU:HG2	5:G:382:ILE:HG13	2.06	0.49
7:Q:522:ASP:OD2	8:Z:45:LYS:NZ	2.44	0.49
3:D:285:ASN:HB2	3:D:348:ILE:HD12	1.95	0.49
3:D:151:MET:HB3	3:D:489:LYS:HD2	1.94	0.49
3:D:50:THR:OG1	3:D:59:LYS:NZ	2.44	0.49
4:E:167:GLN:HA	4:E:170:LYS:HE2	5.29	0.49
6:H:200:VAL:HB	6:H:375:ARG:HA	1.95	0.49
6:H:280:LYS:HG3	6:H:335:ASN:HA	1.94	0.49
1:A:214:TYR:HB3	1:A:364:ILE:HG13	1.95	0.48
4:E:212:GLU:H	4:E:387:ILE:HD12	1.94	0.48
7:Q:185:GLN:HA	7:Q:188:VAL:HG12	1.95	0.48
5:G:48:MET:HB3	8:Z:521:ILE:HG13	1.94	0.48
1:A:118:ILE:HG23	1:A:522:ILE:HG12	1.96	0.48
1:A:200:ALA:N	1:A:377:LEU:O	2.45	0.48
3:D:140:ALA:HB2	3:D:451:VAL:HG22	1.96	0.48
3:D:197:PRO:HA	3:D:201:THR:HA	2.03	0.48
5:G:466:ARG:NH2	7:Q:436:TYR:OH	71.64	0.48
2:B:201:ILE:HD13	2:B:387:GLU:HA	1.96	0.48
3:D:361:LEU:HG	3:D:377:THR:HG22	1.96	0.48
5:G:245:GLU:OE1	5:G:274:ILE:N	2.46	0.48
5:G:238:VAL:HG22	5:G:342:VAL:HA	1.96	0.48
6:H:448:GLN:NE2	6:H:452:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:218:LEU:HD13	7:Q:222:VAL:HG11	1.95	0.48
7:Q:395:GLY:O	7:Q:398:THR:OG1	2.28	0.48
8:Z:77:ILE:HD11	8:Z:99:ILE:HD13	1.95	0.48
1:A:125:CYS:HB2	1:A:518:THR:HG21	1.95	0.48
2:B:281:ARG:NH2	2:B:336:ASP:O	3.38	0.48
3:D:189:ASN:HA	3:D:192:MET:HB2	2.58	0.48
3:D:50:THR:HG1	3:D:59:LYS:HZ1	3.01	0.48
1:A:232:ALA:HB3	1:A:348:ALA:HB3	2.73	0.48
2:B:181:LYS:HA	2:B:184:VAL:HG12	5.13	0.48
2:B:182:LEU:HA	2:B:185:GLU:HG2	1.95	0.48
2:B:171:LEU:HD22	2:B:382:ILE:HG13	1.96	0.48
1:A:463:LEU:HB3	1:A:488:LEU:HD21	1.94	0.48
3:D:138:GLN:OE1	3:D:527:ARG:NH1	2.46	0.48
3:D:203:VAL:HG23	3:D:416:VAL:HG11	1.98	0.48
3:D:49:ARG:HH11	3:D:464:THR:HG22	1.78	0.48
5:G:510:GLU:HA	5:G:513:VAL:HG22	1.94	0.48
1:A:83:ASP:OD1	1:A:90:THR:OG1	2.29	0.48
3:D:474:ILE:HD13	4:E:126:ARG:HD2	90.14	0.48
5:G:403:ASP:OD1	5:G:403:ASP:N	2.44	0.48
5:G:473:ASN:N	5:G:473:ASN:OD1	2.47	0.48
6:H:421:ARG:O	6:H:421:ARG:NH1	2.46	0.48
8:Z:47:LEU:HB2	8:Z:55:LYS:HB3	1.95	0.48
1:A:318:ARG:HA	1:A:321:LYS:HG2	2.21	0.48
1:A:352:VAL:HB	1:A:363:LEU:HG	3.03	0.48
1:A:529:ASP:N	1:A:529:ASP:OD1	2.45	0.48
2:B:398:ALA:HA	2:B:401:VAL:HG22	1.97	0.48
3:D:202:SER:HB3	3:D:416:VAL:HG13	3.98	0.48
4:E:292:ILE:HG13	4:E:297:ALA:H	4.10	0.48
5:G:296:SER:O	5:G:300:GLN:N	2.42	0.48
5:G:34:ASP:HA	5:G:37:ARG:HB2	1.97	0.48
7:Q:449:PRO:O	7:Q:453:ALA:N	2.47	0.48
8:Z:294:GLN:HG2	8:Z:318:ARG:NH1	2.29	0.48
8:Z:384:LEU:HA	8:Z:387:ILE:HG22	1.96	0.48
1:A:234:ILE:HG23	1:A:287:LEU:HD23	2.10	0.48
3:D:463:SER:O	3:D:467:GLU:N	2.54	0.48
5:G:325:ALA:HB2	5:G:370:ALA:HB3	1.98	0.48
6:H:169:SER:HA	6:H:172:LYS:HB3	1.96	0.48
8:Z:289:PHE:HB3	8:Z:310:ILE:HD12	3.75	0.48
8:Z:80:VAL:O	8:Z:83:ALA:HB3	2.13	0.48
1:A:133:ASN:HA	1:A:136:LEU:HD23	1.96	0.48
2:B:37:ASP:HA	2:B:40:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:290:ILE:HD13	3:D:317:LEU:HD21	1.96	0.48
3:D:233:VAL:HB	3:D:325:ILE:HG13	1.96	0.48
4:E:249:ALA:N	4:E:299:LEU:O	2.97	0.48
5:G:25:ASN:HB3	5:G:515:LEU:HD11	3.37	0.48
6:H:186:LEU:HB2	6:H:190:LEU:HD11	1.95	0.48
6:H:189:LEU:O	6:H:191:GLN:NE2	2.47	0.48
7:Q:221:MET:HB3	7:Q:363:PHE:HB2	1.96	0.48
7:Q:86:ILE:HD13	7:Q:514:ALA:HB1	1.96	0.48
8:Z:416:VAL:HG11	8:Z:466:ILE:HG22	2.02	0.48
1:A:33:LYS:HA	1:A:95:ILE:HD11	1.95	0.47
2:B:323:LEU:O	2:B:329:GLY:N	2.42	0.47
3:D:233:VAL:HG21	3:D:323:MET:HG2	1.95	0.47
4:E:200:GLU:HG3	4:E:201:ARG:HD2	6.03	0.47
2:B:267:ILE:HD11	4:E:272:GLU:HG2	9.49	0.47
5:G:207:ILE:HG23	5:G:209:GLU:H	1.78	0.47
5:G:37:ARG:NH1	5:G:449:THR:OG1	2.62	0.47
8:Z:346:HIS:HB3	8:Z:367:ASN:HB3	1.96	0.47
1:A:180:LYS:HE2	1:A:190:TYR:HB2	1.95	0.47
3:D:287:VAL:HG11	3:D:316:PHE:HB3	1.96	0.47
3:D:245:LYS:HD3	3:D:356:LEU:HG	3.89	0.47
5:G:248:LYS:HG2	5:G:276:GLN:HB2	1.95	0.47
7:Q:168:ILE:HG22	7:Q:391:ALA:HB1	1.96	0.47
8:Z:290:VAL:HG21	8:Z:350:VAL:HG11	3.98	0.47
1:A:328:LEU:HG	1:A:331:LEU:HD13	2.45	0.47
1:A:333:ASN:HD22	1:A:340:PHE:HD2	5.27	0.47
2:B:285:HIS:HB3	2:B:287:ILE:HG23	3.17	0.47
2:B:292:ASN:HD21	2:B:296:ILE:HB	6.58	0.47
3:D:204:ASP:HB3	3:D:206:ARG:HB2	2.11	0.47
8:Z:15:ARG:HH21	8:Z:520:GLU:HG2	8.24	0.47
8:Z:376:ILE:HD13	8:Z:387:ILE:HG23	1.95	0.47
1:A:179:ILE:HD13	1:A:194:SER:HB2	1.96	0.47
1:A:82:GLN:O	1:A:82:GLN:NE2	2.47	0.47
2:B:296:ILE:HG23	2:B:300:PRO:HG2	3.22	0.47
2:B:417:MET:HG3	2:B:504:LEU:HD11	1.97	0.47
8:Z:331:VAL:HB	8:Z:343:CYS:HA	2.11	0.47
8:Z:510:VAL:HA	8:Z:513:THR:HG22	1.95	0.47
1:A:35:SER:HB3	1:A:43:LYS:HZ3	1.79	0.47
2:B:108:GLU:OE1	2:B:111:ARG:NH1	2.67	0.47
2:B:232:ILE:HB	2:B:288:ASN:HB3	1.95	0.47
3:D:424:GLY:H	3:D:509:VAL:HA	1.83	0.47
4:E:418:VAL:HA	4:E:509:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:150:MET:HA	5:G:153:ASN:HB2	2.37	0.47
8:Z:278:LYS:HD3	8:Z:308:GLU:HG3	1.96	0.47
8:Z:305:LEU:HD12	8:Z:310:ILE:HB	2.75	0.47
1:A:222:SER:O	1:A:353:GLN:NE2	2.48	0.47
2:B:147:ASP:HA	2:B:405:ARG:HA	1.96	0.47
2:B:71:LEU:HA	2:B:74:ILE:HD12	2.62	0.47
7:Q:118:LEU:HD22	7:Q:123:LEU:HD12	1.96	0.47
8:Z:133:PHE:HE2	8:Z:417:ALA:HB1	1.78	0.47
3:D:296:ASN:O	3:D:323:MET:N	3.20	0.47
4:E:196:VAL:HG21	4:E:406:LEU:HD21	1.96	0.47
4:E:56:GLY:HA2	4:E:465:ASN:HB3	1.95	0.47
5:G:520:ASP:OD1	5:G:520:ASP:N	2.47	0.47
8:Z:229:TYR:HB3	8:Z:344:LEU:HD13	1.96	0.47
8:Z:301:SER:HA	8:Z:304:ALA:HB3	2.39	0.47
1:A:322:ALA:O	1:A:369:ALA:N	2.39	0.47
5:G:219:ILE:HG22	5:G:221:LYS:H	1.79	0.47
5:G:475:GLU:HB3	5:G:477:TRP:CD1	2.50	0.47
5:G:82:ILE:HD11	5:G:511:THR:HG23	1.96	0.47
1:A:423:LEU:HA	1:A:426:TYR:HB3	1.96	0.47
2:B:141:LEU:HD11	2:B:504:LEU:HD12	1.96	0.47
3:D:253:LEU:HD13	3:D:310:SER:H	1.80	0.47
4:E:158:ASP:HB2	4:E:416:ASN:HD21	2.02	0.47
4:E:183:ARG:HE	4:E:183:ARG:HB3	4.27	0.47
4:E:196:VAL:O	4:E:381:ARG:NH1	2.45	0.47
4:E:271:VAL:HB	4:E:274:TYR:HB3	2.31	0.47
4:E:37:HIS:HB3	4:E:87:ILE:HG13	1.96	0.47
6:H:346:GLN:HB2	6:H:363:GLY:HA3	1.97	0.47
7:Q:190:ILE:HD13	7:Q:219:HIS:HD2	1.80	0.47
7:Q:224:LYS:HA	7:Q:360:VAL:HA	1.97	0.47
1:A:277:LYS:NZ	1:A:341:GLU:OE1	3.48	0.47
2:B:357:ASP:OD1	2:B:376:ARG:NE	5.49	0.47
2:B:71:LEU:HD23	2:B:74:ILE:HD12	1.96	0.47
4:E:35:LYS:NZ	4:E:125:ASP:OD1	2.48	0.47
5:G:159:ILE:HD11	5:G:393:ALA:HB2	2.17	0.47
7:Q:450:ARG:HB2	7:Q:464:ILE:HD11	1.96	0.47
2:B:130:TRP:HE1	2:B:515:LEU:HD22	5.57	0.47
3:D:509:VAL:O	3:D:510:GLN:NE2	2.47	0.47
5:G:155:ILE:HA	5:G:159:ILE:HD13	1.96	0.47
7:Q:293:THR:HG22	7:Q:295:GLY:H	1.79	0.47
7:Q:58:ASN:HD21	7:Q:60:LEU:HG	1.80	0.47
1:A:438:ILE:O	1:A:441:PHE:HB3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:49:LEU:HD13	8:Z:522:MET:H	4.88	0.46
6:H:239:LEU:N	6:H:331:GLN:OE1	2.48	0.46
8:Z:47:LEU:HD11	8:Z:63:LEU:HD23	2.82	0.46
1:A:139:ASN:HD22	1:A:499:LYS:HE2	1.80	0.46
1:A:289:THR:HG23	1:A:311:VAL:HB	2.18	0.46
2:B:498:GLN:HE22	2:B:501:ARG:HH21	4.32	0.46
3:D:431:GLU:HG3	3:D:489:LYS:HG3	1.99	0.46
4:E:311:ASN:HA	4:E:314:LEU:HD12	1.97	0.46
5:G:217:VAL:HG11	5:G:322:ILE:HA	1.97	0.46
8:Z:146:GLU:HA	8:Z:149:ILE:HB	2.26	0.46
8:Z:492:VAL:HG13	8:Z:494:VAL:H	5.31	0.46
1:A:181:TYR:OH	1:A:321:LYS:NZ	2.43	0.46
4:E:200:GLU:HG3	4:E:201:ARG:HH21	6.52	0.46
4:E:344:ARG:HG3	4:E:346:SER:H	1.79	0.46
5:G:127:LYS:HE2	5:G:127:LYS:HB3	1.76	0.46
6:H:524:ARG:HD2	7:Q:59:HIS:HB3	1.98	0.46
1:A:218:CYS:SG	1:A:219:VAL:N	3.73	0.46
1:A:376:ILE:HA	1:A:376:ILE:HD12	1.88	0.46
2:B:113:ALA:HB2	2:B:130:TRP:HZ2	2.26	0.46
7:Q:223:PHE:H	7:Q:361:VAL:HG12	1.81	0.46
8:Z:176:ILE:HG21	8:Z:398:VAL:HG13	1.96	0.46
8:Z:84:GLN:NE2	8:Z:507:SER:OG	2.49	0.46
1:A:313:LYS:HA	1:A:316:LEU:HB3	2.13	0.46
3:D:328:ILE:HG13	3:D:333:ILE:HD11	1.96	0.46
4:E:232:LYS:HD2	4:E:325:VAL:HA	1.98	0.46
5:G:379:SER:OG	5:G:380:LYS:N	4.16	0.46
6:H:213:GLY:HA3	6:H:362:THR:HA	1.96	0.46
8:Z:176:ILE:HD11	8:Z:395:LEU:HB2	2.60	0.46
2:B:456:TYR:HE2	2:B:461:LEU:HD22	1.80	0.46
3:D:249:ILE:HB	3:D:298:LEU:HD21	1.97	0.46
4:E:174:GLY:HA2	4:E:179:ASN:HD21	1.81	0.46
4:E:207:GLU:HG2	4:E:208:LEU:HD12	2.09	0.46
4:E:284:LYS:O	4:E:288:MET:HB2	2.16	0.46
4:E:358:LEU:H	4:E:375:GLU:HB2	1.80	0.46
5:G:520:ASP:HB2	5:G:522:VAL:HG23	1.98	0.46
2:B:399:GLN:HB3	2:B:498:GLN:HB2	1.97	0.46
3:D:281:ALA:HA	3:D:284:LEU:HD12	6.60	0.46
6:H:51:ASP:OD1	6:H:55:LYS:N	3.00	0.46
6:H:86:GLN:HG3	6:H:97:VAL:HG11	1.98	0.46
8:Z:228:ALA:HB3	8:Z:347:ALA:HB3	1.97	0.46
8:Z:91:GLY:O	8:Z:95:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:SER:H	2:B:59:ALA:HB1	2.33	0.46
3:D:209:LYS:HB2	3:D:383:GLY:HA2	3.74	0.46
4:E:158:ASP:HB3	4:E:412:LEU:HD13	2.22	0.46
4:E:161:ASP:HB2	4:E:164:PRO:HB2	2.95	0.46
4:E:221:ASP:HB3	4:E:388:ARG:HB3	2.93	0.46
4:E:132:ARG:HD3	4:E:443:LEU:HD12	3.43	0.46
5:G:224:THR:HG23	5:G:312:ARG:HD2	2.11	0.46
5:G:480:ASN:HD21	5:G:482:GLU:HB2	1.81	0.46
8:Z:408:VAL:HG11	8:Z:501:LYS:HD2	2.05	0.46
1:A:46:VAL:HG22	1:A:52:VAL:HA	1.98	0.46
1:A:47:ASP:N	1:A:47:ASP:OD1	2.52	0.46
2:B:150:SER:HA	2:B:155:PHE:HB2	1.98	0.46
2:B:216:GLU:HG2	2:B:361:HIS:CE1	2.51	0.46
5:G:274:ILE:HG22	5:G:277:LEU:H	1.89	0.46
5:G:396:VAL:HG22	5:G:497:PRO:HG2	2.06	0.46
7:Q:230:ASP:HA	7:Q:311:MET:HB2	1.97	0.46
8:Z:34:LEU:HA	8:Z:37:ASN:HD22	1.80	0.46
1:A:221:GLY:HA3	1:A:306:MET:HG2	2.78	0.45
1:A:323:SER:HA	1:A:368:LYS:HB3	1.97	0.45
2:B:201:ILE:HD13	2:B:387:GLU:HG3	1.97	0.45
3:D:52:LEU:HD21	3:D:461:ILE:HG23	1.99	0.45
3:D:478:THR:HG21	4:E:443:LEU:HA	102.74	0.45
8:Z:82:THR:HA	8:Z:85:ASP:HB2	1.99	0.45
1:A:34:SER:O	1:A:34:SER:OG	2.31	0.45
2:B:50:LYS:HD2	2:B:70:ILE:HD13	2.26	0.45
3:D:237:GLY:H	3:D:321:LYS:HD2	1.81	0.45
4:E:288:MET:HA	4:E:292:ILE:HD13	5.93	0.45
5:G:148:SER:HA	5:G:151:MET:HB2	2.22	0.45
6:H:520:ILE:HD11	7:Q:56:VAL:HG22	1.98	0.45
7:Q:234:VAL:HG21	7:Q:289:ASN:HD22	1.81	0.45
7:Q:402:LEU:HD21	7:Q:408:LEU:HD21	1.99	0.45
1:A:205:GLN:HE21	1:A:385:CYS:HB3	1.80	0.45
2:B:404:SER:O	2:B:404:SER:OG	2.31	0.45
4:E:187:GLU:O	4:E:191:ASN:ND2	2.49	0.45
4:E:389:GLY:HA3	4:E:395:ILE:HD11	2.90	0.45
5:G:281:ILE:HG21	5:G:308:ILE:HD13	1.98	0.45
1:A:356:ILE:HB	1:A:361:LEU:HD12	1.99	0.45
3:D:302:LYS:NZ	3:D:327:ASP:OD2	3.72	0.45
3:D:244:ALA:HB3	3:D:359:ALA:HB3	1.97	0.45
4:E:340:ARG:HD3	4:E:340:ARG:HA	2.13	0.45
2:B:67:GLY:HA2	2:B:70:ILE:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:205:ASP:H	4:E:208:LEU:HD13	1.82	0.45
5:G:183:GLN:HB2	5:G:190:LYS:HB3	2.17	0.45
7:Q:380:SER:OG	7:Q:381:THR:N	2.50	0.45
1:A:480:ARG:HD3	1:A:483:LEU:HD22	3.18	0.45
2:B:320:VAL:HA	2:B:323:LEU:HB2	1.99	0.45
3:D:474:ILE:HG12	4:E:128:ILE:HD11	93.93	0.45
1:A:183:ASP:HB3	1:A:189:ARG:HD3	1.98	0.45
1:A:216:LEU:HB3	1:A:362:ILE:HB	4.08	0.45
2:B:282:ILE:HA	2:B:285:HIS:CD2	3.01	0.45
2:B:292:ASN:HB2	2:B:311:ALA:HB1	4.17	0.45
4:E:100:ASP:N	4:E:100:ASP:OD1	2.50	0.45
4:E:173:LEU:HD13	4:E:178:VAL:HG12	1.99	0.45
1:A:180:LYS:HZ1	1:A:403:LEU:HB3	1.82	0.45
2:B:151:ASP:OD2	2:B:404:SER:OG	3.75	0.45
2:B:186:ALA:HA	2:B:190:LEU:HB2	2.09	0.45
2:B:174:HIS:HB3	2:B:209:LEU:HB3	5.77	0.45
3:D:209:LYS:HG3	3:D:384:LYS:HB2	1.99	0.45
5:G:275:GLN:HA	5:G:278:CYS:HB3	2.17	0.45
6:H:163:LEU:HA	6:H:166:LYS:HZ2	1.81	0.45
1:A:165:GLY:HA2	1:A:168:PHE:HB3	2.18	0.45
1:A:175:ALA:HB1	1:A:195:VAL:HG21	1.99	0.45
1:A:435:GLN:OE1	6:H:465:ARG:NH2	119.75	0.45
2:B:148:HIS:ND1	2:B:158:ASP:OD2	2.50	0.45
2:B:200:HIS:HB3	2:B:372:THR:HA	1.98	0.45
3:D:405:ILE:HD13	3:D:405:ILE:HA	1.81	0.45
4:E:48:MET:O	4:E:51:SER:OG	2.33	0.45
5:G:450:LEU:HD22	5:G:479:VAL:HG13	1.97	0.45
6:H:172:LYS:HE3	6:H:172:LYS:HB3	1.71	0.45
6:H:444:ILE:HA	6:H:447:ARG:HB3	1.99	0.45
7:Q:198:ASN:HD21	7:Q:200:ASP:HB3	1.82	0.45
7:Q:170:SER:OG	9:Q:5000:ADP:O2A	4.72	0.45
8:Z:462:THR:HA	8:Z:465:LYS:HB2	1.98	0.45
1:A:169:ALA:HA	1:A:172:VAL:HG12	2.02	0.45
1:A:155:SER:HB3	1:A:398:VAL:HG21	2.55	0.45
1:A:45:LEU:HD12	5:G:523:SER:HB2	1.99	0.45
2:B:281:ARG:O	2:B:284:LYS:NZ	2.42	0.45
7:Q:276:MET:HG3	7:Q:304:TYR:HE2	1.82	0.45
8:Z:117:ARG:HD2	8:Z:517:LEU:HD22	1.98	0.45
8:Z:77:ILE:HA	8:Z:77:ILE:HD12	1.94	0.45
3:D:244:ALA:HA	3:D:296:ASN:HD21	1.82	0.44
4:E:245:ASP:N	4:E:245:ASP:OD1	4.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:301:ILE:HB	4:E:325:VAL:HG11	1.97	0.44
4:E:96:LYS:HA	4:E:96:LYS:HD2	1.70	0.44
5:G:140:SER:HA	5:G:407:VAL:HG22	1.99	0.44
5:G:383:LEU:HA	5:G:386:VAL:HB	2.18	0.44
7:Q:56:VAL:HG11	7:Q:75:GLU:HG3	1.99	0.44
8:Z:328:CYS:HA	8:Z:366:CYS:HB2	3.35	0.44
5:G:46:MET:N	8:Z:517:LEU:O	2.51	0.44
3:D:284:LEU:HD21	3:D:312:LEU:HG	1.99	0.44
4:E:317:ASN:HB3	4:E:319:LEU:HD13	5.36	0.44
5:G:153:ASN:HA	5:G:156:ASN:HD22	1.82	0.44
8:Z:186:ILE:HG13	8:Z:188:LEU:H	2.90	0.44
8:Z:189:PHE:HD1	8:Z:190:MET:HB3	5.88	0.44
2:B:354:ILE:HB	2:B:359:LEU:HD23	5.96	0.44
7:Q:188:VAL:HG23	7:Q:202:ILE:HG13	1.99	0.44
7:Q:326:LYS:HA	7:Q:326:LYS:HD3	1.81	0.44
8:Z:33:VAL:HG13	8:Z:45:LYS:HE3	2.00	0.44
1:A:385:CYS:HB2	1:A:388:MET:HB2	3.62	0.44
3:D:314:LEU:O	3:D:318:ASN:ND2	4.15	0.44
3:D:433:ALA:O	3:D:437:THR:OG1	2.30	0.44
4:E:490:GLY:O	4:E:499:ASN:ND2	2.50	0.44
5:G:32:ILE:HA	5:G:35:ILE:HD12	2.85	0.44
6:H:186:LEU:HD23	6:H:368:LYS:HA	1.99	0.44
8:Z:471:SER:OG	8:Z:475:GLN:NE2	2.46	0.44
3:D:338:LYS:O	3:D:381:SER:OG	2.62	0.44
4:E:188:ILE:HD11	4:E:223:LYS:HA	2.00	0.44
4:E:482:VAL:HG13	4:E:483:LYS:HD3	6.55	0.44
5:G:163:ALA:HB1	5:G:166:ARG:HH22	1.82	0.44
5:G:334:PRO:HA	5:G:337:LEU:HB2	1.98	0.44
5:G:51:ASP:OD1	5:G:55:GLY:N	3.00	0.44
1:A:459:ASP:OD1	1:A:459:ASP:N	4.14	0.44
4:E:292:ILE:HG23	4:E:297:ALA:H	1.83	0.44
1:A:152:ALA:O	1:A:155:SER:OG	2.48	0.44
1:A:85:GLU:HG3	1:A:516:PHE:HE2	1.82	0.44
2:B:264:VAL:HA	2:B:267:ILE:HG22	2.00	0.44
2:B:304:PHE:HB3	2:B:309:VAL:HB	2.71	0.44
5:G:469:HIS:HE1	5:G:476:THR:HA	1.89	0.44
6:H:230:LYS:HA	6:H:348:PHE:HD2	1.82	0.44
8:Z:181:LYS:HE3	8:Z:370:ARG:HH21	1.83	0.44
1:A:467:LEU:HD11	1:A:488:LEU:HG	3.24	0.44
2:B:223:LYS:N	2:B:228:GLN:OE1	4.19	0.44
3:D:100:ILE:O	3:D:413:ARG:NH2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:335:ILE:HG12	4:E:382:ALA:H	1.82	0.44
5:G:465:LEU:HD13	5:G:486:LEU:HD22	2.00	0.44
5:G:74:PRO:HG2	5:G:521:ILE:HG21	2.00	0.44
7:Q:221:MET:HB2	7:Q:372:ILE:HG12	1.99	0.44
7:Q:197:PHE:HD2	7:Q:400:LYS:HE3	1.83	0.44
8:Z:231:LEU:HB3	8:Z:291:VAL:HG12	4.93	0.44
1:A:227:LYS:HD3	1:A:227:LYS:HA	2.20	0.44
4:E:232:LYS:HG3	4:E:325:VAL:HG12	3.41	0.44
5:G:46:MET:HB3	5:G:58:MET:HG2	2.46	0.44
6:H:333:SER:H	6:H:336:ALA:HB2	1.82	0.44
7:Q:99:ASP:OD1	7:Q:99:ASP:N	2.51	0.44
8:Z:319:ARG:O	8:Z:323:ARG:NH1	2.48	0.44
8:Z:232:THR:HG1	8:Z:333:LEU:H	1.63	0.44
8:Z:426:LYS:HA	8:Z:426:LYS:HD3	1.85	0.44
8:Z:446:ILE:HA	8:Z:449:LYS:HB2	2.08	0.44
1:A:323:SER:HB3	1:A:346:GLY:HA3	2.00	0.43
3:D:185:PRO:HA	3:D:188:VAL:HB	1.99	0.43
8:Z:207:ILE:HB	8:Z:373:THR:HB	1.99	0.43
4:E:329:GLU:HB3	4:E:332:LEU:HD23	3.49	0.43
8:Z:374:LEU:HD23	8:Z:374:LEU:HA	1.98	0.43
4:E:235:SER:HB3	4:E:311:ASN:HD21	1.83	0.43
4:E:69:THR:OG1	4:E:70:VAL:N	2.52	0.43
5:G:202:LYS:NZ	5:G:383:LEU:HB2	2.35	0.43
5:G:129:LEU:HB2	5:G:509:VAL:HG11	2.05	0.43
1:A:212:SER:OG	1:A:212:SER:O	3.51	0.43
1:A:46:VAL:H	5:G:523:SER:HB3	3.32	0.43
2:B:187:VAL:HG13	2:B:188:LEU:HD12	9.10	0.43
2:B:319:GLY:HA2	2:B:322:ARG:HD2	2.01	0.43
2:B:49:ASP:OD1	2:B:49:ASP:N	2.53	0.43
3:D:209:LYS:O	3:D:387:THR:OG1	2.34	0.43
4:E:248:ILE:HG12	4:E:299:LEU:HD23	2.09	0.43
4:E:285:PHE:CE2	4:E:289:ILE:HD11	5.98	0.43
4:E:322:VAL:HG21	4:E:372:LEU:HD11	4.54	0.43
4:E:306:PHE:H	4:E:323:ARG:HE	1.67	0.43
5:G:199:ARG:HG2	5:G:217:VAL:HG23	2.71	0.43
5:G:408:PRO:O	5:G:413:SER:OG	4.32	0.43
5:G:129:LEU:HD11	5:G:506:LYS:HG2	2.13	0.43
6:H:176:ALA:HA	6:H:179:VAL:HG12	2.00	0.43
6:H:21:GLN:NE2	6:H:25:ASN:OD1	8.00	0.43
6:H:301:GLN:HA	6:H:304:ALA:HB3	2.01	0.43
6:H:487:ASN:HB3	6:H:492:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:183:LEU:HD13	3:D:405:ILE:HG12	2.04	0.43
3:D:373:LEU:HD13	3:D:391:ARG:HH22	1.83	0.43
4:E:193:VAL:HG11	4:E:409:ILE:HD12	2.00	0.43
4:E:29:MET:O	4:E:33:ALA:N	3.33	0.43
7:Q:170:SER:OG	9:Q:5000:ADP:O1A	2.34	0.43
8:Z:349:LEU:HD23	8:Z:364:GLU:HB2	2.00	0.43
1:A:357:CYS:HB2	1:A:378:ARG:HE	7.00	0.43
2:B:245:ASP:N	2:B:245:ASP:OD1	2.49	0.43
3:D:120:CYS:HA	3:D:123:LEU:HD12	2.01	0.43
3:D:34:ARG:HA	3:D:37:ASN:HD22	1.84	0.43
3:D:74:GLY:HA2	3:D:77:ILE:HD12	2.01	0.43
4:E:224:LEU:HA	4:E:385:ILE:HD11	1.99	0.43
6:H:316:GLU:HA	6:H:319:LEU:HD12	2.01	0.43
7:Q:193:ASP:N	7:Q:193:ASP:OD1	2.51	0.43
8:Z:206:LEU:HD11	8:Z:372:VAL:HB	2.81	0.43
1:A:146:ASP:HA	1:A:149:ILE:HG22	2.00	0.43
1:A:276:GLN:HA	1:A:279:LEU:HB3	2.31	0.43
2:B:224:ILE:HD13	2:B:301:GLU:HG2	2.01	0.43
3:D:246:ILE:HB	3:D:357:GLY:HA3	2.65	0.43
3:D:455:ALA:O	3:D:458:MET:HB2	2.26	0.43
4:E:210:LYS:HE3	4:E:385:ILE:HB	1.99	0.43
4:E:360:GLN:NE2	4:E:375:GLU:OE2	2.52	0.43
4:E:46:ASN:HB3	4:E:49:ARG:HH21	7.38	0.43
4:E:57:LEU:O	4:E:59:LYS:NZ	2.65	0.43
8:Z:469:GLU:HG3	8:Z:474:GLY:HA2	2.00	0.43
8:Z:74:ALA:HA	8:Z:77:ILE:HG22	2.26	0.43
1:A:277:LYS:HE3	1:A:277:LYS:HB3	2.09	0.43
1:A:347:GLN:NE2	1:A:349:GLU:OE1	3.03	0.43
2:B:166:THR:O	2:B:170:LYS:NZ	2.60	0.43
2:B:222:LYS:HE2	2:B:222:LYS:HB2	1.87	0.43
2:B:347:LYS:HD3	2:B:348:LEU:HB2	2.00	0.43
3:D:51:SER:OG	3:D:72:ASN:O	2.64	0.43
4:E:397:GLU:O	4:E:401:SER:OG	2.34	0.43
5:G:507:THR:HA	5:G:510:GLU:HG3	2.01	0.43
7:Q:340:VAL:HG13	8:Z:256:ARG:HH12	10.51	0.43
8:Z:273:LYS:HE3	8:Z:339:LEU:HB2	3.63	0.43
8:Z:316:ALA:O	8:Z:318:ARG:NH1	2.95	0.43
8:Z:450:VAL:HA	8:Z:453:GLN:HB3	2.01	0.43
1:A:233:LYS:NZ	1:A:342:ALA:O	2.41	0.43
2:B:175:HIS:CD2	2:B:212:SER:H	2.37	0.43
2:B:298:ASN:HB2	3:D:349:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:LYS:HA	2:B:46:LYS:HD3	1.84	0.43
4:E:193:VAL:HA	4:E:196:VAL:HG22	2.00	0.43
5:G:214:LEU:HB3	5:G:372:THR:HB	2.00	0.43
5:G:400:VAL:HA	5:G:404:PRO:HA	2.00	0.43
7:Q:142:ILE:HD13	7:Q:422:GLN:HB3	2.01	0.43
8:Z:271:VAL:HA	8:Z:274:ILE:HD12	2.01	0.43
1:A:238:ASP:HB2	1:A:329:SER:HA	2.01	0.43
1:A:530:LEU:HD21	3:D:60:MET:H	1.84	0.43
2:B:388:ARG:HA	2:B:388:ARG:HD2	1.94	0.43
3:D:250:GLN:HB2	3:D:346:ALA:HB2	2.01	0.43
5:G:30:LYS:HD3	5:G:106:SER:HB3	2.34	0.43
8:Z:469:GLU:OE2	8:Z:475:GLN:N	2.49	0.43
1:A:367:THR:OG1	1:A:369:ALA:O	3.54	0.42
1:A:482:ASN:OD1	1:A:482:ASN:N	2.52	0.42
1:A:458:GLN:HG3	1:A:493:GLY:HA3	2.00	0.42
4:E:154:SER:OG	4:E:418:VAL:N	2.99	0.42
4:E:46:ASN:HA	4:E:49:ARG:HB2	4.62	0.42
1:A:242:GLN:HB2	5:G:338:ARG:HD2	3.42	0.42
6:H:100:LEU:HD11	6:H:442:LEU:HD23	2.00	0.42
6:H:177:LYS:HE3	6:H:177:LYS:HB2	1.75	0.42
6:H:349:GLU:HB3	6:H:360:PHE:HB2	2.00	0.42
8:Z:129:LYS:HD2	8:Z:425:HIS:CG	2.54	0.42
8:Z:59:ASP:HB2	8:Z:159:LYS:HE2	2.01	0.42
8:Z:98:ILE:HD11	8:Z:447:ILE:HG12	2.01	0.42
1:A:386:ASP:N	1:A:386:ASP:OD1	4.06	0.42
1:A:529:ASP:OD2	3:D:50:THR:OG1	2.30	0.42
3:D:52:LEU:O	3:D:468:ASN:ND2	2.84	0.42
3:D:90:MET:HB2	3:D:529:ILE:HD11	2.45	0.42
4:E:161:ASP:O	4:E:165:LEU:N	2.89	0.42
4:E:200:GLU:O	4:E:202:ARG:NH2	3.03	0.42
4:E:245:ASP:HB2	4:E:247:LYS:H	4.08	0.42
5:G:230:ARG:HG2	5:G:351:ILE:HD11	2.14	0.42
6:H:153:LYS:O	6:H:156:GLU:HB2	2.19	0.42
7:Q:348:ASP:HB3	7:Q:365:HIS:HB2	2.01	0.42
8:Z:278:LYS:HE3	8:Z:308:GLU:HG3	4.10	0.42
8:Z:327:ALA:HB2	8:Z:371:SER:H	1.83	0.42
8:Z:458:ASP:HB3	8:Z:461:GLU:HB2	2.00	0.42
8:Z:480:ASP:OD2	8:Z:483:THR:OG1	2.30	0.42
1:A:274:ARG:NH1	1:A:330:THR:OG1	2.96	0.42
1:A:181:TYR:HH	1:A:371:THR:HG1	1.64	0.42
1:A:481:LYS:HD3	1:A:481:LYS:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:PRO:HA	2:B:126:ILE:HD12	2.24	0.42
2:B:235:ALA:HB1	2:B:289:CYS:HB2	3.41	0.42
5:G:278:CYS:HA	5:G:281:ILE:HD12	2.01	0.42
8:Z:442:ASP:N	8:Z:442:ASP:OD1	2.95	0.42
8:Z:77:ILE:HD11	8:Z:99:ILE:HG21	2.01	0.42
1:A:224:GLY:HA3	1:A:301:VAL:HG22	2.00	0.42
1:A:272:LYS:HE3	1:A:272:LYS:HB3	1.89	0.42
1:A:293:ASP:HB3	1:A:296:CYS:HB3	2.01	0.42
2:B:97:ASP:N	2:B:392:ASP:OD1	2.50	0.42
3:D:416:VAL:HA	3:D:419:ARG:HG2	2.65	0.42
4:E:426:GLU:HG3	4:E:455:LEU:HD22	2.00	0.42
4:E:531:ASP:N	4:E:531:ASP:OD1	2.48	0.42
5:G:312:ARG:HG3	5:G:313:ARG:HH11	2.23	0.42
7:Q:154:LEU:HA	7:Q:160:VAL:HG11	2.02	0.42
1:A:174:ASP:HA	1:A:177:LEU:HG	2.00	0.42
1:A:274:ARG:HE	1:A:274:ARG:HB3	1.63	0.42
2:B:375:LEU:HD12	2:B:376:ARG:H	1.84	0.42
4:E:479:ALA:HA	4:E:482:VAL:HG12	2.01	0.42
6:H:156:GLU:HG2	6:H:180:VAL:HG21	2.01	0.42
8:Z:276:GLU:O	8:Z:280:LYS:HB2	2.19	0.42
1:A:173:VAL:HA	1:A:176:VAL:HG12	2.12	0.42
1:A:18:ARG:HE	1:A:18:ARG:HB2	3.34	0.42
1:A:236:CYS:HA	1:A:287:LEU:HB2	2.35	0.42
1:A:243:LYS:HE3	1:A:243:LYS:HB3	1.85	0.42
3:D:208:ILE:O	3:D:387:THR:OG1	2.55	0.42
6:H:238:ALA:O	6:H:290:LEU:N	2.37	0.42
7:Q:198:ASN:ND2	7:Q:201:ASN:OD1	2.38	0.42
7:Q:340:VAL:HG23	7:Q:343:GLU:H	1.85	0.42
8:Z:149:ILE:HA	8:Z:173:VAL:HG11	4.01	0.42
8:Z:217:ARG:HH22	8:Z:314:ARG:H	1.67	0.42
8:Z:284:ASP:OD2	8:Z:284:ASP:N	4.06	0.42
8:Z:34:LEU:HD13	8:Z:96:VAL:HG11	3.40	0.42
4:E:498:THR:OG1	4:E:499:ASN:N	2.53	0.42
4:E:87:ILE:HG23	4:E:527:ILE:HD12	2.02	0.42
5:G:386:VAL:O	5:G:390:LEU:HB2	2.20	0.42
5:G:73:HIS:HA	5:G:74:PRO:HD3	1.92	0.42
6:H:69:LEU:HD23	6:H:69:LEU:HA	1.92	0.42
7:Q:80:HIS:HA	7:Q:81:PRO:HD3	1.93	0.42
3:D:58:ASP:N	3:D:58:ASP:OD1	2.53	0.42
5:G:117:HIS:CE1	5:G:119:THR:HG1	2.38	0.42
5:G:239:LEU:HB2	5:G:330:ILE:HB	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:33:ILE:HD12	7:Q:116:GLU:HB3	2.02	0.42
8:Z:277:LEU:HD22	8:Z:339:LEU:HB3	2.04	0.42
1:A:275:ILE:HA	1:A:278:ILE:HG22	2.65	0.42
1:A:412:GLY:HA2	1:A:490:LEU:HD21	2.02	0.42
1:A:78:LEU:HD13	1:A:520:ALA:HA	2.02	0.42
2:B:425:ALA:HB2	2:B:436:MET:HB2	2.01	0.42
4:E:147:HIS:HD2	4:E:429:CYS:HA	1.84	0.42
6:H:228:GLN:HG2	6:H:309:PHE:CG	2.54	0.42
7:Q:298:ALA:HB3	7:Q:301:ALA:HB3	2.02	0.42
7:Q:58:ASN:OD1	7:Q:62:LYS:N	2.48	0.42
1:A:18:ARG:HE	1:A:528:ASP:HB2	1.83	0.42
2:B:221:ASP:HB2	2:B:360:ILE:HD11	2.02	0.42
4:E:78:LEU:HA	4:E:81:MET:HG2	2.49	0.42
6:H:216:PHE:HB2	6:H:359:ASN:HB3	2.01	0.42
7:Q:387:ASP:HA	7:Q:390:ARG:HG2	2.02	0.42
7:Q:442:ALA:O	7:Q:445:PHE:HB2	2.20	0.42
8:Z:101:GLU:HB2	8:Z:446:ILE:HD13	2.76	0.42
8:Z:497:ASN:HD21	8:Z:500:VAL:HG23	1.85	0.42
8:Z:84:GLN:HE22	8:Z:503:GLN:HB3	3.43	0.42
1:A:222:SER:HB2	1:A:224:GLY:H	2.40	0.41
2:B:244:MET:HB3	2:B:303:LEU:HD23	2.00	0.41
3:D:238:ILE:HG13	3:D:240:ARG:H	2.32	0.41
3:D:314:LEU:O	3:D:318:ASN:N	2.53	0.41
4:E:204:VAL:HB	4:E:406:LEU:HD22	2.02	0.41
4:E:431:LEU:HD23	4:E:431:LEU:HA	1.93	0.41
4:E:536:PRO:HA	4:E:538:GLU:HG2	7.39	0.41
5:G:439:VAL:HA	5:G:442:ALA:HB3	2.02	0.41
8:Z:275:ILE:HA	8:Z:278:LYS:HB2	2.02	0.41
2:B:199:ILE:HG22	2:B:201:ILE:HD11	2.02	0.41
2:B:223:LYS:NZ	2:B:313:GLU:H	3.13	0.41
4:E:132:ARG:NH1	6:H:482:GLU:OE1	2.52	0.41
4:E:394:ILE:HA	4:E:397:GLU:HG3	2.02	0.41
4:E:419:VAL:HB	4:E:510:LEU:HD22	7.86	0.41
5:G:523:SER:OG	5:G:523:SER:O	2.50	0.41
6:H:322:THR:HG21	6:H:361:PHE:HD2	1.84	0.41
4:E:132:ARG:NH2	6:H:454:GLY:O	2.53	0.41
7:Q:293:THR:HB	7:Q:314:ARG:HD3	2.02	0.41
1:A:267:GLU:OE1	1:A:273:GLU:N	2.47	0.41
1:A:235:ALA:HB2	1:A:345:LEU:HD13	2.57	0.41
1:A:205:GLN:HE22	1:A:384:MET:HG2	1.84	0.41
2:B:35:ILE:HG23	2:B:71:LEU:HD22	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:287:VAL:HA	3:D:290:ILE:HD12	2.01	0.41
5:G:160:THR:HG22	5:G:161:THR:H	1.85	0.41
5:G:333:ARG:HA	5:G:334:PRO:HD3	1.94	0.41
5:G:353:LYS:HE3	5:G:358:TYR:HD1	2.31	0.41
7:Q:365:HIS:HA	7:Q:369:ASP:HA	2.03	0.41
8:Z:180:LYS:HE2	8:Z:402:ILE:HD13	2.02	0.41
1:A:233:LYS:HB3	1:A:345:LEU:HB2	2.02	0.41
1:A:483:LEU:HG	1:A:486:ILE:HG13	2.03	0.41
2:B:162:ILE:HA	2:B:165:THR:HG22	5.36	0.41
3:D:201:THR:HG23	3:D:419:ARG:HH22	1.85	0.41
3:D:449:TYR:O	3:D:452:ARG:HB3	2.20	0.41
3:D:496:ARG:HH11	3:D:508:VAL:HG22	2.41	0.41
4:E:248:ILE:HA	4:E:299:LEU:H	1.85	0.41
7:Q:476:LYS:HG3	7:Q:476:LYS:H	1.55	0.41
1:A:274:ARG:HB3	1:A:331:LEU:HD23	3.55	0.41
3:D:154:PRO:HA	3:D:420:ALA:HA	2.02	0.41
5:G:164:ILE:HG23	5:G:386:VAL:HG22	2.03	0.41
5:G:140:SER:HB2	5:G:405:GLN:HE21	1.85	0.41
7:Q:155:ARG:NH1	7:Q:192:PRO:O	2.53	0.41
7:Q:398:THR:HA	7:Q:401:VAL:HG12	2.02	0.41
2:B:120:LYS:HD2	2:B:120:LYS:HA	1.87	0.41
2:B:296:ILE:HA	2:B:296:ILE:HD13	1.94	0.41
2:B:33:ILE:HA	2:B:107:ALA:HB1	2.04	0.41
2:B:450:ILE:HG13	2:B:450:ILE:H	1.71	0.41
3:D:338:LYS:HB3	3:D:384:LYS:HZ2	1.85	0.41
3:D:339:THR:HG23	3:D:382:PRO:HB3	2.02	0.41
3:D:497:LYS:HA	3:D:497:LYS:HD3	1.92	0.41
4:E:84:ASP:OD1	4:E:84:ASP:N	2.42	0.41
5:G:144:ASP:OD1	5:G:144:ASP:N	2.54	0.41
5:G:275:GLN:NE2	5:G:302:TYR:HB3	2.46	0.41
5:G:449:THR:O	5:G:452:GLN:HB3	2.21	0.41
6:H:105:LEU:HA	6:H:108:VAL:HG12	2.02	0.41
6:H:145:LYS:HD3	6:H:145:LYS:HA	1.72	0.41
6:H:40:LEU:O	6:H:452:ASN:ND2	2.40	0.41
7:Q:280:VAL:HG21	7:Q:304:TYR:HB3	2.03	0.41
8:Z:350:VAL:HA	8:Z:362:PHE:O	2.21	0.41
1:A:420:SER:HA	1:A:442:ALA:HB1	2.92	0.41
2:B:515:LEU:HD12	2:B:515:LEU:HA	1.95	0.41
3:D:251:PHE:HD2	3:D:286:LEU:HD22	3.16	0.41
4:E:306:PHE:O	4:E:323:ARG:NE	2.52	0.41
4:E:480:ARG:HA	4:E:483:LYS:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:348:LEU:HB3	5:G:363:THR:HG23	2.26	0.41
5:G:214:LEU:O	5:G:372:THR:N	2.53	0.41
5:G:455:GLY:HA3	8:Z:118:ILE:HD11	2.02	0.41
8:Z:295:LYS:HA	8:Z:295:LYS:HD3	1.67	0.41
1:A:235:ALA:HB3	1:A:286:ILE:HA	2.10	0.41
2:B:327:THR:HA	2:B:365:VAL:HB	2.95	0.41
4:E:30:GLY:O	4:E:33:ALA:HB3	2.21	0.41
5:G:66:LEU:HD13	5:G:80:ILE:HG23	2.02	0.41
6:H:231:LYS:HA	6:H:231:LYS:HD2	1.92	0.41
6:H:431:GLN:HA	6:H:434:LEU:HD12	2.01	0.41
6:H:51:ASP:OD1	6:H:54:GLY:N	3.05	0.41
8:Z:98:ILE:O	8:Z:102:LEU:HB2	2.37	0.41
8:Z:211:VAL:HB	8:Z:373:THR:HG21	2.64	0.41
8:Z:432:ARG:HE	8:Z:432:ARG:HB2	1.69	0.41
3:D:309:LEU:HD11	3:D:317:LEU:HD12	2.08	0.41
5:G:393:ALA:HA	5:G:396:VAL:HB	2.02	0.41
6:H:199:LYS:HA	6:H:374:LEU:HB3	2.02	0.41
6:H:420:LEU:HA	6:H:423:TYR:HB2	2.03	0.41
8:Z:97:LEU:HD11	8:Z:447:ILE:HD13	2.03	0.41
1:A:279:LEU:HA	1:A:283:ALA:HB3	2.22	0.41
2:B:224:ILE:HB	2:B:228:GLN:HB2	2.40	0.41
3:D:284:LEU:O	3:D:288:LYS:HG2	2.30	0.41
3:D:394:ASN:HB2	3:D:397:VAL:HG22	2.02	0.41
3:D:408:ALA:HA	3:D:411:VAL:HG12	5.46	0.41
4:E:38:ILE:HG12	4:E:117:LEU:HD13	2.03	0.41
4:E:40:ALA:O	4:E:43:ALA:HB3	2.20	0.41
4:E:94:LEU:HD11	4:E:523:MET:HE3	2.02	0.41
5:G:283:GLN:HE22	5:G:337:LEU:HB3	6.73	0.41
5:G:390:LEU:HA	5:G:393:ALA:HB3	2.03	0.41
7:Q:157:ILE:HG12	7:Q:185:GLN:HE22	1.86	0.41
7:Q:342:GLU:OE1	8:Z:239:TYR:OH	2.47	0.41
8:Z:160:VAL:HB	8:Z:164:LEU:HD23	2.03	0.41
1:A:485:TRP:HD1	1:A:498:ASN:H	1.68	0.41
3:D:238:ILE:H	3:D:321:LYS:HD2	4.62	0.41
6:H:349:GLU:OE2	6:H:351:THR:OG1	2.31	0.41
8:Z:230:ILE:HA	8:Z:290:VAL:HG23	2.02	0.41
8:Z:305:LEU:O	8:Z:309:GLY:N	3.23	0.41
8:Z:327:ALA:HB2	8:Z:371:SER:HB2	2.03	0.41
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.92	0.40
1:A:191:PRO:HG2	1:A:194:SER:HB3	2.02	0.40
1:A:473:GLU:HG3	1:A:483:LEU:HD23	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:OE1	5:G:523:SER:OG	2.41	0.40
2:B:287:ILE:HD11	2:B:309:VAL:HG13	2.04	0.40
2:B:451:ALA:HB2	2:B:478:LEU:HD21	3.08	0.40
4:E:314:LEU:O	4:E:318:ASN:N	2.59	0.40
4:E:356:ALA:HB1	4:E:376:GLN:H	1.86	0.40
5:G:215:ARG:HA	5:G:371:CYS:HB3	2.03	0.40
1:A:198:LEU:H	1:A:377:LEU:HD13	1.86	0.40
2:B:192:GLY:H	2:B:195:ASN:HB2	1.85	0.40
2:B:84:LEU:HD12	2:B:84:LEU:HA	3.16	0.40
3:D:175:VAL:HG12	3:D:400:GLU:HG2	4.78	0.40
3:D:207:ASP:H	3:D:386:VAL:HG22	2.77	0.40
2:B:226:VAL:HG21	3:D:354:ASP:HB2	5.11	0.40
3:D:421:LEU:HD21	3:D:509:VAL:HB	2.03	0.40
4:E:301:ILE:HG22	4:E:322:VAL:H	2.97	0.40
4:E:402:LEU:HA	4:E:402:LEU:HD23	1.90	0.40
7:Q:359:GLN:HG3	7:Q:359:GLN:H	1.75	0.40
7:Q:522:ASP:N	7:Q:522:ASP:OD1	2.54	0.40
8:Z:144:ASP:HB3	8:Z:147:THR:HG23	3.59	0.40
1:A:78:LEU:O	1:A:81:LEU:HB2	2.83	0.40
2:B:191:LYS:HA	2:B:195:ASN:H	2.34	0.40
3:D:210:ILE:N	3:D:385:THR:O	2.54	0.40
4:E:403:HIS:HA	4:E:406:LEU:HB2	2.03	0.40
5:G:234:ASN:HA	5:G:347:GLY:HA2	2.03	0.40
6:H:47:LYS:HA	6:H:47:LYS:HD3	3.82	0.40
7:Q:208:LEU:O	7:Q:378:ARG:NH2	2.43	0.40
7:Q:212:ILE:H	7:Q:212:ILE:HG13	1.72	0.40
8:Z:303:ASP:N	8:Z:303:ASP:OD1	3.01	0.40
1:A:488:LEU:HA	1:A:488:LEU:HD23	1.91	0.40
2:B:122:HIS:O	2:B:125:THR:OG1	2.35	0.40
2:B:282:ILE:HD12	2:B:309:VAL:HG21	3.27	0.40
3:D:289:GLN:HA	3:D:292:LYS:HD3	2.03	0.40
8:Z:299:PRO:HA	8:Z:302:LEU:HB2	2.03	0.40
8:Z:75:SER:O	8:Z:78:ALA:HB3	2.21	0.40
2:B:467:ALA:O	2:B:470:SER:OG	2.46	0.40
3:D:418:LYS:HA	3:D:418:LYS:HD2	1.97	0.40
4:E:306:PHE:O	4:E:323:ARG:NH2	3.50	0.40
4:E:210:LYS:HD2	4:E:384:THR:HA	2.03	0.40
5:G:198:ALA:O	5:G:321:ARG:NH2	2.55	0.40
6:H:294:PRO:HG3	6:H:313:ARG:HE	1.86	0.40
7:Q:246:PHE:HE1	7:Q:336:LEU:HD21	1.87	0.40
8:Z:20:LEU:O	8:Z:24:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:408:VAL:HG22	8:Z:414:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	488/556 (88%)	453 (93%)	35 (7%)	0	100	100
1	a	484/556 (87%)	450 (93%)	34 (7%)	0	100	100
2	B	488/535 (91%)	447 (92%)	41 (8%)	0	100	100
2	b	474/535 (89%)	432 (91%)	42 (9%)	0	100	100
3	D	483/539 (90%)	440 (91%)	43 (9%)	0	100	100
3	d	485/539 (90%)	452 (93%)	33 (7%)	0	100	100
4	E	499/541 (92%)	448 (90%)	51 (10%)	0	100	100
4	e	501/541 (93%)	448 (89%)	53 (11%)	0	100	100
5	G	481/544 (88%)	443 (92%)	38 (8%)	0	100	100
5	g	473/544 (87%)	438 (93%)	35 (7%)	0	100	100
6	H	495/543 (91%)	453 (92%)	42 (8%)	0	100	100
6	h	496/543 (91%)	452 (91%)	44 (9%)	0	100	100
7	Q	479/548 (87%)	441 (92%)	38 (8%)	0	100	100
7	q	479/548 (87%)	441 (92%)	38 (8%)	0	100	100
8	Z	493/531 (93%)	453 (92%)	39 (8%)	1 (0%)	49	83
8	z	504/531 (95%)	471 (94%)	33 (6%)	0	100	100
All	All	7802/8674 (90%)	7162 (92%)	639 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Z	430	LYS

### 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 PDB entries followed by that with respect to all EM entries.

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	409/463 (88%)	407 (100%)	2 (0%)	90	95
1	a	405/463 (88%)	404 (100%)	1 (0%)	94	97
2	B	391/427 (92%)	390 (100%)	1 (0%)	93	96
2	b	380/427 (89%)	379 (100%)	1 (0%)	93	96
3	D	413/452 (91%)	412 (100%)	1 (0%)	94	97
3	d	415/452 (92%)	413 (100%)	2 (0%)	90	95
4	E	422/456 (92%)	421 (100%)	1 (0%)	94	97
4	e	424/456 (93%)	424 (100%)	0	100	100
5	G	416/468 (89%)	415 (100%)	1 (0%)	94	97
5	g	409/468 (87%)	408 (100%)	1 (0%)	94	97
6	H	408/443 (92%)	406 (100%)	2 (0%)	90	95
6	h	409/443 (92%)	407 (100%)	2 (0%)	90	95
7	Q	402/452 (89%)	384 (96%)	18 (4%)	30	62
7	q	402/452 (89%)	384 (96%)	18 (4%)	30	62
8	Z	416/442 (94%)	414 (100%)	2 (0%)	90	95
8	z	425/442 (96%)	424 (100%)	1 (0%)	94	97
All	All	6546/7206 (91%)	6492 (99%)	54 (1%)	84	92

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	309	ARG
2	b	284	LYS
3	d	55	LYS
3	d	240	ARG

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Mol	Chain	Res	Type
5	g	315	ARG
6	h	53	ARG
6	h	507	LEU
7	q	126	SER
7	q	152	LYS
7	q	187	CYS
7	q	213	SER
7	q	215	SER
7	q	233	SER
7	q	235	LYS
7	q	285	ASP
7	q	296	LYS
7	q	318	LYS
7	q	353	SER
7	q	358	THR
7	q	382	ASP
7	q	386	ASP
7	q	393	ASP
7	q	456	SER
7	q	465	SER
7	q	499	ASP
8	z	381	LYS
1	A	309	ARG
1	A	400	LYS
2	B	520	ILE
3	D	55	LYS
4	E	183	ARG
5	G	315	ARG
6	H	344	ARG
6	H	503	LEU
7	Q	126	SER
7	Q	152	LYS
7	Q	187	CYS
7	Q	213	SER
7	Q	215	SER
7	Q	233	SER
7	Q	235	LYS
7	Q	285	ASP
7	Q	296	LYS
7	Q	318	LYS
7	Q	353	SER
7	Q	358	THR

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Mol	Chain	Res	Type
7	Q	382	ASP
7	Q	386	ASP
7	Q	393	ASP
7	Q	456	SER
7	Q	465	SER
7	Q	499	ASP
8	Z	217	ARG
8	Z	395	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	135	ASN
1	a	164	ASN
1	a	353	GLN
1	a	472	ASN
2	b	174	HIS
2	b	175	HIS
2	b	285	HIS
2	b	292	ASN
2	b	298	ASN
2	b	426	ASN
2	b	453	ASN
2	b	473	ASN
3	d	172	ASN
3	d	231	GLN
3	d	318	ASN
3	d	472	ASN
4	e	290	GLN
4	e	495	HIS
5	g	25	ASN
5	g	275	GLN
5	g	300	GLN
5	g	405	GLN
5	g	433	GLN
5	g	480	ASN
5	g	503	GLN
6	h	30	GLN
6	h	245	ASN
6	h	335	GLN
6	h	384	GLN
6	h	505	ASN

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Mol	Chain	Res	Type
7	q	41	GLN
7	q	145	ASN
7	q	219	HIS
7	q	274	ASN
7	q	306	ASN
7	q	383	ASN
7	q	461	ASN
8	z	68	GLN
8	z	84	GLN
8	z	105	GLN
8	z	346	HIS
8	z	460	GLN
1	A	30	ASN
1	A	135	ASN
1	A	139	ASN
1	A	150	ASN
1	A	193	ASN
1	A	196	ASN
1	A	242	GLN
1	A	276	GLN
1	A	472	ASN
2	B	78	ASN
3	D	37	ASN
3	D	85	HIS
3	D	172	ASN
3	D	231	GLN
3	D	318	ASN
3	D	472	ASN
4	E	37	HIS
4	E	86	GLN
4	E	98	GLN
4	E	191	ASN
4	E	311	ASN
4	E	312	HIS
4	E	316	GLN
4	E	411	ASN
4	E	481	GLN
5	G	25	ASN
5	G	156	ASN
5	G	405	GLN
5	G	480	ASN
6	H	25	ASN

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Mol	Chain	Res	Type
6	H	119	GLN
6	H	134	ASN
6	H	241	ASN
7	Q	41	GLN
7	Q	145	ASN
7	Q	219	HIS
7	Q	274	ASN
7	Q	306	ASN
7	Q	383	ASN
8	Z	37	ASN
8	Z	65	HIS
8	Z	84	GLN
8	Z	497	ASN
8	Z	514	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ADP	Q	5000	-	24,29,29	0.93	1 (4%)	25,45,45	1.65	4 (16%)
9	ADP	q	5000	-	24,29,29	0.94	1 (4%)	25,45,45	1.65	4 (16%)

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
9	ADP	Q	5000	-	-	2/12/32/32	0/3/3/3
9	ADP	q	5000	-	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	5000	ADP	C5-C4	2.82	1.46	1.40
9	q	5000	ADP	C5-C4	2.80	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	5000	ADP	PA-O3A-PB	-4.31	118.87	132.57
9	q	5000	ADP	PA-O3A-PB	-4.30	118.90	132.57
9	Q	5000	ADP	N3-C2-N1	-3.34	123.29	128.68
9	q	5000	ADP	N3-C2-N1	-3.30	123.36	128.68
9	q	5000	ADP	C4'-O4'-C1'	-2.83	106.88	109.83
9	Q	5000	ADP	C4'-O4'-C1'	-2.79	106.92	109.83
9	q	5000	ADP	C4-C5-N7	-2.63	106.65	109.40
9	Q	5000	ADP	C4-C5-N7	-2.61	106.67	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

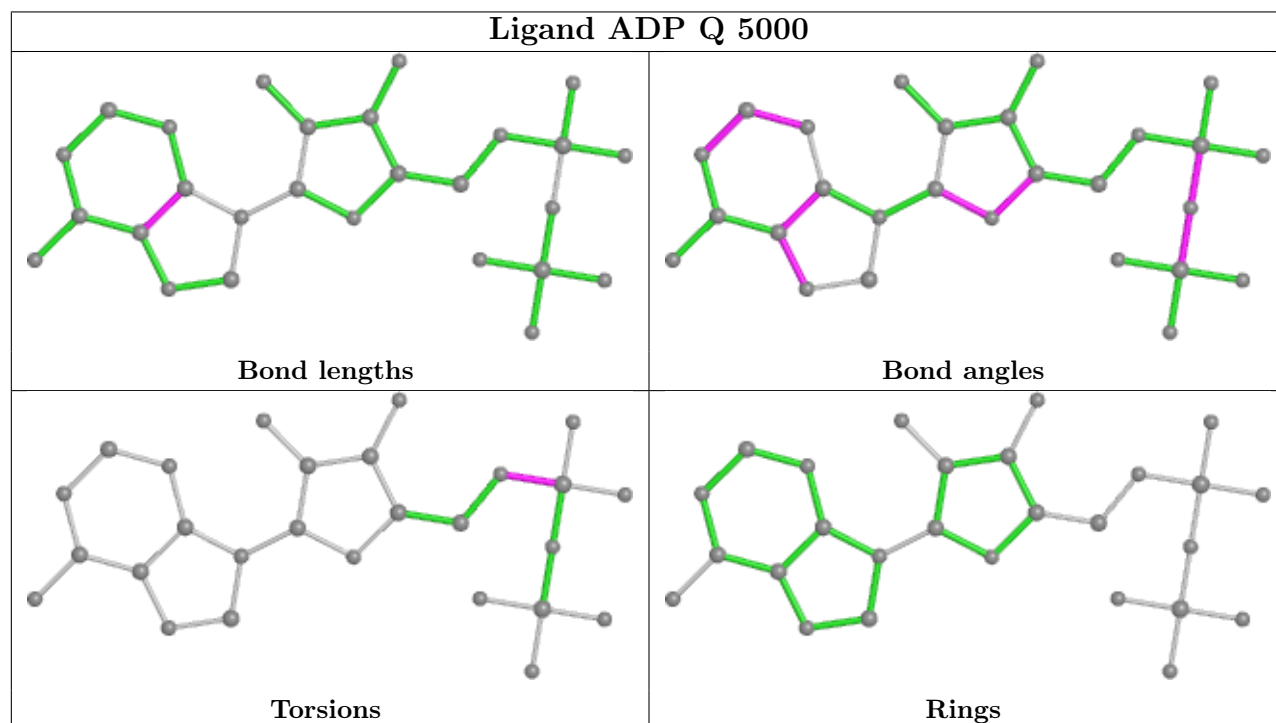
Mol	Chain	Res	Type	Atoms
9	q	5000	ADP	C5'-O5'-PA-O2A
9	q	5000	ADP	C5'-O5'-PA-O3A
9	Q	5000	ADP	C5'-O5'-PA-O3A
9	Q	5000	ADP	C5'-O5'-PA-O1A

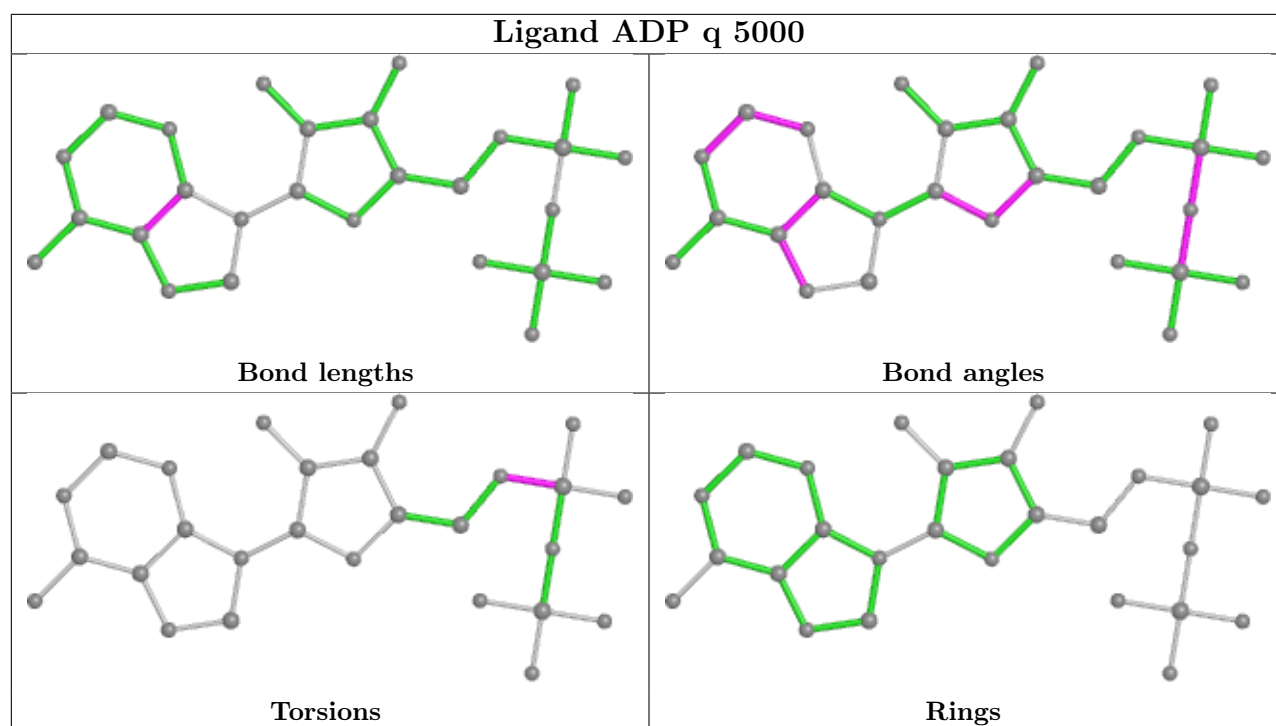
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	5000	ADP	5	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.