



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

Jan 16, 2017 – 03:00 PM EST

PDB ID : 5H3O  
EMDB ID: : EMD-6656  
Title : Structure of a eukaryotic cyclic nucleotide-gated channel  
Authors : Li, M.; Zhou, X.; Wang, S.; Michailidis, I.; Gong, Y.; Su, D.; Li, H.; Li, X.;  
Yang, J.  
Deposited on : 2016-10-26  
Resolution : 3.50 Å(reported)

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  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

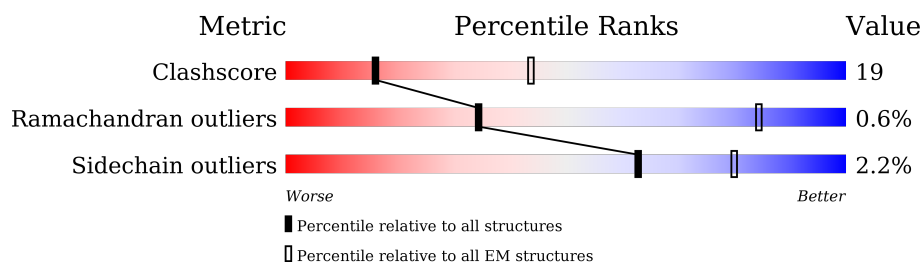
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	738	42% 26% 31%
1	B	738	42% 26% 31%
1	C	738	41% 27% 31%
1	D	738	42% 27% 31%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16958 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 Cyclic nucleotide-gated cation channel.

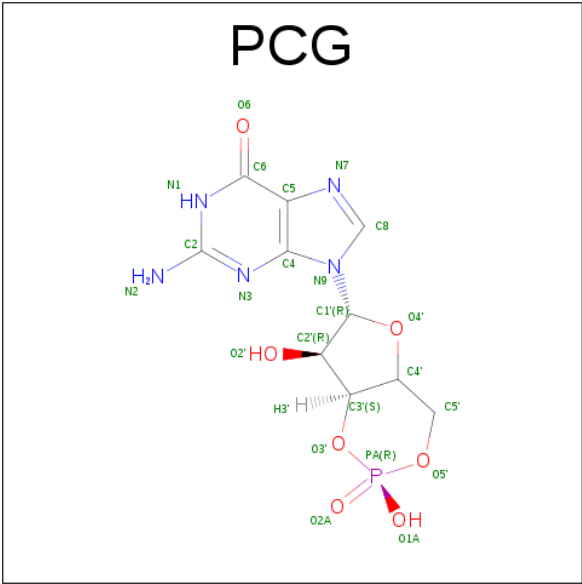
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	510	Total	C	N	O	S	0	0
			4215	2742	708	741	24		
1	B	510	Total	C	N	O	S	0	0
			4216	2742	708	742	24		
1	C	510	Total	C	N	O	S	0	0
			4216	2742	708	742	24		
1	D	510	Total	C	N	O	S	0	0
			4216	2742	708	742	24		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q03611
A	-3	GLY	-	expression tag	UNP Q03611
A	-2	GLY	-	expression tag	UNP Q03611
A	-1	GLY	-	expression tag	UNP Q03611
A	0	SER	-	expression tag	UNP Q03611
B	-4	GLY	-	expression tag	UNP Q03611
B	-3	GLY	-	expression tag	UNP Q03611
B	-2	GLY	-	expression tag	UNP Q03611
B	-1	GLY	-	expression tag	UNP Q03611
B	0	SER	-	expression tag	UNP Q03611
C	-4	GLY	-	expression tag	UNP Q03611
C	-3	GLY	-	expression tag	UNP Q03611
C	-2	GLY	-	expression tag	UNP Q03611
C	-1	GLY	-	expression tag	UNP Q03611
C	0	SER	-	expression tag	UNP Q03611
D	-4	GLY	-	expression tag	UNP Q03611
D	-3	GLY	-	expression tag	UNP Q03611
D	-2	GLY	-	expression tag	UNP Q03611
D	-1	GLY	-	expression tag	UNP Q03611
D	0	SER	-	expression tag	UNP Q03611

- Molecule 2 is CYCLIC GUANOSINE MONOPHOSPHATE (three-letter code: PCG) (for-

mula: C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>7</sub>P).



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

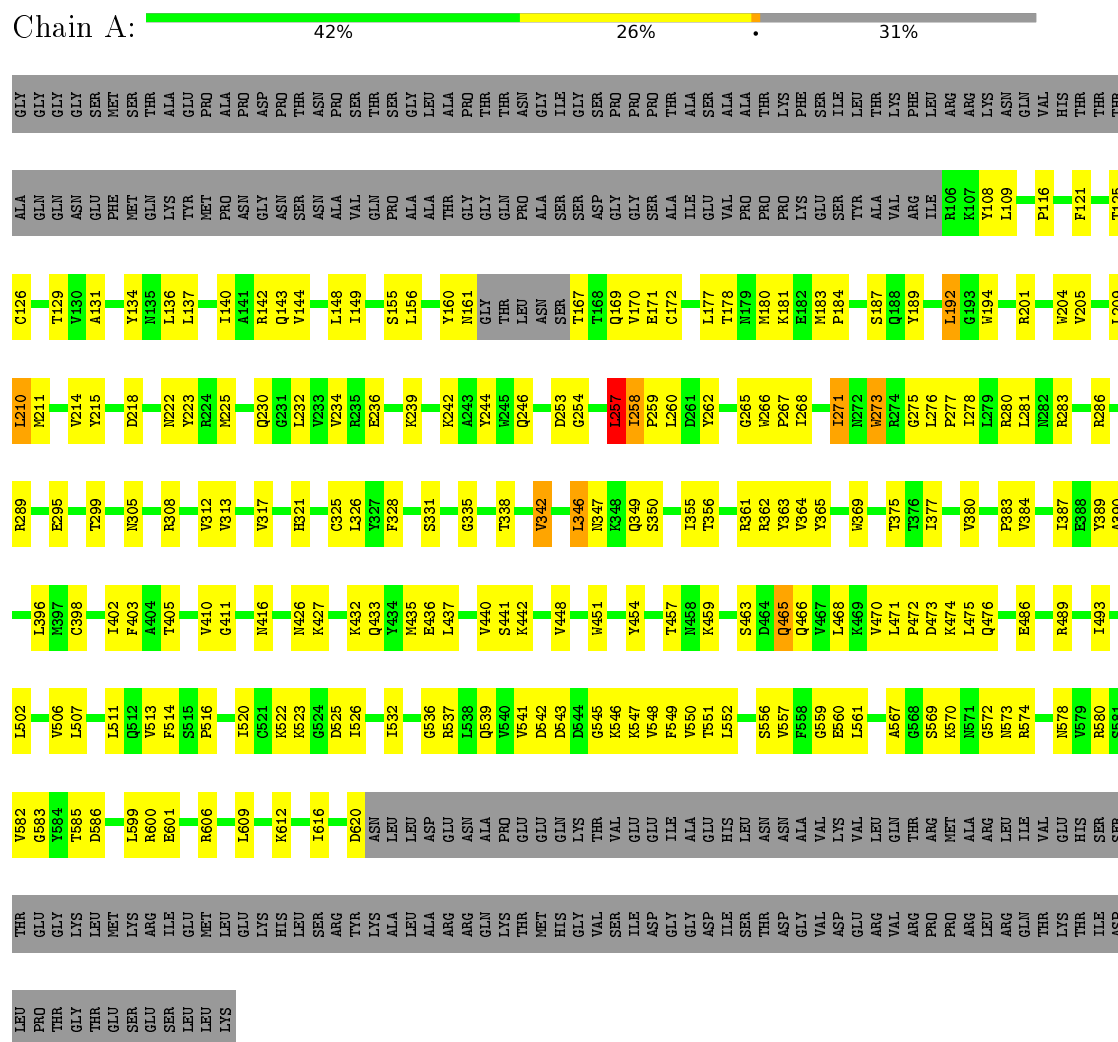
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Na	0
			1	1	
3	A	2	Total	Na	0
			2	2	

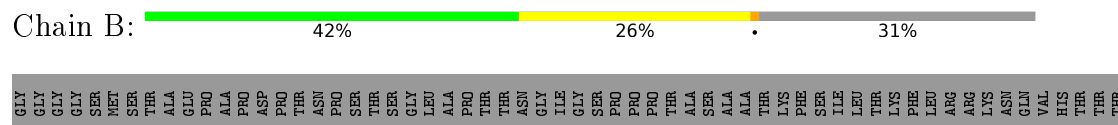
### 3 Residue-property plots

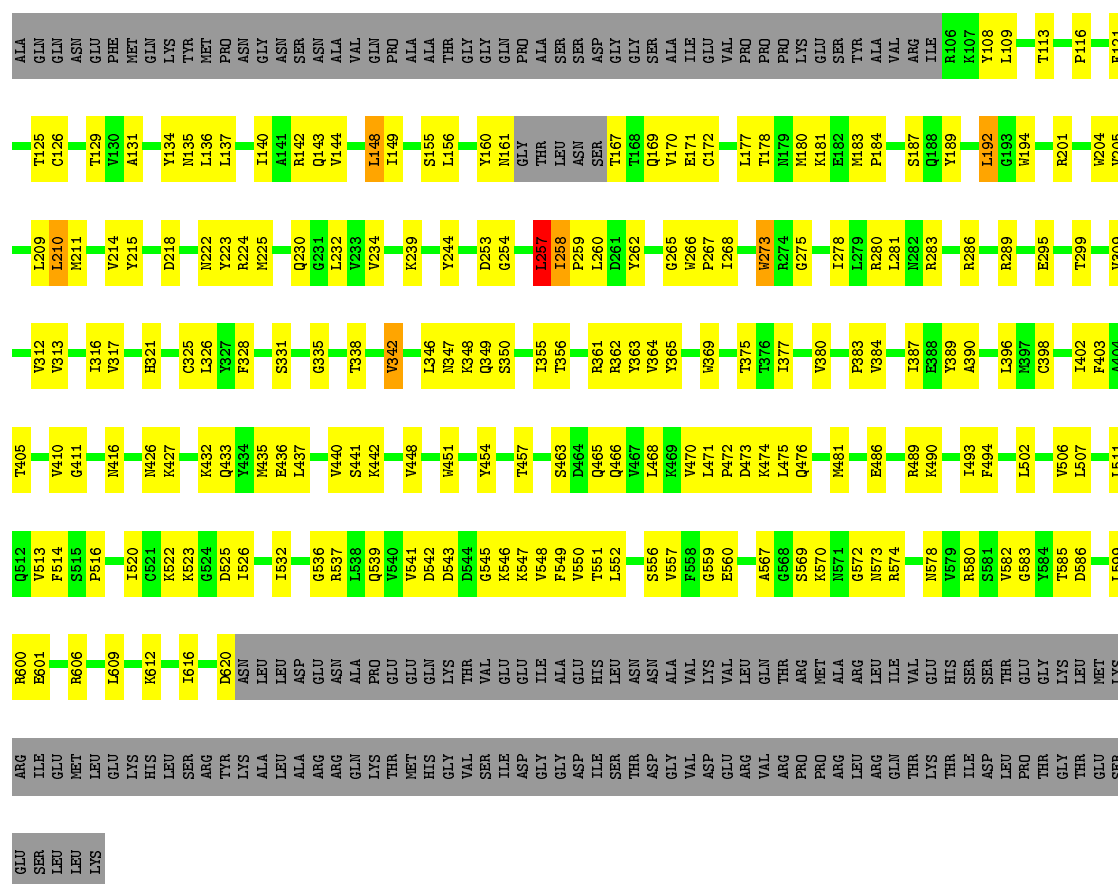
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Cyclic nucleotide-gated cation channel



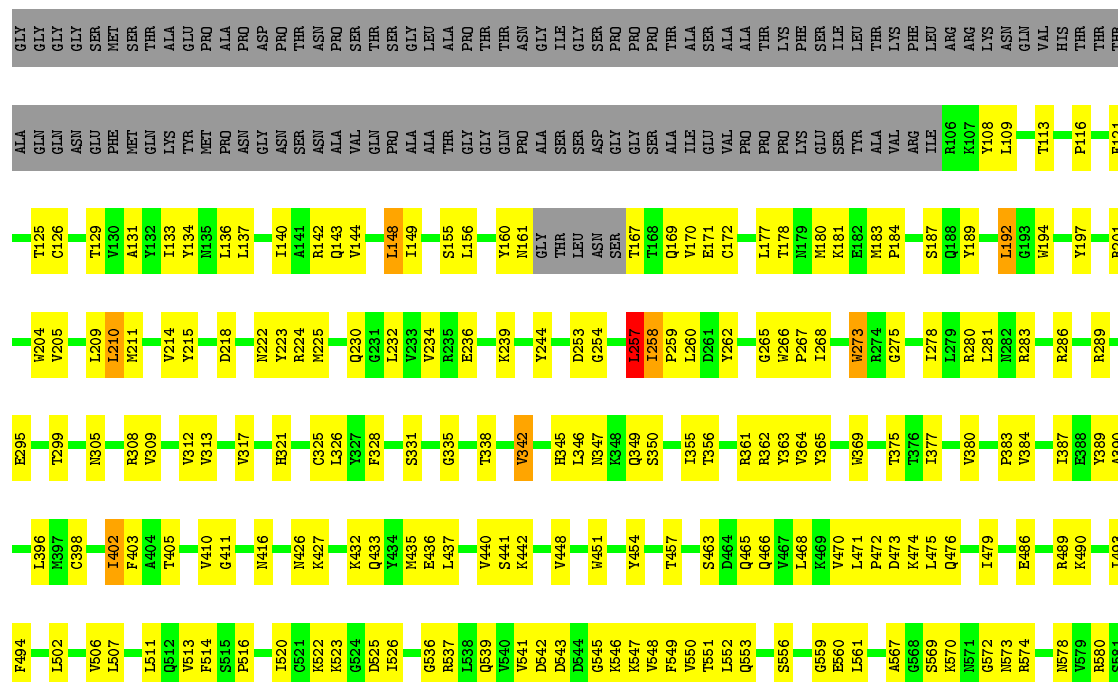
- Molecule 1: Cyclic nucleotide-gated cation channel

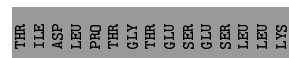
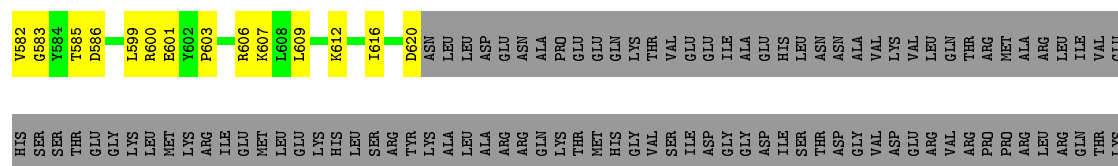




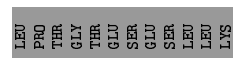
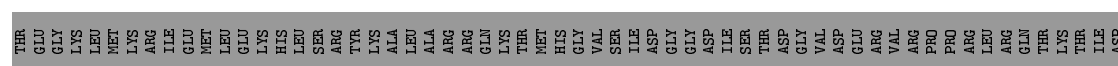
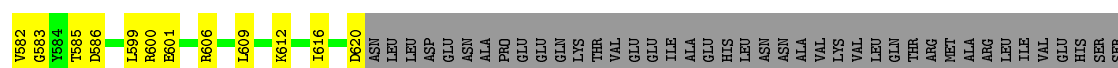
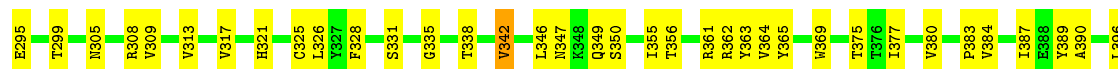
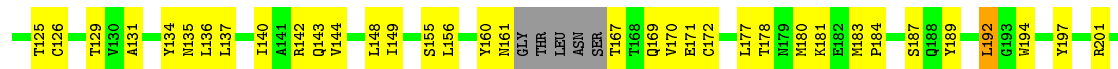
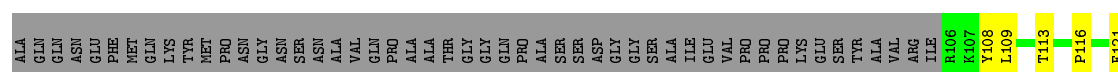
• Molecule 1: Cyclic nucleotide-gated cation channel

Chain C: 41% 27% 31%





- Molecule 1: Cyclic nucleotide-gated cation channel



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	99934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	22500	Depositor
Image detector	Not provided	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.51	0/4317	0.66	3/5854 (0.1%)
1	B	0.51	0/4318	0.67	2/5856 (0.0%)
1	C	0.51	0/4318	0.66	2/5856 (0.0%)
1	D	0.51	0/4318	0.67	2/5856 (0.0%)
All	All	0.51	0/17271	0.67	9/23422 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LEU	CA-CB-CG	5.29	127.46	115.30
1	D	136	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	257	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	136	LEU	CA-CB-CG	5.14	127.11	115.30
1	C	136	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	257	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	257	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	257	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	346	LEU	CB-CA-C	5.05	119.80	110.20

There are no chirality outliers.

There are no planarity outliers.

### 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	4215	0	4253	167	0
1	B	4216	0	4254	169	0
1	C	4216	0	4254	176	0
1	D	4216	0	4254	170	0
2	A	23	0	11	2	0
2	B	23	0	11	2	0
2	C	23	0	11	2	0
2	D	23	0	11	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	16958	0	17059	641	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 19.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:LYS:HG2	1:D:548:VAL:H	1.46	0.80
1:B:547:LYS:HG2	1:B:548:VAL:H	1.47	0.80
1:C:547:LYS:HG2	1:C:548:VAL:H	1.47	0.78
1:A:547:LYS:HG2	1:A:548:VAL:H	1.47	0.78
1:C:541:VAL:HG22	1:C:549:PHE:HD1	1.50	0.77
1:A:472:PRO:HG3	1:D:451:TRP:CZ2	2.20	0.76
1:B:541:VAL:HG22	1:B:549:PHE:HD1	1.51	0.76
1:B:451:TRP:CZ2	1:C:472:PRO:HG3	2.21	0.76
1:A:451:TRP:CZ2	1:B:472:PRO:HG3	2.22	0.75
1:C:523:LYS:HE2	1:C:542:ASP:OD2	1.86	0.75
1:D:541:VAL:HG22	1:D:549:PHE:HD1	1.50	0.75
1:C:451:TRP:CZ2	1:D:472:PRO:HG3	2.22	0.74
1:B:523:LYS:HE2	1:B:542:ASP:OD2	1.87	0.74
1:B:257:LEU:HD21	1:B:286:ARG:HE	1.53	0.74
1:A:257:LEU:HD21	1:A:286:ARG:HE	1.52	0.73
1:B:260:LEU:HD13	1:B:262:TYR:HE2	1.54	0.73
1:B:349:GLN:HG2	1:B:365:TYR:HE1	1.54	0.73
1:D:257:LEU:HD21	1:D:286:ARG:HE	1.54	0.73
1:C:260:LEU:HD13	1:C:262:TYR:HE2	1.54	0.73
1:A:541:VAL:HG22	1:A:549:PHE:HD1	1.52	0.72
1:C:257:LEU:HD21	1:C:286:ARG:HE	1.54	0.72
1:C:349:GLN:HG2	1:C:365:TYR:HE1	1.54	0.72
1:D:523:LYS:HE2	1:D:542:ASP:OD2	1.90	0.71
1:D:260:LEU:HD13	1:D:262:TYR:HE2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD13	1:A:262:TYR:HE2	1.55	0.71
1:D:349:GLN:HG2	1:D:365:TYR:HE1	1.55	0.71
1:A:537:ARG:NH2	1:B:230:GLN:OE1	2.24	0.70
1:A:523:LYS:HE2	1:A:542:ASP:OD2	1.91	0.70
1:A:572:GLY:O	1:A:574:ARG:N	2.23	0.70
1:D:572:GLY:O	1:D:574:ARG:N	2.24	0.70
1:A:349:GLN:HG2	1:A:365:TYR:HE1	1.57	0.69
1:A:183:MET:HG3	1:A:184:PRO:HD2	1.74	0.69
1:D:183:MET:HG3	1:D:184:PRO:HD2	1.75	0.69
1:C:183:MET:HG3	1:C:184:PRO:HD2	1.76	0.68
1:B:537:ARG:NH2	1:C:230:GLN:OE1	2.27	0.68
1:B:572:GLY:O	1:B:574:ARG:N	2.24	0.67
1:A:465:GLN:HA	1:A:468:LEU:HD12	1.75	0.67
1:B:183:MET:HG3	1:B:184:PRO:HD2	1.76	0.67
1:B:465:GLN:HA	1:B:468:LEU:HD12	1.75	0.67
1:C:465:GLN:HA	1:C:468:LEU:HD12	1.76	0.67
1:C:215:TYR:CD1	1:C:286:ARG:HD2	2.29	0.67
1:A:215:TYR:CD1	1:A:286:ARG:HD2	2.29	0.67
1:A:149:ILE:HG12	1:A:204:TRP:CD1	2.29	0.66
1:C:572:GLY:O	1:C:574:ARG:N	2.24	0.66
1:C:473:ASP:OD1	1:C:507:LEU:HD21	1.95	0.66
1:D:465:GLN:HA	1:D:468:LEU:HD12	1.75	0.66
1:C:328:PHE:HZ	1:C:362:ARG:HE	1.43	0.66
1:A:328:PHE:HZ	1:A:362:ARG:HE	1.43	0.66
1:B:473:ASP:OD1	1:B:507:LEU:HD21	1.96	0.66
1:C:523:LYS:CE	1:C:542:ASP:OD2	2.44	0.66
1:D:149:ILE:HG12	1:D:204:TRP:CD1	2.31	0.66
1:C:537:ARG:NH2	1:D:230:GLN:OE1	2.27	0.66
1:D:194:TRP:CZ2	1:D:268:ILE:HB	2.31	0.65
1:D:215:TYR:CD1	1:D:286:ARG:HD2	2.31	0.65
1:B:257:LEU:HD22	1:B:258:ILE:HG23	1.79	0.65
1:D:328:PHE:HZ	1:D:362:ARG:HE	1.45	0.65
1:A:599:LEU:HD22	1:A:606:ARG:HG3	1.79	0.65
1:C:194:TRP:CZ2	1:C:268:ILE:HB	2.32	0.65
1:B:215:TYR:CD1	1:B:286:ARG:HD2	2.31	0.64
1:C:149:ILE:HG12	1:C:204:TRP:CD1	2.32	0.64
1:C:257:LEU:HD22	1:C:258:ILE:HG23	1.80	0.64
1:A:257:LEU:HD22	1:A:258:ILE:HG23	1.80	0.64
1:C:599:LEU:HD22	1:C:606:ARG:HG3	1.80	0.64
1:D:170:VAL:HG12	1:D:171:GLU:H	1.63	0.64
1:B:194:TRP:CZ2	1:B:268:ILE:HB	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ILE:HG12	1:B:204:TRP:CD1	2.33	0.63
1:B:170:VAL:HG12	1:B:171:GLU:H	1.64	0.63
1:D:257:LEU:HD22	1:D:258:ILE:HG23	1.80	0.63
1:A:257:LEU:HG	1:A:286:ARG:HG3	1.79	0.63
1:B:523:LYS:CE	1:B:542:ASP:OD2	2.46	0.63
1:B:599:LEU:HD22	1:B:606:ARG:HG3	1.79	0.63
1:A:194:TRP:CZ2	1:A:268:ILE:HB	2.32	0.63
1:C:257:LEU:HG	1:C:286:ARG:HG3	1.81	0.63
1:B:448:VAL:HG22	1:C:475:LEU:HD13	1.81	0.63
1:B:257:LEU:HG	1:B:286:ARG:HG3	1.80	0.63
1:D:523:LYS:CE	1:D:542:ASP:OD2	2.47	0.63
1:A:230:GLN:OE1	1:D:537:ARG:NH2	2.31	0.63
1:D:599:LEU:HD22	1:D:606:ARG:HG3	1.80	0.63
1:B:355:ILE:HD12	1:B:361:ARG:NH1	2.14	0.63
1:C:468:LEU:O	1:C:476:GLN:NE2	2.32	0.63
1:C:448:VAL:HG22	1:D:475:LEU:HD13	1.81	0.63
1:B:468:LEU:O	1:B:476:GLN:NE2	2.33	0.62
1:A:435:MET:HE1	1:A:448:VAL:HG11	1.80	0.62
1:A:170:VAL:HG12	1:A:171:GLU:H	1.63	0.62
1:D:257:LEU:HG	1:D:286:ARG:HG3	1.81	0.62
1:C:170:VAL:HG12	1:C:171:GLU:H	1.64	0.62
1:B:328:PHE:HZ	1:B:362:ARG:HE	1.45	0.62
1:A:426:ASN:OD1	1:B:416:ASN:ND2	2.33	0.62
1:A:355:ILE:HD12	1:A:361:ARG:NH1	2.14	0.62
1:A:448:VAL:HG22	1:B:475:LEU:HD13	1.81	0.62
1:B:546:LYS:H	1:B:549:PHE:HZ	1.48	0.62
1:D:468:LEU:O	1:D:476:GLN:NE2	2.33	0.62
1:A:473:ASP:OD1	1:A:507:LEU:HD21	2.00	0.61
1:C:435:MET:HE1	1:C:448:VAL:HG11	1.81	0.61
1:C:355:ILE:HD12	1:C:361:ARG:NH1	2.16	0.61
1:A:475:LEU:HD13	1:D:448:VAL:HG22	1.82	0.61
1:C:546:LYS:H	1:C:549:PHE:HZ	1.49	0.61
1:A:468:LEU:O	1:A:476:GLN:NE2	2.33	0.61
1:B:435:MET:HE1	1:B:448:VAL:HG11	1.81	0.61
1:D:435:MET:HE1	1:D:448:VAL:HG11	1.82	0.60
1:C:125:THR:HG22	1:C:289:ARG:HD2	1.83	0.60
1:B:426:ASN:OD1	1:C:416:ASN:ND2	2.34	0.60
1:A:140:ILE:O	1:A:144:VAL:HG23	2.02	0.60
1:A:125:THR:HG22	1:A:289:ARG:HD2	1.82	0.60
1:A:405:THR:HG22	1:D:411:GLY:HA2	1.84	0.60
1:C:426:ASN:OD1	1:D:416:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ILE:O	1:D:144:VAL:HG23	2.02	0.60
1:D:473:ASP:OD1	1:D:507:LEU:HD21	2.00	0.60
1:C:160:TYR:HA	1:C:167:THR:HA	1.84	0.60
1:D:355:ILE:HD12	1:D:361:ARG:NH1	2.16	0.60
1:C:140:ILE:O	1:C:144:VAL:HG23	2.02	0.60
1:B:160:TYR:HA	1:B:167:THR:HA	1.83	0.59
1:D:215:TYR:CE1	1:D:286:ARG:HD2	2.37	0.59
1:A:416:ASN:ND2	1:D:426:ASN:OD1	2.34	0.59
1:A:215:TYR:CE1	1:A:286:ARG:HD2	2.37	0.59
1:D:194:TRP:HZ2	1:D:268:ILE:HB	1.67	0.59
1:A:160:TYR:HA	1:A:167:THR:HA	1.84	0.59
1:B:140:ILE:O	1:B:144:VAL:HG23	2.02	0.59
1:D:155:SER:HB2	1:D:172:CYS:HB2	1.85	0.59
1:D:546:LYS:H	1:D:549:PHE:HZ	1.50	0.59
1:C:215:TYR:CE1	1:C:286:ARG:HD2	2.38	0.58
1:D:125:THR:HG22	1:D:289:ARG:HD2	1.84	0.58
1:A:542:ASP:O	1:A:543:ASP:HB2	2.02	0.58
1:D:160:TYR:HA	1:D:167:THR:HA	1.84	0.58
1:C:542:ASP:O	1:C:543:ASP:HB2	2.04	0.58
1:D:545:GLY:HA2	1:D:549:PHE:HE1	1.68	0.58
1:A:545:GLY:HA2	1:A:549:PHE:HE1	1.69	0.58
1:B:215:TYR:CE1	1:B:286:ARG:HD2	2.38	0.58
1:D:369:TRP:NE1	1:D:380:VAL:HG11	2.19	0.58
1:B:542:ASP:O	1:B:543:ASP:HB2	2.03	0.58
1:D:260:LEU:HD13	1:D:262:TYR:CE2	2.39	0.58
1:C:545:GLY:HA2	1:C:549:PHE:CE1	2.38	0.58
1:A:260:LEU:HD13	1:A:262:TYR:CE2	2.38	0.58
1:B:537:ARG:HH11	1:C:232:LEU:HD12	1.69	0.57
1:D:486:GLU:HG2	1:D:489:ARG:HH21	1.68	0.57
1:D:545:GLY:HA2	1:D:549:PHE:CE1	2.39	0.57
1:C:155:SER:HB2	1:C:172:CYS:HB2	1.86	0.57
1:C:260:LEU:HD13	1:C:262:TYR:CE2	2.37	0.57
1:A:411:GLY:HA2	1:B:405:THR:HG22	1.85	0.57
1:C:537:ARG:HH11	1:D:232:LEU:HD12	1.69	0.57
1:A:545:GLY:HA2	1:A:549:PHE:CE1	2.39	0.57
1:A:369:TRP:NE1	1:A:380:VAL:HG11	2.19	0.57
1:B:474:LYS:HE2	1:B:474:LYS:HA	1.86	0.57
1:A:432:LYS:O	1:A:436:GLU:HG2	2.05	0.57
1:A:546:LYS:H	1:A:549:PHE:HZ	1.51	0.57
1:A:234:VAL:HG11	1:A:239:LYS:HD3	1.87	0.57
1:D:474:LYS:HE2	1:D:474:LYS:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:HB2	1:A:172:CYS:HB2	1.85	0.56
1:A:194:TRP:HZ2	1:A:268:ILE:HB	1.70	0.56
1:B:545:GLY:HA2	1:B:549:PHE:CE1	2.39	0.56
1:B:194:TRP:HZ2	1:B:268:ILE:HB	1.69	0.56
1:B:125:THR:HG22	1:B:289:ARG:HD2	1.86	0.56
1:C:369:TRP:NE1	1:C:380:VAL:HG11	2.20	0.56
1:C:432:LYS:O	1:C:436:GLU:HG2	2.05	0.56
1:C:545:GLY:HA2	1:C:549:PHE:HE1	1.69	0.56
1:B:234:VAL:HG11	1:B:239:LYS:HD3	1.87	0.56
1:B:432:LYS:O	1:B:436:GLU:HG2	2.05	0.56
1:A:369:TRP:CD1	1:A:380:VAL:HG11	2.40	0.56
1:B:454:TYR:HA	1:B:457:THR:HG22	1.88	0.56
1:C:539:GLN:OE1	1:C:580:ARG:NH2	2.36	0.56
1:C:411:GLY:HA2	1:D:405:THR:HG22	1.86	0.56
1:A:537:ARG:HH11	1:B:232:LEU:HD12	1.70	0.56
1:B:155:SER:HB2	1:B:172:CYS:HB2	1.86	0.56
1:B:369:TRP:NE1	1:B:380:VAL:HG11	2.21	0.56
1:D:542:ASP:O	1:D:543:ASP:HB2	2.05	0.56
1:C:194:TRP:HZ2	1:C:268:ILE:HB	1.69	0.56
1:C:369:TRP:CD1	1:C:380:VAL:HG11	2.41	0.56
1:C:536:GLY:HA3	1:C:585:THR:HG22	1.88	0.56
1:A:541:VAL:HG22	1:A:549:PHE:CD1	2.39	0.56
1:B:545:GLY:HA2	1:B:549:PHE:HE1	1.70	0.55
1:C:454:TYR:HA	1:C:457:THR:HG22	1.89	0.55
1:B:411:GLY:HA2	1:C:405:THR:HG22	1.89	0.55
1:D:432:LYS:O	1:D:436:GLU:HG2	2.05	0.55
1:A:525:ASP:OD1	1:A:526:ILE:N	2.40	0.55
1:C:578:ASN:OD1	1:C:578:ASN:N	2.40	0.55
1:A:536:GLY:HA3	1:A:585:THR:HG22	1.89	0.55
1:A:516:PRO:HB3	1:A:583:GLY:HA2	1.88	0.55
1:C:335:GLY:O	1:C:338:THR:HG22	2.07	0.55
1:B:210:LEU:HB3	1:B:211:MET:HE1	1.89	0.55
1:D:522:LYS:HA	1:D:578:ASN:HB3	1.89	0.55
1:B:525:ASP:OD1	1:B:526:ILE:N	2.39	0.55
1:C:569:SER:HB3	1:C:620:ASP:OD2	2.07	0.55
1:D:234:VAL:HG11	1:D:239:LYS:HD3	1.89	0.55
1:D:536:GLY:HA3	1:D:585:THR:HG22	1.89	0.55
1:A:523:LYS:CE	1:A:542:ASP:OD2	2.54	0.54
1:B:578:ASN:OD1	1:B:578:ASN:N	2.40	0.54
1:D:149:ILE:HG23	1:D:201:ARG:HG2	1.89	0.54
1:A:474:LYS:HA	1:A:474:LYS:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LYS:HA	1:C:474:LYS:HE2	1.89	0.54
1:D:454:TYR:HA	1:D:457:THR:HG22	1.89	0.54
1:A:578:ASN:OD1	1:A:578:ASN:N	2.40	0.54
1:C:486:GLU:HG2	1:C:489:ARG:HH21	1.72	0.54
1:C:522:LYS:HA	1:C:578:ASN:HB3	1.89	0.54
1:B:335:GLY:O	1:B:338:THR:HG22	2.08	0.54
1:B:369:TRP:CD1	1:B:380:VAL:HG11	2.42	0.54
1:C:525:ASP:OD1	1:C:526:ILE:N	2.40	0.54
1:A:335:GLY:O	1:A:338:THR:HG22	2.08	0.54
1:B:149:ILE:HG23	1:B:201:ARG:HG2	1.90	0.54
1:B:516:PRO:HB3	1:B:583:GLY:HA2	1.90	0.54
1:D:369:TRP:CD1	1:D:380:VAL:HG11	2.43	0.54
1:B:257:LEU:HB2	1:B:283:ARG:HA	1.89	0.54
1:B:569:SER:HB3	1:B:620:ASP:OD2	2.08	0.54
1:B:156:LEU:HD12	1:B:169:GLN:HB3	1.90	0.53
1:B:486:GLU:HG2	1:B:489:ARG:HH21	1.72	0.53
1:D:266:TRP:CD1	1:D:267:PRO:HG2	2.44	0.53
1:D:335:GLY:O	1:D:338:THR:HG22	2.08	0.53
1:D:578:ASN:N	1:D:578:ASN:OD1	2.41	0.53
1:A:232:LEU:HD12	1:D:537:ARG:HH11	1.71	0.53
1:D:525:ASP:OD1	1:D:526:ILE:N	2.41	0.53
1:A:149:ILE:HG23	1:A:201:ARG:HG2	1.91	0.53
1:A:266:TRP:CD1	1:A:267:PRO:HG2	2.44	0.53
1:A:486:GLU:HG2	1:A:489:ARG:HH21	1.73	0.53
1:C:142:ARG:HD3	1:C:149:ILE:CD1	2.39	0.53
1:A:232:LEU:HD21	1:D:582:VAL:HG12	1.91	0.53
1:A:454:TYR:HA	1:A:457:THR:HG22	1.90	0.53
1:B:522:LYS:HA	1:B:578:ASN:HB3	1.90	0.53
1:C:234:VAL:HG11	1:C:239:LYS:HD3	1.89	0.53
1:C:569:SER:CB	1:C:620:ASP:OD2	2.57	0.53
1:B:266:TRP:CD1	1:B:267:PRO:HG2	2.44	0.53
1:B:539:GLN:HB3	1:B:551:THR:HG22	1.91	0.53
1:A:142:ARG:HD3	1:A:149:ILE:CD1	2.39	0.53
1:A:522:LYS:HA	1:A:578:ASN:HB3	1.89	0.53
1:C:433:GLN:O	1:C:437:LEU:HD13	2.09	0.53
1:D:569:SER:HB3	1:D:620:ASP:OD2	2.09	0.53
1:B:541:VAL:HG22	1:B:549:PHE:CD1	2.39	0.53
1:C:131:ALA:O	1:C:134:TYR:HB3	2.09	0.53
1:C:149:ILE:HG23	1:C:201:ARG:HG2	1.91	0.53
1:D:257:LEU:HB2	1:D:283:ARG:HA	1.91	0.52
1:D:539:GLN:HB3	1:D:551:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ALA:O	1:B:134:TYR:HB3	2.09	0.52
1:A:253:ASP:OD1	1:A:254:GLY:N	2.43	0.52
1:B:260:LEU:HD13	1:B:262:TYR:CE2	2.38	0.52
1:D:108:TYR:CZ	1:D:109:LEU:HD13	2.45	0.52
1:D:253:ASP:OD1	1:D:254:GLY:N	2.43	0.52
1:B:142:ARG:HD3	1:B:149:ILE:CD1	2.40	0.52
1:B:536:GLY:HA3	1:B:585:THR:HG22	1.92	0.52
1:C:516:PRO:HB3	1:C:583:GLY:HA2	1.90	0.52
1:A:321:HIS:CE1	1:A:363:TYR:HH	2.23	0.52
1:D:156:LEU:HD12	1:D:169:GLN:HB3	1.92	0.52
1:A:131:ALA:O	1:A:134:TYR:HB3	2.10	0.52
1:C:266:TRP:CD1	1:C:267:PRO:HG2	2.44	0.52
1:C:253:ASP:OD1	1:C:254:GLY:N	2.43	0.52
1:D:383:PRO:HB2	1:D:389:TYR:CE2	2.45	0.52
1:A:156:LEU:HA	1:A:170:VAL:O	2.09	0.52
1:A:433:GLN:O	1:A:437:LEU:HD13	2.09	0.52
1:B:433:GLN:O	1:B:437:LEU:HD13	2.10	0.52
1:B:569:SER:CB	1:B:620:ASP:OD2	2.59	0.52
1:B:582:VAL:HG12	1:C:232:LEU:HD21	1.93	0.51
1:C:156:LEU:HD12	1:C:169:GLN:HB3	1.92	0.51
1:D:433:GLN:O	1:D:437:LEU:HD13	2.10	0.51
1:A:435:MET:HG2	1:A:440:VAL:HG11	1.92	0.51
1:A:559:GLY:H	2:A:801:PCG:H4'	1.76	0.51
1:D:131:ALA:O	1:D:134:TYR:HB3	2.10	0.51
1:A:470:VAL:HG11	1:D:427:LYS:HB3	1.93	0.51
1:B:253:ASP:OD1	1:B:254:GLY:N	2.44	0.51
1:C:156:LEU:HA	1:C:170:VAL:O	2.10	0.51
1:C:383:PRO:HB2	1:C:389:TYR:CE2	2.46	0.51
1:C:547:LYS:HG2	1:C:548:VAL:N	2.23	0.51
1:C:567:ALA:HB1	1:C:570:LYS:HA	1.93	0.51
1:B:466:GLN:O	1:B:470:VAL:HG23	2.10	0.51
1:C:313:VAL:O	1:C:317:VAL:HG23	2.11	0.51
1:D:516:PRO:HB3	1:D:583:GLY:HA2	1.92	0.51
1:A:156:LEU:HD12	1:A:169:GLN:HB3	1.93	0.51
1:B:156:LEU:HA	1:B:170:VAL:O	2.11	0.51
1:B:144:VAL:HG21	1:B:325:CYS:HB3	1.93	0.51
1:A:427:LYS:HB3	1:B:470:VAL:HG11	1.93	0.51
1:C:435:MET:HG2	1:C:440:VAL:HG11	1.93	0.51
1:D:265:GLY:HA2	1:D:273:TRP:HE1	1.75	0.51
1:A:257:LEU:HB2	1:A:283:ARG:HA	1.93	0.51
1:B:218:ASP:OD1	1:B:289:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:VAL:HG22	1:C:549:PHE:CD1	2.38	0.51
1:D:466:GLN:O	1:D:470:VAL:HG23	2.10	0.51
1:A:567:ALA:HB1	1:A:570:LYS:HA	1.91	0.51
1:C:427:LYS:HB3	1:D:470:VAL:HG11	1.93	0.51
1:D:142:ARG:HD3	1:D:149:ILE:CD1	2.41	0.51
1:A:569:SER:HB3	1:A:620:ASP:OD2	2.12	0.50
1:C:539:GLN:HB3	1:C:551:THR:HG22	1.93	0.50
1:A:313:VAL:O	1:A:317:VAL:HG23	2.11	0.50
1:B:567:ALA:HB1	1:B:570:LYS:HA	1.93	0.50
1:B:313:VAL:O	1:B:317:VAL:HG23	2.10	0.50
1:B:383:PRO:HB2	1:B:389:TYR:CE2	2.46	0.50
1:C:265:GLY:HA2	1:C:273:TRP:HE1	1.77	0.50
1:D:116:PRO:HA	1:D:121:PHE:CD2	2.46	0.50
1:A:170:VAL:HG12	1:A:171:GLU:N	2.27	0.50
1:C:265:GLY:O	1:C:275:GLY:HA2	2.12	0.50
1:B:265:GLY:HA2	1:B:273:TRP:HE1	1.77	0.50
1:C:108:TYR:CZ	1:C:109:LEU:HD13	2.46	0.50
1:C:257:LEU:HB2	1:C:283:ARG:HA	1.92	0.50
1:D:156:LEU:HA	1:D:170:VAL:O	2.12	0.50
1:B:427:LYS:HB3	1:C:470:VAL:HG11	1.94	0.50
1:D:547:LYS:HG2	1:D:548:VAL:N	2.22	0.50
1:A:116:PRO:HA	1:A:121:PHE:CD2	2.47	0.50
1:A:582:VAL:HG12	1:B:232:LEU:HD21	1.94	0.50
1:D:567:ALA:HB1	1:D:570:LYS:HA	1.93	0.50
1:C:210:LEU:HB3	1:C:211:MET:HE1	1.94	0.50
1:D:541:VAL:HG22	1:D:549:PHE:CD1	2.39	0.50
1:B:116:PRO:HA	1:B:121:PHE:CD2	2.47	0.49
1:D:273:TRP:CE3	1:D:273:TRP:HA	2.47	0.49
1:D:569:SER:CB	1:D:620:ASP:OD2	2.60	0.49
1:B:108:TYR:CZ	1:B:109:LEU:HD13	2.47	0.49
1:B:273:TRP:HA	1:B:273:TRP:CE3	2.47	0.49
1:B:547:LYS:CG	1:B:548:VAL:H	2.21	0.49
1:D:313:VAL:O	1:D:317:VAL:HG23	2.12	0.49
1:B:493:ILE:HD11	1:B:609:LEU:HD21	1.94	0.49
1:C:170:VAL:HG12	1:C:171:GLU:N	2.27	0.49
1:A:539:GLN:HB3	1:A:551:THR:HG22	1.93	0.49
1:D:349:GLN:HG2	1:D:365:TYR:CE1	2.42	0.49
1:D:435:MET:HG2	1:D:440:VAL:HG11	1.93	0.49
1:A:108:TYR:CZ	1:A:109:LEU:HD13	2.47	0.49
1:A:383:PRO:HB2	1:A:389:TYR:CE2	2.47	0.49
1:D:215:TYR:HD1	1:D:286:ARG:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:LEU:O	1:A:506:VAL:HG23	2.13	0.49
1:D:126:CYS:O	1:D:129:THR:HB	2.12	0.49
1:A:223:TYR:HA	1:A:244:TYR:CD1	2.48	0.49
1:B:194:TRP:CD1	1:B:194:TRP:N	2.79	0.49
1:A:569:SER:CB	1:A:620:ASP:OD2	2.61	0.49
1:B:435:MET:HG2	1:B:440:VAL:HG11	1.94	0.49
1:B:126:CYS:O	1:B:129:THR:HB	2.13	0.49
1:B:539:GLN:OE1	1:B:580:ARG:NH2	2.39	0.49
1:A:194:TRP:CD1	1:A:194:TRP:N	2.80	0.48
1:A:326:LEU:HA	1:A:326:LEU:HD23	1.59	0.48
1:B:170:VAL:HG12	1:B:171:GLU:N	2.27	0.48
1:B:222:ASN:HA	1:B:225:MET:HG2	1.95	0.48
1:B:502:LEU:O	1:B:506:VAL:HG23	2.13	0.48
1:C:116:PRO:HA	1:C:121:PHE:CD2	2.48	0.48
1:C:349:GLN:HG2	1:C:365:TYR:CE1	2.41	0.48
1:C:502:LEU:O	1:C:506:VAL:HG23	2.12	0.48
1:C:612:LYS:O	1:C:616:ILE:HG13	2.13	0.48
1:D:559:GLY:H	2:D:801:PCG:H4'	1.79	0.48
1:D:218:ASP:OD1	1:D:289:ARG:NH1	2.45	0.48
1:C:582:VAL:HG12	1:D:232:LEU:HD21	1.95	0.48
1:C:493:ILE:HD11	1:C:609:LEU:HD21	1.95	0.48
1:D:539:GLN:OE1	1:D:580:ARG:NH2	2.38	0.48
1:A:350:SER:O	1:A:361:ARG:NH1	2.46	0.48
1:A:514:PHE:CD1	1:A:520:ILE:HG13	2.49	0.48
1:B:265:GLY:O	1:B:275:GLY:HA2	2.14	0.48
1:C:559:GLY:H	2:C:801:PCG:H4'	1.79	0.48
1:D:142:ARG:HD3	1:D:149:ILE:HD11	1.95	0.48
1:A:547:LYS:CG	1:A:548:VAL:H	2.21	0.48
1:C:126:CYS:O	1:C:129:THR:HB	2.14	0.48
1:C:466:GLN:O	1:C:470:VAL:HG23	2.13	0.48
1:A:273:TRP:CE3	1:A:273:TRP:HA	2.48	0.48
1:A:612:LYS:O	1:A:616:ILE:HG13	2.14	0.48
1:B:349:GLN:HG2	1:B:365:TYR:CE1	2.41	0.48
1:B:514:PHE:CD1	1:B:520:ILE:HG13	2.48	0.48
1:D:170:VAL:HG12	1:D:171:GLU:N	2.26	0.48
1:C:361:ARG:NH2	1:D:389:TYR:CE2	2.82	0.48
1:B:612:LYS:O	1:B:616:ILE:HG13	2.14	0.48
1:A:126:CYS:O	1:A:129:THR:HB	2.14	0.48
1:B:361:ARG:NH2	1:C:389:TYR:CE2	2.82	0.48
1:D:144:VAL:HG21	1:D:325:CYS:HB3	1.96	0.48
1:D:194:TRP:CD1	1:D:194:TRP:N	2.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TYR:HA	1:B:244:TYR:CD1	2.49	0.47
1:D:511:LEU:HD23	1:D:511:LEU:HA	1.64	0.47
1:D:539:GLN:HA	1:D:550:VAL:O	2.14	0.47
1:B:331:SER:HA	1:B:342:VAL:HG22	1.96	0.47
1:B:600:ARG:HB2	1:B:601:GLU:OE1	2.13	0.47
1:C:273:TRP:HA	1:C:273:TRP:CE3	2.48	0.47
1:D:493:ILE:HD11	1:D:609:LEU:HD21	1.94	0.47
1:A:466:GLN:O	1:A:470:VAL:HG23	2.14	0.47
1:A:473:ASP:CG	1:A:507:LEU:HD21	2.35	0.47
1:B:143:GLN:O	1:B:143:GLN:NE2	2.48	0.47
1:B:451:TRP:CE2	1:C:472:PRO:HG3	2.49	0.47
1:C:144:VAL:HG21	1:C:325:CYS:HB3	1.97	0.47
1:D:223:TYR:HA	1:D:244:TYR:CD1	2.49	0.47
1:D:514:PHE:CD1	1:D:520:ILE:HG13	2.49	0.47
1:A:222:ASN:HA	1:A:225:MET:HG2	1.96	0.47
1:A:222:ASN:OD1	1:A:289:ARG:NH2	2.44	0.47
1:A:493:ILE:HD11	1:A:609:LEU:HD21	1.95	0.47
1:B:559:GLY:H	2:B:801:PCG:H4'	1.80	0.47
1:C:222:ASN:HA	1:C:225:MET:HG2	1.97	0.47
1:C:473:ASP:CG	1:C:507:LEU:HD21	2.35	0.47
1:C:547:LYS:CG	1:C:548:VAL:H	2.22	0.47
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.60	0.47
1:D:326:LEU:HA	1:D:326:LEU:HD23	1.56	0.47
1:D:612:LYS:O	1:D:616:ILE:HG13	2.14	0.47
1:C:215:TYR:HD1	1:C:286:ARG:HD2	1.75	0.47
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.61	0.47
1:A:156:LEU:HD23	1:A:187:SER:HB2	1.97	0.47
1:A:361:ARG:NH2	1:B:389:TYR:CE2	2.82	0.47
1:A:305:ASN:OD1	1:A:308:ARG:NH1	2.47	0.47
1:D:265:GLY:O	1:D:275:GLY:HA2	2.15	0.47
1:B:526:ILE:HD12	1:B:526:ILE:H	1.80	0.47
1:C:259:PRO:O	1:C:260:LEU:HB2	2.15	0.47
1:D:350:SER:O	1:D:361:ARG:NH1	2.48	0.47
1:B:547:LYS:HG2	1:B:548:VAL:N	2.23	0.47
1:C:222:ASN:OD1	1:C:289:ARG:NH2	2.44	0.47
1:A:560:GLU:OE1	2:A:801:PCG:O2'	2.33	0.46
1:C:181:LYS:N	1:C:181:LYS:HD2	2.30	0.46
1:D:547:LYS:CG	1:D:548:VAL:H	2.21	0.46
1:B:326:LEU:HA	1:B:326:LEU:HD23	1.58	0.46
1:C:223:TYR:HA	1:C:244:TYR:CD1	2.48	0.46
1:C:305:ASN:OD1	1:C:308:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLN:NE2	1:D:143:GLN:O	2.48	0.46
1:A:349:GLN:HG2	1:A:365:TYR:CE1	2.44	0.46
1:B:156:LEU:HD23	1:B:187:SER:HB2	1.97	0.46
1:C:398:CYS:O	1:C:402:ILE:HB	2.16	0.46
1:C:514:PHE:CD1	1:C:520:ILE:HG13	2.50	0.46
1:D:398:CYS:O	1:D:402:ILE:HB	2.16	0.46
1:B:259:PRO:O	1:B:260:LEU:HB2	2.15	0.46
1:B:215:TYR:HD1	1:B:286:ARG:HD2	1.77	0.46
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.68	0.46
1:C:331:SER:HA	1:C:342:VAL:HG22	1.97	0.46
1:C:539:GLN:HA	1:C:550:VAL:O	2.16	0.46
1:D:473:ASP:CG	1:D:507:LEU:HD21	2.36	0.46
1:D:502:LEU:O	1:D:506:VAL:HG23	2.15	0.46
1:D:560:GLU:OE1	2:D:801:PCG:O2'	2.34	0.46
1:A:375:THR:O	1:A:377:ILE:HD12	2.16	0.46
1:A:331:SER:HA	1:A:342:VAL:HG22	1.97	0.46
1:B:312:VAL:HG11	1:B:410:VAL:HG22	1.98	0.46
1:B:350:SER:O	1:B:361:ARG:NH1	2.48	0.46
1:B:475:LEU:HD23	1:B:475:LEU:HA	1.59	0.46
1:D:441:SER:OG	1:D:442:LYS:N	2.49	0.46
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.68	0.46
1:A:215:TYR:HD1	1:A:286:ARG:HD2	1.75	0.46
1:A:387:ILE:O	1:A:390:ALA:HB3	2.15	0.46
1:A:539:GLN:OE1	1:A:580:ARG:NH2	2.37	0.46
1:B:134:TYR:CD2	1:B:211:MET:HG3	2.51	0.46
1:C:387:ILE:O	1:C:390:ALA:HB3	2.16	0.46
1:D:222:ASN:OD1	1:D:289:ARG:NH2	2.45	0.46
1:A:389:TYR:CE2	1:D:361:ARG:NH2	2.82	0.46
1:D:526:ILE:HD12	1:D:526:ILE:H	1.81	0.46
1:A:265:GLY:HA2	1:A:273:TRP:HE1	1.80	0.46
1:A:142:ARG:HD3	1:A:149:ILE:HD11	1.97	0.46
1:A:155:SER:CB	1:A:172:CYS:HB2	2.46	0.46
1:C:451:TRP:CE2	1:D:472:PRO:HG3	2.51	0.46
1:C:526:ILE:H	1:C:526:ILE:HD12	1.81	0.46
1:C:560:GLU:OE1	2:C:801:PCG:O2'	2.33	0.46
1:D:432:LYS:HB3	1:D:432:LYS:HE3	1.80	0.46
1:D:600:ARG:HB2	1:D:601:GLU:OE1	2.16	0.46
1:A:259:PRO:O	1:A:260:LEU:HB2	2.15	0.45
1:B:375:THR:O	1:B:377:ILE:HD12	2.16	0.45
1:B:473:ASP:CG	1:B:507:LEU:HD21	2.36	0.45
1:D:222:ASN:HA	1:D:225:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HG21	1:A:325:CYS:HB3	1.97	0.45
1:A:600:ARG:HB2	1:A:601:GLU:OE1	2.16	0.45
1:A:181:LYS:N	1:A:181:LYS:HD2	2.30	0.45
1:A:398:CYS:O	1:A:402:ILE:HB	2.16	0.45
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.81	0.45
1:B:539:GLN:HA	1:B:550:VAL:O	2.16	0.45
1:C:156:LEU:HD23	1:C:187:SER:HB2	1.96	0.45
1:A:137:LEU:HA	1:A:137:LEU:HD23	1.63	0.45
1:A:539:GLN:HA	1:A:550:VAL:O	2.16	0.45
1:B:441:SER:OG	1:B:442:LYS:N	2.50	0.45
1:C:142:ARG:HD3	1:C:149:ILE:HD11	1.97	0.45
1:A:346:LEU:HA	1:A:346:LEU:HD23	1.85	0.45
1:B:142:ARG:HD3	1:B:149:ILE:HD11	1.98	0.45
1:A:451:TRP:CE2	1:B:472:PRO:HG3	2.50	0.45
1:C:155:SER:CB	1:C:172:CYS:HB2	2.46	0.45
1:C:194:TRP:N	1:C:194:TRP:CD1	2.79	0.45
1:C:350:SER:O	1:C:361:ARG:NH1	2.49	0.45
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.68	0.45
1:C:511:LEU:HA	1:C:511:LEU:HD23	1.66	0.45
1:D:259:PRO:O	1:D:260:LEU:HB2	2.16	0.45
1:B:511:LEU:HD23	1:B:511:LEU:HA	1.63	0.45
1:C:441:SER:OG	1:C:442:LYS:N	2.50	0.45
1:C:600:ARG:HB2	1:C:601:GLU:OE1	2.17	0.45
1:D:331:SER:HA	1:D:342:VAL:HG22	1.97	0.45
1:D:375:THR:O	1:D:377:ILE:HD12	2.17	0.45
1:D:475:LEU:HA	1:D:475:LEU:HD23	1.58	0.45
1:A:526:ILE:HD12	1:A:526:ILE:H	1.81	0.45
1:D:387:ILE:O	1:D:390:ALA:HB3	2.17	0.45
1:A:280:ARG:NH2	1:A:283:ARG:HD3	2.32	0.45
1:A:218:ASP:OD1	1:A:289:ARG:NH1	2.50	0.45
1:A:441:SER:OG	1:A:442:LYS:N	2.50	0.45
1:B:473:ASP:OD1	1:B:507:LEU:CD2	2.65	0.45
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.61	0.45
1:B:257:LEU:HD21	1:B:286:ARG:NE	2.29	0.44
1:B:387:ILE:O	1:B:390:ALA:HB3	2.17	0.44
1:D:134:TYR:CD2	1:D:211:MET:HG3	2.52	0.44
1:D:156:LEU:HD23	1:D:187:SER:HB2	1.97	0.44
1:D:181:LYS:N	1:D:181:LYS:HD2	2.32	0.44
1:D:552:LEU:HD23	1:D:556:SER:HB2	1.99	0.44
1:D:346:LEU:HD23	1:D:346:LEU:HA	1.85	0.44
1:A:143:GLN:NE2	1:A:143:GLN:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASP:OD1	1:A:507:LEU:CD2	2.65	0.44
1:C:143:GLN:O	1:C:143:GLN:NE2	2.51	0.44
1:C:280:ARG:NH2	1:C:283:ARG:HD3	2.32	0.44
1:D:295:GLU:O	1:D:299:THR:HG23	2.18	0.44
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.65	0.44
1:B:560:GLU:OE1	2:B:801:PCG:O2'	2.35	0.44
1:C:473:ASP:OD1	1:C:507:LEU:CD2	2.63	0.44
1:C:475:LEU:HD23	1:C:475:LEU:HA	1.62	0.44
1:D:209:LEU:HD12	1:D:209:LEU:HA	1.86	0.44
1:B:295:GLU:O	1:B:299:THR:HG23	2.18	0.44
1:B:321:HIS:ND1	1:B:363:TYR:OH	2.36	0.44
1:A:295:GLU:O	1:A:299:THR:HG23	2.18	0.44
1:A:513:VAL:HG22	1:A:586:ASP:OD1	2.18	0.44
1:C:134:TYR:CD2	1:C:211:MET:HG3	2.53	0.44
1:C:257:LEU:HD21	1:C:286:ARG:NE	2.29	0.44
1:C:375:THR:O	1:C:377:ILE:HD12	2.18	0.44
1:D:177:LEU:HA	1:D:177:LEU:HD23	1.68	0.44
1:D:321:HIS:CE1	1:D:363:TYR:HH	2.29	0.44
1:A:236:GLU:OE1	1:A:239:LYS:HD2	2.17	0.44
1:A:552:LEU:HD23	1:A:556:SER:HB2	2.00	0.44
1:C:209:LEU:HA	1:C:209:LEU:HD12	1.86	0.44
1:B:155:SER:CB	1:B:172:CYS:HB2	2.48	0.44
1:C:312:VAL:HG11	1:C:410:VAL:HG22	2.00	0.44
1:D:513:VAL:HG22	1:D:586:ASP:OD1	2.18	0.44
1:A:542:ASP:O	1:A:543:ASP:CB	2.65	0.43
1:B:398:CYS:O	1:B:402:ILE:HB	2.17	0.43
1:B:348:LYS:HB2	1:B:348:LYS:HE2	1.84	0.43
1:C:553:GLN:O	1:C:556:SER:OG	2.26	0.43
1:D:280:ARG:NH2	1:D:283:ARG:HD3	2.33	0.43
1:A:475:LEU:HD23	1:A:475:LEU:HA	1.61	0.43
1:B:181:LYS:N	1:B:181:LYS:HD2	2.33	0.43
1:B:280:ARG:NH2	1:B:283:ARG:HD3	2.33	0.43
1:D:210:LEU:O	1:D:214:VAL:HG23	2.19	0.43
1:B:513:VAL:HG22	1:B:586:ASP:OD1	2.19	0.43
1:C:178:THR:OG1	1:C:356:THR:HG22	2.18	0.43
1:C:513:VAL:HG22	1:C:586:ASP:OD1	2.18	0.43
1:C:572:GLY:C	1:C:574:ARG:N	2.72	0.43
1:D:305:ASN:OD1	1:D:308:ARG:NH1	2.52	0.43
1:C:189:TYR:HB2	1:C:192:LEU:HA	2.00	0.43
1:C:295:GLU:O	1:C:299:THR:HG23	2.18	0.43
1:C:607:LYS:HA	1:C:607:LYS:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TYR:HB2	1:A:192:LEU:HA	1.98	0.43
1:B:178:THR:OG1	1:B:356:THR:HG22	2.18	0.43
1:B:494:PHE:CD1	1:B:502:LEU:HD12	2.54	0.43
1:B:257:LEU:H	1:B:257:LEU:HD13	1.83	0.43
1:B:490:LYS:HB3	1:B:490:LYS:HE2	1.89	0.43
1:D:178:THR:OG1	1:D:356:THR:HG22	2.18	0.43
1:C:218:ASP:OD1	1:C:289:ARG:NH1	2.52	0.43
1:A:205:VAL:O	1:A:209:LEU:HB2	2.19	0.43
1:A:402:ILE:HG22	1:A:403:PHE:CD1	2.54	0.43
1:A:547:LYS:HG2	1:A:548:VAL:N	2.23	0.43
1:B:572:GLY:C	1:B:574:ARG:N	2.72	0.43
1:A:134:TYR:CD2	1:A:211:MET:HG3	2.53	0.43
1:A:542:ASP:N	1:A:547:LYS:HD2	2.33	0.43
1:B:402:ILE:HG22	1:B:403:PHE:CD1	2.54	0.43
1:A:347:ASN:OD1	1:A:347:ASN:O	2.37	0.42
1:B:205:VAL:O	1:B:209:LEU:HB2	2.19	0.42
1:A:257:LEU:H	1:A:257:LEU:HD13	1.84	0.42
1:A:459:LYS:HD2	1:A:459:LYS:HA	1.78	0.42
1:B:160:TYR:O	1:B:161:ASN:HB2	2.19	0.42
1:B:347:ASN:OD1	1:B:347:ASN:O	2.37	0.42
1:C:402:ILE:HG22	1:C:403:PHE:CD1	2.54	0.42
1:C:472:PRO:HD2	1:C:475:LEU:HB2	2.01	0.42
1:D:236:GLU:OE1	1:D:239:LYS:HD2	2.20	0.42
1:D:473:ASP:OD1	1:D:507:LEU:CD2	2.67	0.42
1:A:472:PRO:HG3	1:D:451:TRP:CE2	2.53	0.42
1:A:532:ILE:HG12	1:A:557:VAL:HG22	2.02	0.42
1:B:472:PRO:HD2	1:B:475:LEU:HB2	2.00	0.42
1:B:364:VAL:HG12	1:B:365:TYR:N	2.35	0.42
1:C:542:ASP:N	1:C:547:LYS:HD2	2.34	0.42
1:A:265:GLY:O	1:A:275:GLY:HA2	2.19	0.42
1:D:572:GLY:C	1:D:574:ARG:N	2.72	0.42
1:D:160:TYR:O	1:D:161:ASN:HB2	2.20	0.42
1:D:552:LEU:HB3	1:D:556:SER:OG	2.19	0.42
1:B:542:ASP:N	1:B:547:LYS:HD2	2.35	0.42
1:C:494:PHE:CD1	1:C:502:LEU:HD12	2.55	0.42
1:C:552:LEU:HD23	1:C:556:SER:HB2	2.02	0.42
1:A:210:LEU:O	1:A:214:VAL:HG23	2.20	0.42
1:C:257:LEU:HD13	1:C:257:LEU:H	1.85	0.42
1:C:561:LEU:HD23	1:C:561:LEU:HA	1.82	0.42
1:D:155:SER:CB	1:D:172:CYS:HB2	2.47	0.42
1:D:459:LYS:HD2	1:D:459:LYS:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HG22	1:A:403:PHE:HD1	1.85	0.42
1:A:552:LEU:HB3	1:A:556:SER:OG	2.20	0.42
1:D:257:LEU:HD13	1:D:257:LEU:H	1.84	0.42
1:D:309:VAL:O	1:D:313:VAL:HG23	2.19	0.42
1:A:257:LEU:HD21	1:A:286:ARG:NE	2.28	0.41
1:B:222:ASN:OD1	1:B:289:ARG:NH2	2.44	0.41
1:C:262:TYR:O	1:C:266:TRP:N	2.53	0.41
1:C:309:VAL:O	1:C:313:VAL:HG23	2.20	0.41
1:A:160:TYR:O	1:A:161:ASN:HB2	2.20	0.41
1:A:364:VAL:HG12	1:A:365:TYR:N	2.36	0.41
1:B:346:LEU:HA	1:B:346:LEU:HD23	1.85	0.41
1:C:552:LEU:HB3	1:C:556:SER:OG	2.19	0.41
1:D:532:ILE:HG12	1:D:557:VAL:HG22	2.01	0.41
1:B:189:TYR:HB2	1:B:192:LEU:HA	2.02	0.41
1:B:135:ASN:HD21	1:B:215:TYR:HE2	1.68	0.41
1:B:309:VAL:O	1:B:313:VAL:HG23	2.20	0.41
1:B:532:ILE:HG12	1:B:557:VAL:HG22	2.02	0.41
1:C:205:VAL:O	1:C:209:LEU:HB2	2.20	0.41
1:D:402:ILE:HG22	1:D:403:PHE:CD1	2.56	0.41
1:C:148:LEU:HD21	1:C:204:TRP:CZ2	2.56	0.41
1:C:160:TYR:O	1:C:161:ASN:HB2	2.19	0.41
1:C:347:ASN:OD1	1:C:347:ASN:O	2.38	0.41
1:D:205:VAL:O	1:D:209:LEU:HB2	2.19	0.41
1:D:472:PRO:HD2	1:D:475:LEU:HB2	2.03	0.41
1:A:178:THR:OG1	1:A:356:THR:HG22	2.20	0.41
1:C:236:GLU:OE1	1:C:239:LYS:HD2	2.20	0.41
1:C:278:ILE:O	1:C:281:LEU:HG	2.21	0.41
1:C:402:ILE:HG22	1:C:403:PHE:N	2.36	0.41
1:D:271:ILE:H	1:D:271:ILE:HG13	1.66	0.41
1:D:364:VAL:HG12	1:D:365:TYR:N	2.35	0.41
1:C:361:ARG:NH2	1:D:389:TYR:CZ	2.88	0.41
1:D:553:GLN:O	1:D:556:SER:OG	2.27	0.41
1:A:384:VAL:O	1:A:384:VAL:HG12	2.21	0.41
1:A:572:GLY:C	1:A:574:ARG:N	2.73	0.41
1:B:273:TRP:HE3	1:B:273:TRP:HA	1.86	0.41
1:B:552:LEU:HD23	1:B:556:SER:HB2	2.03	0.41
1:C:192:LEU:HD23	1:C:192:LEU:H	1.85	0.41
1:C:194:TRP:HA	1:C:197:TYR:O	2.21	0.41
1:C:210:LEU:O	1:C:214:VAL:HG23	2.21	0.41
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.59	0.41
1:D:347:ASN:OD1	1:D:347:ASN:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:MET:SD	1:D:502:LEU:HD21	2.61	0.41
1:A:312:VAL:HG11	1:A:410:VAL:HG22	2.02	0.41
1:C:384:VAL:HG12	1:C:384:VAL:O	2.21	0.41
1:C:402:ILE:HG22	1:C:403:PHE:HD1	1.85	0.41
1:D:113:THR:HA	1:D:224:ARG:HB3	2.02	0.41
1:C:364:VAL:HG12	1:C:365:TYR:N	2.35	0.41
1:C:427:LYS:HD2	1:C:427:LYS:HA	1.94	0.41
1:D:135:ASN:HD21	1:D:215:TYR:HE2	1.69	0.41
1:D:384:VAL:O	1:D:384:VAL:HG12	2.21	0.41
1:D:402:ILE:HG22	1:D:403:PHE:HD1	1.86	0.41
1:C:479:ILE:HG21	1:C:479:ILE:HD13	1.84	0.41
1:D:194:TRP:H	1:D:194:TRP:HD1	1.65	0.41
1:B:402:ILE:HG22	1:B:403:PHE:HD1	1.86	0.41
1:B:442:LYS:HA	1:B:442:LYS:HD2	1.89	0.41
1:C:113:THR:HA	1:C:224:ARG:HB3	2.03	0.41
1:C:321:HIS:ND1	1:C:363:TYR:OH	2.36	0.41
1:D:143:GLN:HA	1:D:277:PRO:HG2	2.03	0.41
1:D:210:LEU:HB3	1:D:211:MET:HE1	2.02	0.41
1:A:156:LEU:CD2	1:A:187:SER:HB2	2.51	0.41
1:B:210:LEU:O	1:B:214:VAL:HG23	2.20	0.40
1:B:313:VAL:HA	1:B:316:ILE:HD12	2.03	0.40
1:C:490:LYS:HE2	1:C:490:LYS:HB3	1.88	0.40
1:C:603:PRO:O	1:C:606:ARG:HB2	2.21	0.40
1:A:242:LYS:O	1:A:246:GLN:HG2	2.21	0.40
1:A:265:GLY:O	1:A:276:LEU:N	2.52	0.40
1:A:271:ILE:HG13	1:A:271:ILE:H	1.65	0.40
1:D:265:GLY:O	1:D:276:LEU:N	2.53	0.40
1:A:143:GLN:HA	1:A:277:PRO:HG2	2.03	0.40
1:B:331:SER:OG	1:B:342:VAL:HG22	2.22	0.40
1:A:278:ILE:O	1:A:281:LEU:HG	2.20	0.40
1:A:331:SER:OG	1:A:342:VAL:HG22	2.22	0.40
1:B:148:LEU:HD21	1:B:204:TRP:CZ2	2.56	0.40
1:B:266:TRP:CG	1:B:267:PRO:HD2	2.56	0.40
1:B:384:VAL:O	1:B:384:VAL:HG12	2.21	0.40
1:B:481:MET:SD	1:B:502:LEU:HD21	2.62	0.40
1:C:345:HIS:CD2	1:C:346:LEU:HG	2.56	0.40
1:D:494:PHE:CD1	1:D:502:LEU:HD12	2.56	0.40
1:A:273:TRP:HE3	1:A:273:TRP:HA	1.87	0.40
1:B:113:THR:HA	1:B:224:ARG:HB3	2.02	0.40
1:B:278:ILE:O	1:B:281:LEU:HG	2.22	0.40
1:C:129:THR:O	1:C:133:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:TYR:HB2	1:D:192:LEU:HA	2.02	0.40
1:D:194:TRP:HA	1:D:197:TYR:O	2.22	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	506/738 (69%)	474 (94%)	29 (6%)	3 (1%)	30	75
1	B	506/738 (69%)	472 (93%)	31 (6%)	3 (1%)	30	75
1	C	506/738 (69%)	473 (94%)	30 (6%)	3 (1%)	30	75
1	D	506/738 (69%)	472 (93%)	31 (6%)	3 (1%)	30	75
All	All	2024/2952 (69%)	1891 (93%)	121 (6%)	12 (1%)	34	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	573	ASN
1	B	573	ASN
1	C	573	ASN
1	D	573	ASN
1	A	148	LEU
1	B	148	LEU
1	C	148	LEU
1	D	148	LEU
1	A	258	ILE
1	D	258	ILE
1	B	258	ILE
1	C	258	ILE

### 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	462/652 (71%)	451 (98%)	11 (2%)	57	85
1	B	462/652 (71%)	453 (98%)	9 (2%)	65	87
1	C	462/652 (71%)	452 (98%)	10 (2%)	60	85
1	D	462/652 (71%)	452 (98%)	10 (2%)	60	85
All	All	1848/2608 (71%)	1808 (98%)	40 (2%)	63	85

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	MET
1	A	192	LEU
1	A	210	LEU
1	A	257	LEU
1	A	271	ILE
1	A	273	TRP
1	A	342	VAL
1	A	396	LEU
1	A	463	SER
1	A	465	GLN
1	A	471	LEU
1	B	180	MET
1	B	192	LEU
1	B	210	LEU
1	B	257	LEU
1	B	273	TRP
1	B	342	VAL
1	B	396	LEU
1	B	463	SER
1	B	471	LEU
1	C	180	MET
1	C	192	LEU
1	C	210	LEU
1	C	257	LEU

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Mol	Chain	Res	Type
1	C	273	TRP
1	C	342	VAL
1	C	396	LEU
1	C	402	ILE
1	C	463	SER
1	C	471	LEU
1	D	180	MET
1	D	192	LEU
1	D	210	LEU
1	D	257	LEU
1	D	273	TRP
1	D	342	VAL
1	D	396	LEU
1	D	463	SER
1	D	471	LEU
1	D	507	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	ASN
1	B	571	ASN
1	C	571	ASN
1	D	571	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 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$
2	PCG	A	801	-	20,26,26	1.84	3 (15%)	21,41,41	2.14	6 (28%)
2	PCG	B	801	-	20,26,26	1.84	3 (15%)	21,41,41	2.15	6 (28%)
2	PCG	C	801	-	20,26,26	1.83	3 (15%)	21,41,41	2.13	6 (28%)
2	PCG	D	801	-	20,26,26	1.83	3 (15%)	21,41,41	2.14	6 (28%)

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
2	PCG	A	801	-	-	0/0/31/31	0/4/4/4
2	PCG	B	801	-	-	0/0/31/31	0/4/4/4
2	PCG	C	801	-	-	0/0/31/31	0/4/4/4
2	PCG	D	801	-	-	0/0/31/31	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	PCG	C2-N1	3.04	1.41	1.35
2	A	801	PCG	C2-N1	3.04	1.41	1.35
2	D	801	PCG	C2-N1	3.07	1.41	1.35
2	B	801	PCG	C2-N1	3.11	1.41	1.35
2	C	801	PCG	C6-N1	4.35	1.40	1.33
2	B	801	PCG	C6-N1	4.37	1.40	1.33
2	A	801	PCG	C6-N1	4.38	1.40	1.33
2	D	801	PCG	C6-N1	4.41	1.41	1.33
2	D	801	PCG	O4'-C1'	4.91	1.48	1.41
2	A	801	PCG	O4'-C1'	4.98	1.48	1.41
2	B	801	PCG	O4'-C1'	4.98	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	PCG	O4'-C1'	4.98	1.48	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	PCG	N3-C2-N1	-5.12	120.60	127.56
2	D	801	PCG	N3-C2-N1	-5.10	120.62	127.56
2	A	801	PCG	N3-C2-N1	-5.09	120.64	127.56
2	C	801	PCG	N3-C2-N1	-5.07	120.66	127.56
2	B	801	PCG	C4'-O4'-C1'	-4.02	105.39	109.64
2	D	801	PCG	C4'-O4'-C1'	-3.97	105.44	109.64
2	A	801	PCG	O3'-C3'-C4'	-3.92	107.59	110.72
2	C	801	PCG	C4'-O4'-C1'	-3.85	105.57	109.64
2	A	801	PCG	C4'-O4'-C1'	-3.80	105.61	109.64
2	B	801	PCG	O3'-C3'-C4'	-3.79	107.69	110.72
2	D	801	PCG	O3'-C3'-C4'	-3.76	107.72	110.72
2	C	801	PCG	O3'-C3'-C4'	-3.72	107.75	110.72
2	D	801	PCG	C5-C6-N1	-3.36	119.12	123.52
2	C	801	PCG	C5-C6-N1	-3.36	119.13	123.52
2	B	801	PCG	C5-C6-N1	-3.35	119.15	123.52
2	A	801	PCG	C5-C6-N1	-3.30	119.21	123.52
2	A	801	PCG	C6-N1-C2	2.41	118.71	115.88
2	B	801	PCG	C6-N1-C2	2.46	118.77	115.88
2	D	801	PCG	C6-N1-C2	2.47	118.77	115.88
2	C	801	PCG	C6-N1-C2	2.47	118.78	115.88
2	B	801	PCG	O1A-PA-O2A	2.91	118.28	108.67
2	D	801	PCG	O1A-PA-O2A	2.93	118.33	108.67
2	C	801	PCG	O1A-PA-O2A	2.93	118.33	108.67
2	A	801	PCG	O1A-PA-O2A	2.93	118.34	108.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PCG	2	0
2	B	801	PCG	2	0
2	C	801	PCG	2	0
2	D	801	PCG	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.