



# Full wwPDB X-ray Structure Validation Report

Sep 21, 2014 – 10:43 AM EDT

PDB ID : 1VY9  
Title : Crystal structure of the E. coli CRISPR RNA-guided surveillance complex, Cascade  
Authors : Jackson, R.N.; Golden, S.M.; Carter, J.; Wiedenheft, B.  
Deposited on : 2014-06-28  
Resolution : 3.24 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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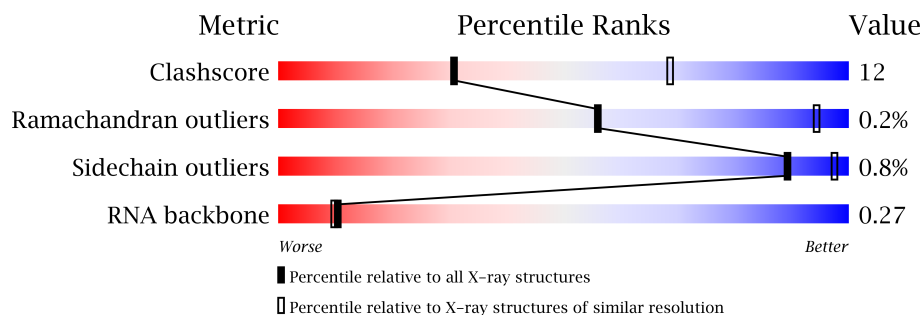
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 3.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RNA backbone	1838	1006 (3.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	J	165	
1	K	165	
2	B	363	
2	C	363	
2	D	363	
2	E	363	
2	F	363	
2	G	363	
3	A	199	
4	H	224	
5	L	61	
6	I	502	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 51732 atoms, of which 25183 are hydrogens and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR system Cascade subunit CasB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	K	157	Total	C	H	N	O	S	0	0	0
			2524	795	1254	245	223	7			
1	J	157	Total	C	H	N	O	S	0	0	0
			2551	800	1280	248	216	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	GLY	-	expression tag	UNP P76632
K	-3	PRO	-	expression tag	UNP P76632
K	-2	GLY	-	expression tag	UNP P76632
K	-1	TYR	-	expression tag	UNP P76632
K	0	GLN	-	expression tag	UNP P76632
J	-4	GLY	-	expression tag	UNP P76632
J	-3	PRO	-	expression tag	UNP P76632
J	-2	GLY	-	expression tag	UNP P76632
J	-1	TYR	-	expression tag	UNP P76632
J	0	GLN	-	expression tag	UNP P76632

- Molecule 2 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	356	Total	C	H	N	O	S	0	0	0
			5396	1702	2681	487	511	15			
2	D	356	Total	C	H	N	O	S	0	0	0
			5165	1660	2518	476	497	14			
2	E	351	Total	C	H	N	O	S	0	0	0
			5237	1664	2582	476	501	14			
2	C	347	Total	C	H	N	O	S	0	0	0
			5023	1610	2455	469	475	14			
2	B	345	Total	C	H	N	O	S	0	0	0
			4922	1590	2389	458	471	14			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	353	Total	C	H	N	O	S	0	0	0
			5306	1681	2621	482	507	15			

- Molecule 3 is a protein called CRISPR system Cascade subunit CasE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	192	Total	C	H	N	O	S	0	0	0
			2991	954	1506	262	262	7			

- Molecule 4 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	219	Total	C	H	N	O	S	0	0	0
			3434	1093	1708	307	317	9			

- Molecule 5 is a RNA chain called Escherichia coli strain ECOR44 cluster 1 CRISPR region.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	L	61	Total	C	H	N	O	P	0	0	0
			1957	580	657	233	426	61			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	42	A	C	conflict	GB 50811866
L	53	C	U	conflict	GB 50811866

- Molecule 6 is a protein called CRISPR system Cascade subunit CasA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	I	493	Total	C	H	N	O	S	0	0	0
			7225	2356	3532	658	660	19			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Zn	0	0
			1	1		

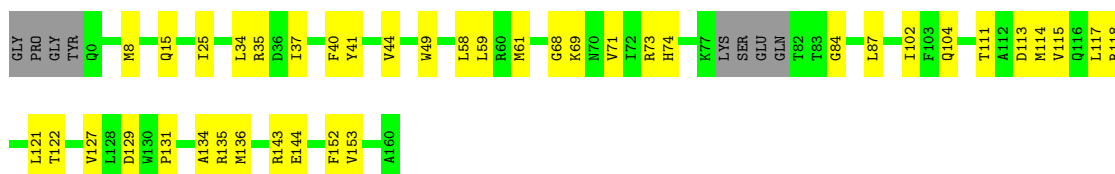
### 3 Residue-property plots

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

Note EDS was not executed.

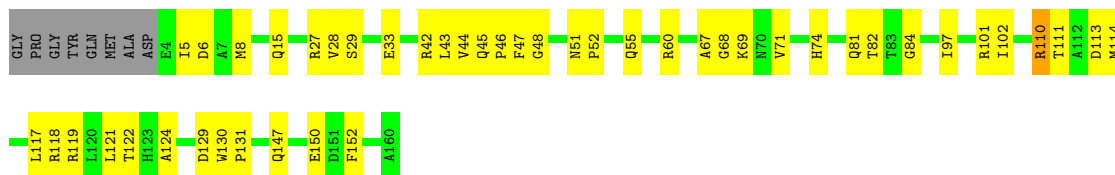
- Molecule 1: CRISPR system Cascade subunit CasB

Chain K: 



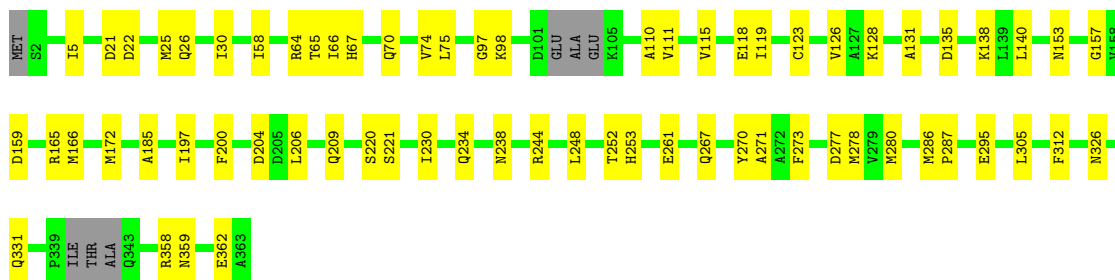
- Molecule 1: CRISPR system Cascade subunit CasB

Chain J: 



- Molecule 2: CRISPR system Cascade subunit CasC

Chain F: 



- Molecule 2: CRISPR system Cascade subunit CasC

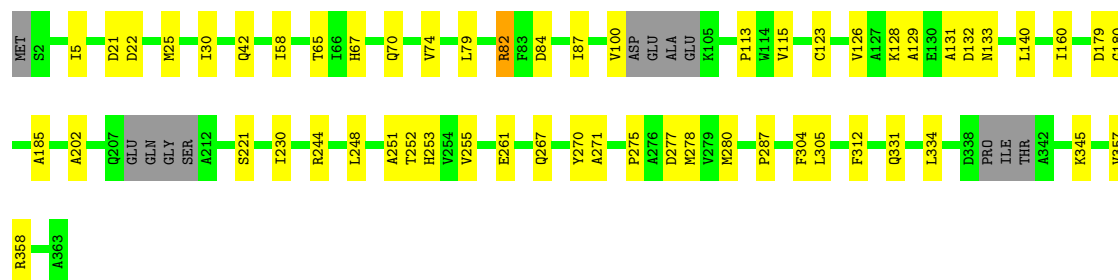
Chain D: 





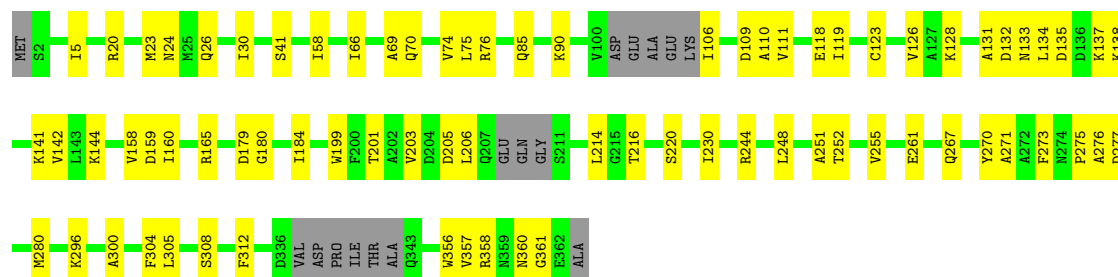
• Molecule 2: CRISPR system Cascade subunit CasC

Chain E:



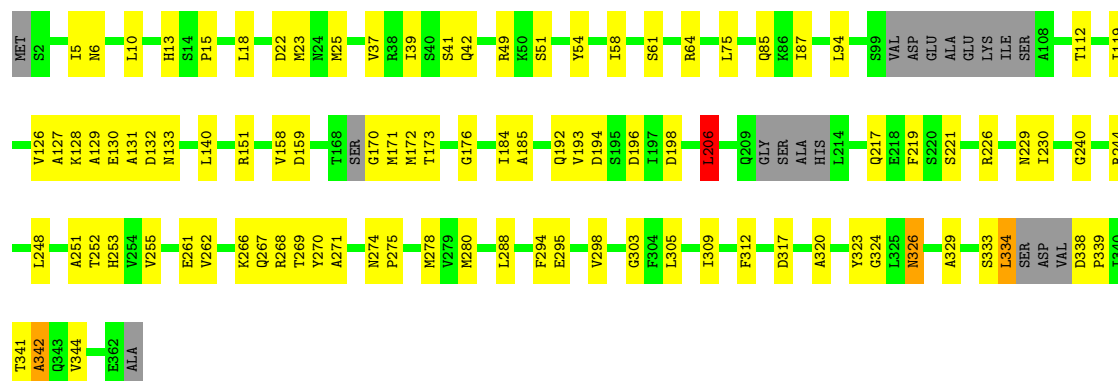
• Molecule 2: CRISPR system Cascade subunit CasC

Chain C:



• Molecule 2: CRISPR system Cascade subunit CasC

Chain B:



• Molecule 2: CRISPR system Cascade subunit CasC

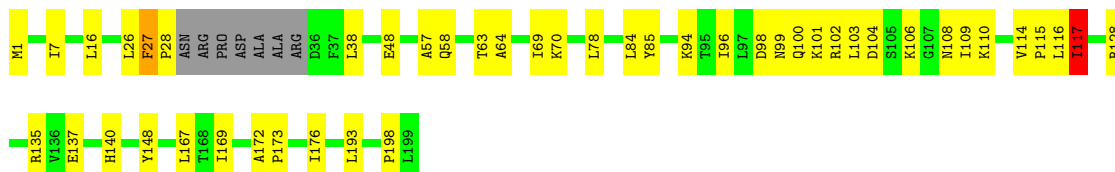
Chain G:





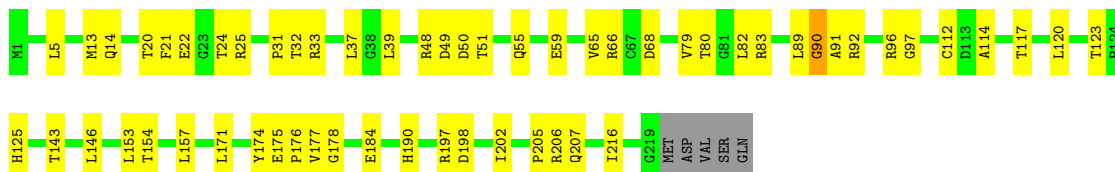
• Molecule 3: CRISPR system Cascade subunit CasE

Chain A:



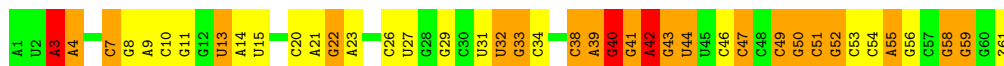
• Molecule 4: CRISPR system Cascade subunit CasD

Chain H:



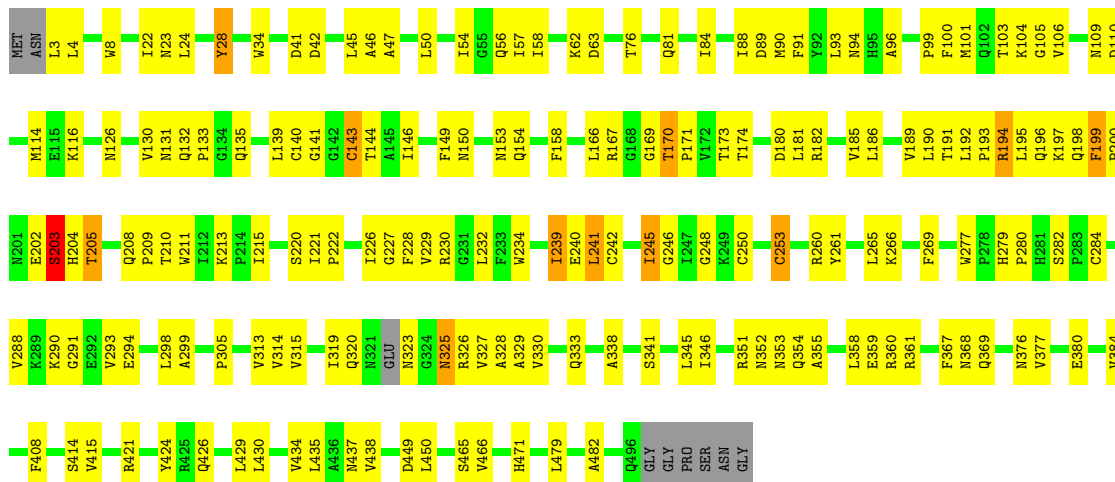
• Molecule 5: Escherichia coli strain ECOR44 cluster 1 CRISPR region

Chain L:



• Molecule 6: CRISPR system Cascade subunit CasA

Chain I:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.85Å 214.54Å 217.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.61 – 3.24	Depositor
% Data completeness (in resolution range)	99.8 (39.61-3.24)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, $R_{free}$	0.234 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 23G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	J	0.28	0/1296	0.53	0/1751
1	K	0.29	0/1294	0.55	0/1751
2	B	0.31	0/2573	0.65	2/3491 (0.1%)
2	C	0.30	0/2608	0.59	0/3530
2	D	0.29	0/2690	0.58	0/3649
2	E	0.31	0/2696	0.58	2/3648 (0.1%)
2	F	0.31	0/2757	0.59	0/3723
2	G	0.32	0/2728	0.65	2/3687 (0.1%)
3	A	0.28	0/1516	0.55	0/2056
4	H	0.28	0/1768	0.58	1/2402 (0.0%)
5	L	0.38	0/1423	1.02	4/2216 (0.2%)
6	I	0.33	0/3782	0.65	2/5159 (0.0%)
All	All	0.31	0/27131	0.64	13/37063 (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
2	B	0	3
2	E	0	1
2	F	0	1
2	G	0	1
3	A	0	1
4	H	0	2
6	I	0	3
All	All	0	12

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	194	ARG	NE-CZ-NH1	8.31	124.46	120.30
2	G	86	LYS	CD-CE-NZ	-7.60	94.22	111.70
2	E	82	ARG	NE-CZ-NH1	7.44	124.02	120.30
6	I	194	ARG	NE-CZ-NH2	-6.94	116.83	120.30
4	H	90	GLY	N-CA-C	-5.61	99.07	113.10
2	B	303	GLY	N-CA-C	-5.58	99.16	113.10
5	L	20	C	C2-N1-C1'	5.51	124.86	118.80
5	L	42	A	O4'-C1'-N9	5.50	112.60	108.20
5	L	3	A	O5'-P-OP2	-5.40	100.84	105.70
2	G	210	GLY	N-CA-C	-5.12	100.30	113.10
2	B	206	LEU	CA-CB-CG	5.11	127.05	115.30
5	L	40	G	O4'-C1'-N9	5.08	112.27	108.20
2	E	82	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	106	LYS	Peptide
2	B	206	LEU	Peptide
2	B	221	SER	Peptide
2	B	342	ALA	Peptide
2	E	132	ASP	Peptide
2	F	326	ASN	Peptide
2	G	166	MET	Peptide
4	H	174	TYR	Peptide
4	H	89	LEU	Peptide
6	I	203	SER	Peptide
6	I	245	ILE	Peptide
6	I	76	THR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1271	1280	0	35	0
1	K	1270	1254	3	24	0
2	B	2533	2389	0	79	0
2	C	2568	2455	1	62	0
2	D	2647	2518	0	46	0
2	E	2655	2582	1	49	0
2	F	2715	2681	1	59	0
2	G	2685	2621	1	58	0
3	A	1485	1506	0	36	0
4	H	1726	1708	0	43	0
5	L	1300	657	0	39	0
6	I	3693	3532	1	156	0
7	I	1	0	0	0	0
All	All	26549	25183	8	609	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (609) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:73:ASP:OD1	2:D:77:GLN:NE2	1.90	1.03
5:L:52:G:N7	5:L:55:A:N6	2.06	1.03
2:B:64:ARG:NH2	2:B:159:ASP:OD2	2.02	0.92
2:B:58:ILE:HG22	2:B:158:VAL:HG11	1.52	0.92
2:G:244:ARG:NH1	2:G:360:ASN:OD1	2.05	0.89
2:B:58:ILE:CG2	2:B:158:VAL:HG11	2.07	0.85
1:J:27:ARG:NH2	2:B:22:ASP:OD1	2.12	0.83
2:G:179:ASP:OD2	4:H:48:ARG:NH2	2.12	0.82
6:I:359:GLU:OE1	6:I:361:ARG:NH1	2.12	0.81
2:B:326:ASN:ND2	2:B:326:ASN:O	2.13	0.79
2:D:66:ILE:HG23	2:D:111:VAL:HG12	1.63	0.79
2:F:66:ILE:CG2	2:F:111:VAL:HG22	2.13	0.78
2:C:276:ALA:O	2:B:323:TYR:OH	2.02	0.77
6:I:139:LEU:O	6:I:261:TYR:N	2.16	0.77
2:G:168:THR:OG1	4:H:92:ARG:N	2.18	0.76
2:E:79:LEU:HD22	2:E:82:ARG:NH2	2.01	0.76
6:I:351:ARG:NH1	6:I:359:GLU:OE2	2.20	0.75
6:I:57:ILE:HD11	6:I:229:VAL:HG22	1.69	0.73
6:I:210:THR:HG22	6:I:215:ILE:HD11	1.72	0.72
2:C:58:ILE:HG22	2:C:158:VAL:HG21	1.72	0.72
2:G:153:ASN:ND2	2:G:169:SER:OG	2.22	0.72
4:H:146:LEU:HD12	4:H:146:LEU:O	1.90	0.71
2:G:199:TRP:CH2	2:G:214:LEU:HD22	2.25	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:37:VAL:HG23	2:B:193:VAL:HG21	1.71	0.71
6:I:250:CYS:SG	6:I:253:CYS:HB2	2.31	0.70
2:G:158:VAL:HA	2:G:239:LEU:HD21	1.72	0.70
4:H:21:PHE:O	6:I:131:ASN:ND2	2.24	0.70
2:F:206:LEU:HD12	2:E:65:THR:HG21	1.74	0.69
6:I:57:ILE:HD11	6:I:229:VAL:CG2	2.22	0.69
3:A:172:ALA:HB3	3:A:173:PRO:HD3	1.74	0.69
2:C:20:ARG:NH1	2:C:24:ASN:OD1	2.26	0.69
5:L:42:A:O2'	5:L:43:G:O5'	2.11	0.69
2:G:202:ALA:HB2	5:L:13:U:H1'	1.74	0.68
2:C:159:ASP:OD1	2:C:160:ILE:HD12	1.91	0.68
6:I:22:ILE:HG21	6:I:34:TRP:HZ3	1.58	0.68
2:B:342:ALA:HB1	2:B:344:VAL:H	1.57	0.68
6:I:181:LEU:O	6:I:185:VAL:HG23	1.94	0.67
6:I:22:ILE:HG21	6:I:34:TRP:CZ3	2.29	0.67
2:C:58:ILE:HG21	2:C:158:VAL:HG11	1.77	0.67
6:I:191:THR:HG22	6:I:194:ARG:HD2	1.76	0.67
2:F:70:GLN:O	2:F:74:VAL:HG23	1.95	0.66
2:F:166:MET:HE1	5:L:11:G:C2	2.30	0.66
5:L:46:C:H2'	5:L:47:C:H5''	1.77	0.66
6:I:126:ASN:O	6:I:130:VAL:HG22	1.95	0.66
1:J:15:GLN:NE2	1:J:69:LYS:O	2.22	0.66
2:F:185:ALA:HB2	2:G:271:ALA:HB3	1.77	0.66
4:H:51:THR:HG23	4:H:202:ILE:HG22	1.78	0.66
6:I:315:VAL:O	6:I:325:ASN:ND2	2.25	0.66
2:B:268:ARG:NH1	2:B:274:ASN:O	2.29	0.65
2:D:206:LEU:HD13	2:C:70:GLN:HB3	1.79	0.65
2:F:277:ASP:OD2	2:F:305:LEU:HD21	1.97	0.65
1:J:113:ASP:OD1	1:J:114:MET:N	2.30	0.65
2:G:25:MET:HE1	6:I:414:SER:O	1.95	0.65
2:B:206:LEU:O	2:B:206:LEU:HD12	1.96	0.65
3:A:99:ASN:N	5:L:44:U:O4	2.28	0.65
6:I:88:ILE:HG23	6:I:91:PHE:CE2	2.31	0.65
2:D:185:ALA:HB2	2:E:271:ALA:HB3	1.78	0.65
6:I:210:THR:CG2	6:I:215:ILE:HD11	2.25	0.65
4:H:13:MET:HE3	4:H:82:LEU:HD12	1.77	0.65
2:B:51:SER:OG	2:B:261:GLU:OE1	2.09	0.65
2:E:277:ASP:OD2	2:E:305:LEU:HD21	1.97	0.64
1:K:104:GLN:HB2	2:F:197:ILE:HD11	1.79	0.64
1:K:113:ASP:OD1	1:K:114:MET:N	2.30	0.64
2:B:192:GLN:NE2	2:B:196:ASP:OD2	2.31	0.64
2:C:244:ARG:NH2	2:C:360:ASN:OD1	2.29	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:35:ARG:NH1	1:K:59:LEU:HD11	2.13	0.64
2:C:58:ILE:CG2	2:C:158:VAL:HG21	2.28	0.64
1:J:147:GLN:NE2	1:J:150:GLU:OE1	2.31	0.63
2:B:18:LEU:HD22	2:B:39:ILE:HD11	1.81	0.63
2:C:138:LYS:O	2:C:142:VAL:HG23	1.98	0.63
2:B:23:MET:HE1	2:B:25:MET:HE2	1.80	0.63
2:F:271:ALA:HB3	2:E:185:ALA:HB2	1.81	0.63
6:I:193:PRO:O	6:I:197:LYS:N	2.31	0.63
2:F:65:THR:HG21	2:G:206:LEU:HD12	1.80	0.62
6:I:3:LEU:N	6:I:90:MET:O	2.31	0.62
6:I:47:ALA:HB2	6:I:146:ILE:HD13	1.82	0.62
6:I:314:VAL:HG11	6:I:367:PHE:HE2	1.61	0.62
2:C:248:LEU:O	2:C:252:THR:HG23	1.99	0.62
2:D:172:MET:O	2:D:176:GLY:N	2.25	0.62
4:H:80:THR:N	4:H:112:CYS:O	2.33	0.62
6:I:114:MET:HB3	6:I:139:LEU:HD12	1.80	0.62
6:I:100:PHE:HB2	6:I:211:TRP:CD2	2.35	0.61
2:C:123:CYS:HA	2:C:126:VAL:HG12	1.81	0.61
2:B:13:HIS:CD2	2:B:18:LEU:HD21	2.35	0.61
6:I:28:TYR:HE1	6:I:186:LEU:HD21	1.65	0.61
6:I:62:LYS:HB3	6:I:63:ASP:HA	1.83	0.61
6:I:139:LEU:HD22	6:I:143:CYS:SG	2.41	0.61
2:C:300:ALA:HB2	2:C:304:PHE:CE1	2.36	0.60
2:C:26:GLN:NE2	2:C:220:SER:OG	2.32	0.60
3:A:78:LEU:HB3	3:A:169:ILE:HD13	1.81	0.60
2:D:90:LYS:O	2:D:94:LEU:HD12	2.01	0.60
2:G:336:ASP:HB3	2:G:337:VAL:HA	1.83	0.60
2:E:58:ILE:HD11	2:E:253:HIS:HB3	1.84	0.60
6:I:56:GLN:HA	6:I:189:VAL:HG13	1.83	0.60
3:A:26:LEU:HD23	3:A:63:THR:HG23	1.82	0.60
2:F:58:ILE:HD11	2:F:253:HIS:HB3	1.83	0.60
6:I:288:VAL:HG23	6:I:323:ASN:OD1	2.01	0.60
2:E:70:GLN:O	2:E:74:VAL:HG23	2.02	0.60
2:F:209:GLN:OE1	5:L:22:G:O2'	2.18	0.60
5:L:32:U:H2'	5:L:33:G:H4'	1.84	0.59
2:B:269:THR:HG23	2:B:270:TYR:HD1	1.66	0.59
2:E:79:LEU:HD22	2:E:82:ARG:HH22	1.65	0.59
2:F:166:MET:HE1	5:L:11:G:N2	2.16	0.59
6:I:4:LEU:HD22	6:I:24:LEU:HD13	1.83	0.59
6:I:245:ILE:N	6:I:260:ARG:O	2.28	0.59
2:B:226:ARG:NH1	2:B:261:GLU:O	2.33	0.59
2:F:221:SER:OG	2:E:30:ILE:O	2.21	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:79:LEU:HD11	2:G:119:ILE:CD1	2.33	0.59
6:I:239:ILE:HG22	6:I:266:LYS:HB3	1.85	0.59
2:B:329:ALA:CB	2:B:344:VAL:HG22	2.33	0.59
6:I:241:LEU:HD12	6:I:242:CYS:N	2.17	0.59
1:J:60:ARG:HG2	1:J:114:MET:HE3	1.85	0.59
2:D:202:ALA:HB1	2:C:111:VAL:HG21	1.83	0.59
2:E:277:ASP:OD1	2:E:334:LEU:HD12	2.03	0.58
6:I:196:GLN:O	6:I:200:PRO:HA	2.02	0.58
2:C:159:ASP:OD1	2:C:160:ILE:N	2.36	0.58
2:G:3:ASN:ND2	2:G:231:ASN:OD1	2.36	0.58
4:H:33:ARG:NH1	4:H:37:LEU:HD11	2.18	0.58
6:I:104:LYS:HD3	6:I:105:GLY:H	1.68	0.58
2:C:70:GLN:O	2:C:74:VAL:HG23	2.02	0.58
2:G:338:ASP:OD2	2:G:346:GLN:NE2	2.37	0.58
6:I:4:LEU:CD2	6:I:24:LEU:HD13	2.33	0.58
2:C:201:THR:HG21	5:L:39:A:N3	2.18	0.58
6:I:167:ARG:HH12	6:I:173:THR:HG22	1.69	0.58
4:H:175:GLU:HB2	4:H:176:PRO:HD3	1.85	0.58
6:I:195:LEU:HD11	6:I:228:PHE:CD1	2.39	0.57
6:I:195:LEU:HD12	6:I:199:PHE:CE1	2.39	0.57
6:I:277:TRP:HZ3	6:I:279:HIS:HA	1.69	0.57
2:G:79:LEU:HD11	2:G:119:ILE:HD11	1.86	0.57
6:I:8:TRP:CH2	6:I:50:LEU:HD23	2.39	0.57
6:I:141:GLY:O	6:I:144:THR:HG22	2.04	0.57
6:I:195:LEU:HD12	6:I:199:PHE:HE1	1.70	0.57
6:I:195:LEU:HD11	6:I:228:PHE:CE1	2.39	0.57
3:A:27:PHE:HB2	3:A:28:PRO:HD3	1.86	0.57
2:D:111:VAL:HG21	2:E:202:ALA:HB1	1.86	0.57
6:I:100:PHE:HB2	6:I:211:TRP:CE2	2.40	0.57
2:B:18:LEU:CD2	2:B:39:ILE:HD11	2.34	0.57
2:C:66:ILE:HG23	2:C:111:VAL:HG12	1.86	0.57
2:F:206:LEU:CD1	2:E:65:THR:HG21	2.35	0.57
6:I:88:ILE:O	6:I:88:ILE:HG22	2.05	0.57
2:F:252:THR:HG21	2:F:358:ARG:CG	2.35	0.57
2:G:74:VAL:HG11	2:G:111:VAL:HG23	1.87	0.57
2:G:122:PHE:HE2	2:G:147:ILE:HG22	1.69	0.57
2:B:192:GLN:NE2	2:B:194:ASP:O	2.38	0.56
2:B:267:GLN:N	2:B:267:GLN:OE1	2.38	0.56
4:H:31:PRO:HD2	4:H:65:VAL:HG11	1.87	0.56
2:D:248:LEU:O	2:D:252:THR:HG23	2.05	0.56
4:H:22:GLU:OE2	6:I:360:ARG:NH1	2.39	0.56
2:E:248:LEU:O	2:E:252:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:81:GLN:O	1:J:82:THR:OG1	2.19	0.56
2:B:329:ALA:C	2:B:344:VAL:HG13	2.25	0.56
2:G:286:MET:HE3	4:H:157:LEU:HG	1.87	0.56
2:E:126:VAL:O	2:E:129:ALA:HB3	2.06	0.56
2:G:286:MET:HE1	4:H:153:LEU:CD1	2.36	0.56
6:I:81:GLN:HA	6:I:84:ILE:HD12	1.88	0.56
2:G:194:ASP:HB3	6:I:471:HIS:CD2	2.41	0.56
6:I:192:LEU:O	6:I:192:LEU:HD23	2.06	0.56
1:K:87:LEU:HD23	1:K:136:MET:HE1	1.88	0.56
2:E:5:ILE:HG22	2:E:230:ILE:HB	1.88	0.55
6:I:325:ASN:C	6:I:325:ASN:HD21	2.10	0.55
1:J:60:ARG:CG	1:J:114:MET:HE3	2.36	0.55
2:B:127:ALA:O	2:B:130:GLU:N	2.38	0.55
2:F:5:ILE:HG22	2:F:230:ILE:HB	1.87	0.55
2:F:66:ILE:HG22	2:F:111:VAL:HG22	1.88	0.55
6:I:100:PHE:CG	6:I:101:MET:N	2.74	0.55
2:F:248:LEU:O	2:F:252:THR:HG23	2.07	0.55
2:B:58:ILE:HD11	2:B:253:HIS:HB3	1.89	0.54
2:F:128:LYS:O	2:F:131:ALA:HB3	2.07	0.54
2:G:167:ALA:HA	2:G:169:SER:H	1.72	0.54
6:I:169:GLY:O	6:I:170:THR:OG1	2.22	0.54
6:I:192:LEU:HD23	6:I:192:LEU:C	2.28	0.54
2:F:206:LEU:HD12	2:E:65:THR:CG2	2.35	0.54
2:G:4:PHE:HE1	4:H:143:THR:HG22	1.72	0.54
5:L:40:G:O2'	5:L:41:G:O5'	2.18	0.54
2:B:13:HIS:NE2	2:B:18:LEU:HD21	2.23	0.54
2:B:49:ARG:HA	2:B:54:TYR:CE2	2.42	0.54
2:F:165:ARG:NH1	2:F:172:MET:HE1	2.22	0.54
2:D:359:ASN:HB3	2:D:362:GLU:HB2	1.90	0.54
6:I:298:LEU:HD23	6:I:299:ALA:N	2.22	0.54
6:I:57:ILE:HD11	6:I:229:VAL:HG13	1.90	0.54
2:C:304:PHE:N	2:B:295:GLU:OE1	2.40	0.54
2:C:5:ILE:HG22	2:C:230:ILE:HB	1.90	0.54
6:I:88:ILE:HD12	6:I:91:PHE:HE2	1.73	0.54
5:L:40:G:O2'	5:L:41:G:P	2.65	0.54
4:H:59:GLU:O	4:H:123:THR:HG21	2.08	0.54
2:G:168:THR:N	4:H:91:ALA:HB1	2.23	0.54
6:I:240:GLU:N	6:I:265:LEU:O	2.41	0.54
6:I:191:THR:HG21	6:I:194:ARG:NH1	2.23	0.53
6:I:57:ILE:HD11	6:I:229:VAL:CG1	2.37	0.53
6:I:290:LYS:N	6:I:291:GLY:HA3	2.22	0.53
1:K:117:LEU:O	1:K:121:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:78:LEU:HD12	3:A:176:ILE:HG13	1.89	0.53
6:I:203:SER:N	6:I:204:HIS:HB2	2.23	0.53
3:A:108:ASN:OD1	3:A:109:ILE:N	2.40	0.53
2:B:18:LEU:HD12	2:B:18:LEU:H	1.73	0.53
2:B:333:SER:HB2	2:B:334:LEU:HA	1.91	0.53
2:B:94:LEU:O	2:B:171:MET:CB	2.57	0.53
2:C:128:LYS:O	2:C:131:ALA:HB3	2.09	0.53
2:C:277:ASP:OD2	2:C:305:LEU:HD21	2.10	0.53
2:E:179:ASP:OD1	2:E:180:GLY:N	2.40	0.53
2:F:252:THR:HG21	2:F:358:ARG:HG3	1.91	0.53
1:K:8:MET:SD	1:K:74:HIS:NE2	2.82	0.53
2:C:141:LYS:O	2:C:144:LYS:NZ	2.36	0.52
6:I:353:ASN:OD1	6:I:358:LEU:HD11	2.09	0.52
2:C:132:ASP:CB	2:C:134:LEU:N	2.73	0.52
2:C:76:ARG:NE	2:C:85:GLN:OE1	2.43	0.52
2:E:21:ASP:OD1	2:E:22:ASP:N	2.39	0.52
2:E:84:ASP:HB2	2:E:87:ILE:HG12	1.90	0.52
2:B:248:LEU:O	2:B:252:THR:HG23	2.09	0.52
6:I:210:THR:HG22	6:I:215:ILE:CD1	2.37	0.52
6:I:426:GLN:OE1	6:I:429:LEU:HD12	2.10	0.52
2:B:15:PRO:HB2	3:A:140:HIS:NE2	2.25	0.52
2:F:123:CYS:HA	2:F:126:VAL:HG12	1.91	0.52
4:H:49:ASP:OD1	4:H:50:ASP:N	2.43	0.52
6:I:194:ARG:HH11	6:I:194:ARG:HG3	1.73	0.52
1:K:41:TYR:CE1	1:J:150:GLU:HG2	2.45	0.52
2:B:41:SER:HB2	2:B:184:ILE:HG23	1.92	0.52
6:I:376:ASN:OD1	6:I:377:VAL:N	2.42	0.52
2:C:69:ALA:HB2	2:C:106:ILE:N	2.24	0.52
2:D:172:MET:O	2:D:175:LEU:N	2.42	0.52
2:E:280:MET:HE2	2:E:312:PHE:HZ	1.73	0.52
2:G:315:TYR:CE1	2:G:319:VAL:HG21	2.45	0.52
2:B:128:LYS:O	2:B:131:ALA:HB3	2.10	0.52
2:D:30:ILE:O	2:E:221:SER:OG	2.27	0.52
2:D:166:MET:HE2	5:L:23:A:C4	2.45	0.52
2:E:244:ARG:O	2:E:248:LEU:HD12	2.10	0.51
2:G:167:ALA:HA	2:G:169:SER:N	2.25	0.51
2:G:228:ALA:HB2	2:G:258:LEU:HD21	1.92	0.51
6:I:166:LEU:HD21	6:I:234:TRP:CE2	2.45	0.51
1:J:42:ARG:NH2	3:A:148:TYR:CG	2.78	0.51
2:F:204:ASP:OD2	2:E:67:HIS:CE1	2.63	0.51
2:C:41:SER:HB2	2:C:184:ILE:HG23	1.91	0.51
3:A:38:LEU:N	3:A:38:LEU:HD12	2.24	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:84:LEU:HD12	3:A:169:ILE:HD11	1.93	0.51
2:F:64:ARG:NH2	2:F:159:ASP:OD2	2.43	0.51
2:G:240:GLY:HA2	2:G:241:GLY:C	2.30	0.51
6:I:345:LEU:HD23	6:I:346:ILE:N	2.26	0.51
1:J:52:PRO:HA	1:J:55:GLN:HG3	1.92	0.51
3:A:48:GLU:OE1	3:A:48:GLU:N	2.43	0.51
2:D:41:SER:HB2	2:D:184:ILE:HG23	1.92	0.51
2:B:172:MET:O	2:B:176:GLY:N	2.40	0.51
2:B:6:ASN:ND2	2:B:229:ASN:OD1	2.44	0.51
2:E:128:LYS:O	2:E:131:ALA:HB3	2.11	0.51
6:I:199:PHE:CD1	6:I:199:PHE:N	2.79	0.51
6:I:215:ILE:HB	6:I:269:PHE:HE2	1.76	0.51
3:A:100:GLN:HG3	3:A:101:LYS:H	1.75	0.51
2:B:274:ASN:N	2:B:274:ASN:OD1	2.44	0.51
6:I:368:ASN:OD1	6:I:369:GLN:N	2.43	0.51
6:I:434:VAL:O	6:I:438:VAL:HG13	2.10	0.51
2:C:179:ASP:OD1	2:C:180:GLY:N	2.44	0.51
2:C:5:ILE:CG2	2:C:230:ILE:HB	2.41	0.51
2:D:221:SER:OG	2:C:30:ILE:O	2.29	0.51
2:F:30:ILE:O	2:G:221:SER:OG	2.27	0.51
6:I:245:ILE:O	6:I:260:ARG:N	2.42	0.51
3:A:128:ARG:NH1	5:L:58:G:OP1	2.39	0.51
3:A:115:PRO:HB2	3:A:117:ILE:HG22	1.93	0.50
2:F:244:ARG:HG2	2:F:248:LEU:CD1	2.41	0.50
2:B:10:LEU:HB2	2:B:278:MET:HB3	1.92	0.50
1:K:25:ILE:HG23	1:K:34:LEU:HD11	1.92	0.50
2:E:5:ILE:CG2	2:E:230:ILE:HB	2.40	0.50
2:F:295:GLU:OE1	2:G:304:PHE:N	2.44	0.50
1:J:29:SER:OG	1:J:33:GLU:OE1	2.24	0.50
1:K:118:ARG:O	1:K:122:THR:HG23	2.12	0.50
2:F:280:MET:HE2	2:F:312:PHE:HZ	1.77	0.50
2:E:129:ALA:O	2:E:133:ASN:HB3	2.12	0.50
6:I:88:ILE:HD12	6:I:91:PHE:CE2	2.46	0.50
1:J:44:VAL:O	1:J:44:VAL:HG22	2.12	0.50
6:I:180:ASP:OD1	6:I:181:LEU:N	2.45	0.50
4:H:79:VAL:HG12	4:H:80:THR:H	1.76	0.50
2:B:49:ARG:O	2:B:61:SER:OG	2.26	0.49
6:I:245:ILE:HG22	6:I:246:GLY:N	2.27	0.49
2:B:132:ASP:CB	2:B:133:ASN:C	2.80	0.49
2:D:341:THR:O	2:D:344:VAL:HG22	2.12	0.49
6:I:101:MET:HE1	6:I:241:LEU:H	1.76	0.49
2:B:262:VAL:HB	2:B:266:LYS:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:333:SER:HB2	2:B:334:LEU:CA	2.42	0.49
2:D:90:LYS:C	2:D:94:LEU:HD12	2.33	0.49
2:E:123:CYS:HA	2:E:126:VAL:HG12	1.93	0.49
6:I:116:LYS:HB3	6:I:158:PHE:CZ	2.46	0.49
6:I:226:ILE:N	6:I:227:GLY:HA2	2.27	0.49
3:A:116:LEU:C	3:A:117:ILE:HG23	2.32	0.49
2:F:135:ASP:O	2:F:138:LYS:N	2.46	0.49
6:I:434:VAL:O	6:I:437:ASN:N	2.43	0.49
6:I:89:ASP:C	6:I:90:MET:HE2	2.33	0.49
2:G:132:ASP:CB	2:G:133:ASN:HA	2.43	0.49
2:G:147:ILE:HG13	2:G:148:ALA:N	2.27	0.49
1:K:111:THR:O	1:K:115:VAL:HG23	2.11	0.49
4:H:207:GLN:NE2	6:I:135:GLN:OE1	2.45	0.49
6:I:96:ALA:O	6:I:104:LYS:HG2	2.12	0.49
2:C:135:ASP:O	2:C:138:LYS:N	2.46	0.49
2:C:356:TRP:CE2	2:C:361:GLY:HA2	2.48	0.49
2:B:333:SER:HB2	2:B:334:LEU:CB	2.42	0.49
2:G:139:LEU:O	2:G:142:VAL:HG22	2.12	0.49
6:I:99:PRO:HB2	6:I:100:PHE:C	2.33	0.49
6:I:170:THR:CG2	6:I:352:ASN:HB3	2.43	0.49
1:K:15:GLN:NE2	1:K:69:LYS:O	2.35	0.49
4:H:90:GLY:HA3	4:H:91:ALA:HB2	1.95	0.48
1:J:84:GLY:HA3	1:J:129:ASP:HB2	1.95	0.48
1:J:28:VAL:CG2	1:J:33:GLU:HB3	2.43	0.48
2:E:21:ASP:HB3	2:E:25:MET:H	1.78	0.48
2:G:49:ARG:NH1	2:G:163:SER:HB2	2.27	0.48
6:I:105:GLY:O	6:I:106:VAL:HG22	2.13	0.48
1:J:48:GLY:O	1:J:51:ASN:N	2.46	0.48
4:H:177:VAL:HG12	4:H:178:GLY:N	2.28	0.48
6:I:22:ILE:HG22	6:I:23:ASN:O	2.14	0.48
2:D:244:ARG:O	2:D:248:LEU:HD12	2.14	0.48
2:E:251:ALA:O	2:E:255:VAL:HG23	2.13	0.48
4:H:146:LEU:HD23	4:H:153:LEU:HD23	1.95	0.48
1:J:67:ALA:HB1	1:J:122:THR:HG23	1.95	0.48
4:H:190:HIS:CE1	4:H:216:ILE:HG23	2.48	0.48
6:I:248:GLY:N	6:I:260:ARG:HE	2.11	0.48
1:J:44:VAL:C	1:J:46:PRO:HD2	2.33	0.48
6:I:24:LEU:O	6:I:24:LEU:HD23	2.14	0.48
5:L:50:G:H2'	5:L:51:C:H5'	1.96	0.48
3:A:94:LYS:O	3:A:114:VAL:HG22	2.14	0.48
2:B:320:ALA:O	2:B:324:GLY:HA2	2.14	0.48
2:C:244:ARG:O	2:C:248:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:244:ARG:HG2	2:E:248:LEU:CD1	2.44	0.48
6:I:195:LEU:O	6:I:199:PHE:HD1	1.95	0.48
2:B:317:ASP:CG	2:B:341:THR:HG21	2.34	0.48
6:I:226:ILE:CB	6:I:277:TRP:HE1	2.27	0.48
2:D:251:ALA:O	2:D:255:VAL:HG23	2.14	0.47
2:E:100:VAL:O	2:E:100:VAL:HG13	2.13	0.47
2:E:140:LEU:HD23	2:E:140:LEU:O	2.14	0.47
6:I:208:GLN:CB	6:I:213:LYS:CB	2.92	0.47
6:I:220:SER:HA	6:I:221:ILE:CB	2.44	0.47
6:I:101:MET:CE	6:I:241:LEU:H	2.27	0.47
1:K:143:ARG:HG3	1:K:144:GLU:OE2	2.14	0.47
2:C:252:THR:HG22	2:C:357:VAL:HB	1.96	0.47
6:I:170:THR:HG21	6:I:352:ASN:HB3	1.96	0.47
6:I:415:VAL:HG12	6:I:465:SER:HB3	1.95	0.47
6:I:449:ASP:OD1	6:I:450:LEU:N	2.47	0.47
2:C:251:ALA:O	2:C:255:VAL:HG23	2.15	0.47
2:D:118:GLU:N	2:D:153:ASN:OD1	2.47	0.47
2:F:5:ILE:CG2	2:F:230:ILE:HB	2.44	0.47
3:A:98:ASP:OD1	3:A:100:GLN:N	2.48	0.47
2:E:261:GLU:OE2	2:E:261:GLU:HA	2.14	0.47
1:J:117:LEU:O	1:J:121:LEU:HD12	2.13	0.47
1:K:49:TRP:HZ3	1:J:150:GLU:OE2	1.97	0.47
3:A:102:ARG:NH2	5:L:46:C:OP2	2.48	0.47
2:B:58:ILE:HG22	2:B:158:VAL:CG1	2.36	0.47
2:D:66:ILE:HG21	2:D:109:ASP:O	2.14	0.47
2:D:70:GLN:O	2:D:74:VAL:HG23	2.13	0.47
2:G:292:ASN:OD1	4:H:154:THR:HG21	2.14	0.47
6:I:196:GLN:O	6:I:200:PRO:CA	2.62	0.47
5:L:49:C:H5"	5:L:50:G:OP2	2.15	0.47
1:J:43:LEU:O	1:J:43:LEU:HD23	2.14	0.47
2:E:280:MET:HE2	2:E:312:PHE:CZ	2.49	0.47
2:F:21:ASP:N	2:F:25:MET:O	2.46	0.47
2:G:338:ASP:CG	2:G:339:PRO:HD2	2.34	0.47
1:J:44:VAL:C	1:J:46:PRO:CD	2.82	0.47
6:I:190:LEU:HD23	6:I:333:GLN:OE1	2.14	0.47
6:I:434:VAL:HG23	6:I:435:LEU:N	2.30	0.47
3:A:69:ILE:HG22	3:A:70:LYS:HG3	1.96	0.47
2:C:267:GLN:HA	2:C:270:TYR:O	2.14	0.47
4:H:197:ARG:NH2	6:I:41:ASP:OD1	2.38	0.47
1:J:8:MET:SD	1:J:74:HIS:NE2	2.88	0.47
2:D:20:ARG:NH2	5:L:29:G:OP2	2.47	0.47
2:G:25:MET:HE2	6:I:414:SER:H	1.78	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:I:284:CYS:SG	6:I:326:ARG:NH1	2.88	0.47
6:I:45:LEU:HD23	6:I:154:GLN:HE22	1.79	0.47
3:A:167:LEU:HD12	3:A:167:LEU:C	2.35	0.47
2:F:58:ILE:HG22	2:F:58:ILE:O	2.15	0.47
2:G:77:GLN:HG3	2:G:78:LYS:N	2.30	0.47
4:H:79:VAL:HG12	4:H:80:THR:N	2.30	0.47
2:B:269:THR:HG23	2:B:270:TYR:CD1	2.49	0.46
2:B:280:MET:HE2	2:B:312:PHE:CZ	2.50	0.46
1:K:84:GLY:HA3	1:K:129:ASP:HB2	1.97	0.46
2:B:329:ALA:HB1	2:B:344:VAL:HG22	1.97	0.46
2:C:261:GLU:OE2	2:C:261:GLU:HA	2.15	0.46
1:J:110:ARG:HG3	1:J:111:THR:N	2.30	0.46
5:L:8:G:O2'	5:L:10:C:OP1	2.23	0.46
2:C:199:TRP:CE3	2:C:216:THR:HG22	2.51	0.46
2:D:128:LYS:O	2:D:131:ALA:HB3	2.15	0.46
2:D:91:THR:HA	2:D:94:LEU:HD12	1.96	0.46
2:E:252:THR:HG21	2:E:358:ARG:CG	2.44	0.46
5:L:38:C:H2'	5:L:39:A:H4'	1.96	0.46
2:C:75:LEU:HD13	2:C:119:ILE:HG21	1.97	0.46
2:E:278:MET:SD	2:E:331:GLN:NE2	2.84	0.46
2:F:244:ARG:O	2:F:248:LEU:HD12	2.15	0.46
2:F:261:GLU:HA	2:F:261:GLU:OE2	2.15	0.46
2:F:280:MET:HE2	2:F:312:PHE:CZ	2.50	0.46
6:I:338:ALA:O	6:I:341:SER:OG	2.24	0.46
2:B:42:GLN:HG3	5:L:39:A:OP2	2.15	0.46
5:L:41:G:N3	5:L:41:G:C2'	2.77	0.46
2:C:277:ASP:OD2	2:C:305:LEU:CD2	2.64	0.46
2:D:132:ASP:CB	2:D:134:LEU:N	2.78	0.46
2:E:115:VAL:CG1	2:E:160:ILE:HD12	2.46	0.46
2:F:140:LEU:HD23	2:F:140:LEU:C	2.36	0.46
2:G:280:MET:HE3	2:G:312:PHE:CE1	2.51	0.46
2:G:45:LYS:CE	5:L:7:C:OP2	2.63	0.46
4:H:33:ARG:HD2	4:H:184:GLU:OE2	2.14	0.46
6:I:42:ASP:OD2	6:I:42:ASP:N	2.48	0.46
2:D:278:MET:SD	2:D:331:GLN:NE2	2.79	0.46
2:G:288:LEU:CD1	2:G:325:LEU:HD22	2.46	0.46
4:H:32:THR:HB	4:H:198:ASP:HB2	1.98	0.46
2:F:359:ASN:HB3	2:F:362:GLU:HB2	1.97	0.46
2:F:67:HIS:NE2	2:G:207:GLN:OE1	2.40	0.46
6:I:8:TRP:CZ2	6:I:50:LEU:HD23	2.51	0.46
2:G:139:LEU:HD12	2:G:140:LEU:N	2.30	0.46
6:I:24:LEU:CD2	6:I:28:TYR:CD2	2.99	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:118:ARG:O	1:J:122:THR:HG21	2.16	0.46
1:J:119:ARG:HB3	2:C:23:MET:HE1	1.98	0.46
2:D:190:THR:O	2:D:298:VAL:HG22	2.16	0.46
6:I:57:ILE:CD1	6:I:229:VAL:HG13	2.46	0.46
6:I:479:LEU:HD12	6:I:479:LEU:C	2.36	0.46
1:J:68:GLY:HA3	1:J:71:VAL:HG23	1.97	0.46
2:F:267:GLN:HA	2:F:270:TYR:O	2.16	0.46
2:F:97:GLY:HA2	2:F:98:LYS:HA	1.78	0.46
2:B:54:TYR:OH	2:B:158:VAL:HG23	2.15	0.45
5:L:42:A:O2'	5:L:43:G:P	2.74	0.45
2:G:280:MET:HE3	2:G:312:PHE:HE1	1.82	0.45
4:H:68:ASP:OD2	4:H:117:THR:OG1	2.34	0.45
6:I:479:LEU:HA	6:I:482:ALA:HB3	1.98	0.45
1:K:68:GLY:HA3	1:K:71:VAL:HG23	1.98	0.45
5:L:61:23G:H5'A	5:L:61:23G:H8	1.99	0.45
6:I:103:THR:HG22	6:I:239:ILE:O	2.16	0.45
6:I:239:ILE:HG22	6:I:266:LYS:CB	2.46	0.45
5:L:58:G:C2'	5:L:59:G:H5'	2.45	0.45
2:C:280:MET:HE2	2:C:312:PHE:HZ	1.81	0.45
2:F:75:LEU:HD11	2:F:119:ILE:HD13	1.99	0.45
3:A:63:THR:O	3:A:64:ALA:HB3	2.16	0.45
6:I:226:ILE:O	6:I:230:ARG:HB3	2.17	0.45
6:I:293:VAL:HG22	6:I:294:GLU:N	2.31	0.45
1:J:45:GLN:N	1:J:46:PRO:CD	2.79	0.45
5:L:49:C:C5'	5:L:50:G:OP2	2.65	0.45
3:A:114:VAL:HB	5:L:43:G:H2'	1.99	0.45
2:B:126:VAL:O	2:B:129:ALA:HB3	2.16	0.45
2:D:123:CYS:HA	2:D:126:VAL:HG12	1.97	0.45
2:E:113:PRO:HB2	2:E:160:ILE:HD11	1.97	0.45
6:I:280:PRO:O	6:I:330:VAL:HG23	2.17	0.45
2:C:199:TRP:HB3	2:C:214:LEU:HD23	1.99	0.45
6:I:209:PRO:HB3	6:I:211:TRP:CH2	2.52	0.45
4:H:123:THR:HG23	4:H:125:HIS:N	2.32	0.45
1:K:44:VAL:CG2	1:K:58:LEU:HD13	2.46	0.45
2:B:158:VAL:HG23	2:B:159:ASP:N	2.32	0.45
2:B:267:GLN:HB3	2:B:271:ALA:CB	2.47	0.45
6:I:202:GLU:O	6:I:205:THR:OG1	2.35	0.45
2:D:10:LEU:HD22	2:D:278:MET:HE2	1.98	0.45
2:D:302:ASP:O	2:C:296:LYS:HG3	2.17	0.45
2:F:75:LEU:HD13	2:F:119:ILE:HG21	1.99	0.45
2:B:23:MET:HE1	2:B:25:MET:CE	2.45	0.44
2:D:347:MET:HE3	2:D:352:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:252:THR:HG21	2:E:358:ARG:HG3	1.99	0.44
6:I:327:VAL:HG12	6:I:328:ALA:N	2.31	0.44
5:L:42:A:HI'	5:L:43:G:OP1	2.17	0.44
4:H:25:ARG:CD	5:L:4:A:OP2	2.65	0.44
2:E:252:THR:HG22	2:E:357:VAL:HB	1.99	0.44
2:C:275:PRO:HG3	2:B:288:LEU:CD2	2.47	0.44
6:I:170:THR:N	6:I:171:PRO:CD	2.81	0.44
6:I:198:GLN:HB3	6:I:199:PHE:CE1	2.53	0.44
2:C:203:VAL:CG2	5:L:38:C:C6	3.01	0.44
2:C:252:THR:HG21	2:C:358:ARG:CG	2.48	0.44
6:I:199:PHE:N	6:I:200:PRO:HD3	2.32	0.44
3:A:110:LYS:HE2	5:L:47:C:OP2	2.17	0.44
2:D:140:LEU:HD23	2:D:140:LEU:C	2.38	0.44
2:B:244:ARG:O	2:B:248:LEU:HD12	2.17	0.44
2:C:205:ASP:O	2:C:206:LEU:HB2	2.18	0.44
2:D:20:ARG:NH1	2:D:24:ASN:OD1	2.50	0.44
4:H:20:THR:HG21	4:H:24:THR:O	2.17	0.44
3:A:27:PHE:HD2	3:A:58:GLN:HB3	1.83	0.44
2:C:118:GLU:OE1	2:C:165:ARG:NH2	2.51	0.44
2:F:115:VAL:HG11	2:F:157:GLY:HA3	2.00	0.44
4:H:83:ARG:HE	6:I:421:ARG:CZ	2.31	0.44
2:C:58:ILE:CG2	2:C:158:VAL:HG11	2.45	0.43
2:G:278:MET:HE1	2:G:312:PHE:CD1	2.52	0.43
6:I:101:MET:HE1	6:I:240:GLU:HA	1.99	0.43
6:I:93:LEU:N	6:I:94:ASN:HA	2.33	0.43
2:F:359:ASN:HB3	2:F:362:GLU:CB	2.48	0.43
1:J:5:ILE:HG22	1:J:6:ASP:N	2.33	0.43
2:F:22:ASP:HB3	2:G:199:TRP:CD2	2.54	0.43
4:H:146:LEU:HD23	4:H:153:LEU:CD2	2.47	0.43
1:K:44:VAL:O	1:K:44:VAL:HG22	2.17	0.43
2:D:323:TYR:CE1	2:E:275:PRO:HB3	2.53	0.43
6:I:28:TYR:HE2	6:I:58:ILE:HD11	1.84	0.43
1:J:102:ILE:CD1	1:J:152:PHE:CD2	3.01	0.43
1:K:143:ARG:CZ	1:K:144:GLU:OE2	2.66	0.43
6:I:194:ARG:HA	6:I:197:LYS:HB2	2.00	0.43
1:K:73:ARG:HB2	1:K:127:VAL:HG12	2.00	0.43
5:L:41:G:N2	5:L:42:A:C6	2.86	0.43
2:B:5:ILE:CG2	2:B:230:ILE:HB	2.49	0.43
2:B:58:ILE:HG12	2:B:253:HIS:CD2	2.53	0.43
2:B:261:GLU:OE2	2:B:261:GLU:HA	2.19	0.43
3:A:1:MET:N	3:A:57:ALA:HA	2.33	0.43
2:B:42:GLN:HE21	5:L:39:A:P	2.42	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:153:ASN:CG	2:G:169:SER:HG	2.22	0.43
6:I:280:PRO:HA	6:I:329:ALA:HB3	2.00	0.43
1:K:37:ILE:HD12	1:K:40:PHE:H	1.83	0.43
3:A:84:LEU:HD23	3:A:198:PRO:HA	2.01	0.43
2:D:5:ILE:HD12	2:D:232:LEU:HD21	2.00	0.43
6:I:198:GLN:NE2	6:I:329:ALA:HB2	2.34	0.43
2:G:10:LEU:HD22	2:G:278:MET:HE3	2.00	0.43
2:G:286:MET:HE3	4:H:157:LEU:CG	2.49	0.43
6:I:192:LEU:O	6:I:195:LEU:HB3	2.18	0.43
2:C:137:LYS:O	2:C:141:LYS:HG3	2.19	0.42
2:G:336:ASP:CB	2:G:337:VAL:HA	2.49	0.42
2:B:15:PRO:O	2:B:18:LEU:HD12	2.19	0.42
4:H:39:LEU:HD13	4:H:39:LEU:C	2.39	0.42
6:I:180:ASP:OD2	6:I:182:ARG:HB3	2.19	0.42
6:I:430:LEU:O	6:I:434:VAL:HG13	2.19	0.42
6:I:50:LEU:HD13	6:I:149:PHE:CG	2.54	0.42
4:H:25:ARG:NH1	5:L:3:A:H1'	2.34	0.42
4:H:96:ARG:HG3	4:H:97:GLY:N	2.34	0.42
6:I:354:GLN:O	6:I:355:ALA:HB3	2.20	0.42
3:A:103:LEU:HD23	3:A:104:ASP:N	2.34	0.42
2:B:217:GLN:HB3	3:A:85:TYR:CE1	2.54	0.42
2:B:280:MET:HE2	2:B:312:PHE:CE1	2.55	0.42
2:C:75:LEU:HD11	2:C:119:ILE:HD13	2.02	0.42
2:D:313:ASN:HB3	2:D:341:THR:HG21	2.01	0.42
2:D:66:ILE:HG23	2:D:111:VAL:CG1	2.42	0.42
2:G:201:THR:HA	2:G:213:HIS:O	2.19	0.42
6:I:195:LEU:HD21	6:I:228:PHE:CE2	2.54	0.42
2:B:151:ARG:HB2	2:B:240:GLY:CA	2.49	0.42
2:B:305:LEU:O	2:B:309:ILE:HG12	2.19	0.42
2:B:329:ALA:HB3	2:B:344:VAL:HG22	2.00	0.42
1:J:101:ARG:HG3	2:D:199:TRP:CH2	2.55	0.42
4:H:55:GLN:HA	4:H:202:ILE:HD13	2.00	0.42
6:I:380:GLU:O	6:I:384:VAL:HG23	2.19	0.42
6:I:4:LEU:HD21	6:I:54:ILE:CD1	2.49	0.42
1:K:61:MET:HE3	1:K:134:ALA:HB1	2.02	0.42
2:D:252:THR:HG21	2:D:358:ARG:CG	2.50	0.42
2:F:200:PHE:HB3	2:E:42:GLN:HE21	1.84	0.42
2:G:84:ASP:HB2	2:G:87:ILE:CD1	2.49	0.42
1:K:131:PRO:O	1:K:135:ARG:HG3	2.19	0.42
2:D:206:LEU:HD13	2:C:70:GLN:CB	2.47	0.42
2:F:244:ARG:HG2	2:F:248:LEU:HD11	2.02	0.42
2:G:325:LEU:HD13	2:G:325:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:130:TRP:HB3	1:J:131:PRO:HD3	2.02	0.42
2:C:304:PHE:O	2:C:308:SER:OG	2.28	0.42
2:G:87:ILE:O	2:G:91:THR:HG23	2.19	0.42
6:I:305:PRO:CD	6:I:424:TYR:CD1	3.03	0.42
1:J:29:SER:N	1:J:33:GLU:OE1	2.51	0.42
2:C:66:ILE:HG22	2:C:110:ALA:O	2.19	0.42
2:D:280:MET:HE2	2:D:312:PHE:CZ	2.55	0.42
2:G:199:TRP:CZ2	2:G:214:LEU:HD22	2.55	0.42
6:I:232:LEU:HD11	6:I:277:TRP:HH2	1.85	0.42
6:I:466:VAL:HG11	6:I:479:LEU:HD22	2.01	0.42
2:D:66:ILE:HG22	2:D:111:VAL:HA	2.02	0.41
4:H:66:ARG:HB2	4:H:171:LEU:HD13	2.01	0.41
6:I:132:GLN:NE2	6:I:133:PRO:HD2	2.34	0.41
6:I:22:ILE:HG22	6:I:23:ASN:N	2.35	0.41
6:I:174:THR:HG21	6:I:313:VAL:HG13	2.02	0.41
3:A:135:ARG:NH2	3:A:137:GLU:OE1	2.53	0.41
2:B:64:ARG:HA	2:B:112:THR:O	2.20	0.41
2:B:140:LEU:HD23	2:B:140:LEU:C	2.41	0.41
2:C:271:ALA:HB3	2:B:185:ALA:HB2	2.02	0.41
2:E:115:VAL:HG13	2:E:160:ILE:HD12	2.02	0.41
2:E:277:ASP:OD2	2:E:305:LEU:CD2	2.66	0.41
1:K:153:VAL:HG11	6:I:408:PHE:HE1	1.85	0.41
3:A:96:ILE:HD13	5:L:43:G:N1	2.35	0.41
2:B:75:LEU:HD21	2:B:119:ILE:HD12	2.02	0.41
2:F:118:GLU:N	2:F:153:ASN:OD1	2.54	0.41
2:F:26:GLN:NE2	2:F:220:SER:OG	2.49	0.41
2:B:87:ILE:CG2	2:B:126:VAL:HG11	2.51	0.41
2:B:251:ALA:O	2:B:255:VAL:HG23	2.20	0.41
2:G:87:ILE:HG23	2:G:126:VAL:HG23	2.03	0.41
2:G:67:HIS:HB2	2:G:70:GLN:HG3	2.02	0.41
6:I:90:MET:N	6:I:90:MET:HE2	2.36	0.41
2:B:338:ASP:N	2:B:339:PRO:CD	2.83	0.41
2:C:144:LYS:NZ	2:C:144:LYS:HB2	2.35	0.41
2:F:200:PHE:HB3	2:E:42:GLN:HE22	1.84	0.41
6:I:434:VAL:CG2	6:I:435:LEU:N	2.83	0.41
2:D:306:GLN:N	2:D:307:PRO:HD2	2.35	0.41
2:F:209:GLN:HG3	2:F:209:GLN:O	2.20	0.41
6:I:232:LEU:CD1	6:I:277:TRP:HH2	2.32	0.41
3:A:193:LEU:HD23	3:A:193:LEU:C	2.41	0.41
3:A:7:ILE:HG21	3:A:48:GLU:HB2	2.02	0.41
2:C:280:MET:HE2	2:C:312:PHE:CZ	2.55	0.41
2:G:158:VAL:HG23	2:G:159:ASP:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:I:221:ILE:N	6:I:222:PRO:CD	2.84	0.41
1:J:60:ARG:CD	1:J:114:MET:HE3	2.51	0.41
1:J:43:LEU:O	1:J:46:PRO:CD	2.69	0.41
5:L:40:G:HO2'	5:L:41:G:P	2.40	0.41
5:L:42:A:C2'	5:L:42:A:N3	2.83	0.41
2:E:345:LYS:HB2	2:E:345:LYS:HE3	1.91	0.41
2:F:166:MET:HE1	5:L:11:G:N3	2.36	0.41
2:F:277:ASP:OD2	2:F:305:LEU:CD2	2.65	0.41
6:I:57:ILE:CD1	6:I:229:VAL:HG22	2.44	0.41
2:B:5:ILE:HG22	2:B:230:ILE:HB	2.03	0.41
2:E:267:GLN:HA	2:E:270:TYR:O	2.20	0.41
2:G:320:ALA:HA	2:G:325:LEU:HD23	2.03	0.41
6:I:193:PRO:O	6:I:197:LYS:HG3	2.21	0.41
1:J:97:ILE:HD11	1:J:124:ALA:HB2	2.03	0.41
2:B:219:PHE:HB3	3:A:140:HIS:HB2	2.02	0.40
2:C:132:ASP:CB	2:C:133:ASN:C	2.89	0.40
2:C:141:LYS:HA	2:C:144:LYS:HE3	2.03	0.40
2:C:267:GLN:HB3	2:C:273:PHE:CZ	2.56	0.40
4:H:205:PRO:HA	4:H:206:ARG:HA	1.86	0.40
1:K:102:ILE:CD1	1:K:152:PHE:CD2	3.04	0.40
3:A:16:LEU:N	3:A:16:LEU:HD22	2.36	0.40
2:C:90:LYS:HB3	2:C:90:LYS:NZ	2.36	0.40
2:F:66:ILE:HG22	2:F:110:ALA:O	2.20	0.40
2:F:234:GLN:NE2	2:F:238:ASN:OD1	2.54	0.40
6:I:114:MET:CB	6:I:139:LEU:HD12	2.48	0.40
2:B:170:GLY:O	2:B:173:THR:HG22	2.20	0.40
2:B:206:LEU:HD22	3:A:84:LEU:HD21	2.03	0.40
2:D:252:THR:HG21	2:D:358:ARG:HG3	2.04	0.40
2:F:278:MET:SD	2:F:331:GLN:NE2	2.89	0.40
2:F:286:MET:HG3	2:F:287:PRO:HD2	2.02	0.40
4:H:14:GLN:NE2	4:H:114:ALA:O	2.54	0.40
6:I:109:ASN:HB3	6:I:110:ASP:HA	2.03	0.40
6:I:46:ALA:CB	6:I:150:ASN:HB2	2.52	0.40
6:I:319:ILE:HD12	6:I:320:GLN:N	2.37	0.40
2:B:294:PHE:HD1	2:B:298:VAL:HG21	1.86	0.40
2:D:295:GLU:OE1	2:E:304:PHE:N	2.48	0.40
2:F:273:PHE:CD1	2:E:287:PRO:HB2	2.57	0.40
4:H:5:LEU:O	4:H:120:LEU:HD23	2.21	0.40
6:I:282:SER:C	6:I:328:ALA:HB2	2.42	0.40
6:I:57:ILE:CG2	6:I:58:ILE:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	155/165 (94%)	154 (99%)	1 (1%)	0	100	100
1	K	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
2	B	335/363 (92%)	315 (94%)	18 (5%)	2 (1%)	33	84
2	C	339/363 (93%)	323 (95%)	16 (5%)	0	100	100
2	D	350/363 (96%)	327 (93%)	20 (6%)	3 (1%)	25	77
2	E	343/363 (94%)	328 (96%)	15 (4%)	0	100	100
2	F	350/363 (96%)	330 (94%)	20 (6%)	0	100	100
2	G	347/363 (96%)	322 (93%)	25 (7%)	0	100	100
3	A	188/199 (94%)	182 (97%)	4 (2%)	2 (1%)	21	74
4	H	217/224 (97%)	208 (96%)	9 (4%)	0	100	100
6	I	489/502 (97%)	460 (94%)	28 (6%)	1 (0%)	56	94
All	All	3266/3433 (95%)	3100 (95%)	158 (5%)	8 (0%)	56	94

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	117	ILE
6	I	170	THR
2	D	343	GLN
2	B	198	ASP
3	A	27	PHE
2	D	158	VAL
2	D	15	PRO
2	B	275	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	130/141 (92%)	128 (98%)	2 (2%)	76	95
1	K	130/141 (92%)	130 (100%)	0	100	100
2	B	243/298 (82%)	240 (99%)	3 (1%)	82	96
2	C	249/298 (84%)	248 (100%)	1 (0%)	95	99
2	D	259/298 (87%)	259 (100%)	0	100	100
2	E	271/298 (91%)	271 (100%)	0	100	100
2	F	282/298 (95%)	282 (100%)	0	100	100
2	G	277/298 (93%)	274 (99%)	3 (1%)	84	96
3	A	158/170 (93%)	157 (99%)	1 (1%)	92	98
4	H	185/192 (96%)	185 (100%)	0	100	100
6	I	371/426 (87%)	360 (97%)	11 (3%)	53	89
All	All	2555/2858 (89%)	2534 (99%)	21 (1%)	89	97

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	47	PHE
1	J	110	ARG
2	C	109	ASP
2	B	85	GLN
2	B	326	ASN
2	B	334	LEU
2	G	208	GLU
2	G	279	VAL
2	G	325	LEU
3	A	117	ILE
6	I	28	TYR
6	I	140	CYS
6	I	143	CYS
6	I	153	ASN
6	I	199	PHE
6	I	203	SER
6	I	205	THR
6	I	239	ILE
6	I	241	LEU
6	I	253	CYS

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Mol	Chain	Res	Type
6	I	325	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	42	GLN
2	D	8	HIS
2	D	229	ASN
2	D	292	ASN
2	G	153	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	59/61 (96%)	33 (55%)	3 (5%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L	3	A
5	L	4	A
5	L	7	C
5	L	9	A
5	L	13	U
5	L	14	A
5	L	15	U
5	L	21	A
5	L	22	G
5	L	26	C
5	L	27	U
5	L	31	U
5	L	32	U
5	L	33	G
5	L	34	C
5	L	38	C
5	L	39	A
5	L	40	G
5	L	41	G
5	L	42	A
5	L	43	G

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Mol	Chain	Res	Type
5	L	44	U
5	L	47	C
5	L	49	C
5	L	50	G
5	L	51	C
5	L	52	G
5	L	53	C
5	L	54	C
5	L	55	A
5	L	56	G
5	L	58	G
5	L	59	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L	9	A
5	L	40	G
5	L	42	A

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
5	23G	L	61	5	27,29,30	6.30	16 (59%)	40,45,48	3.68	17 (42%)

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
5	23G	L	61	5	-	1/8/35/36	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	61	23G	PC-O2'	-16.72	1.41	1.58
5	L	61	23G	C2-N3	14.05	1.50	1.33
5	L	61	23G	C2-N2	12.87	1.51	1.32
5	L	61	23G	C4-N3	10.92	1.53	1.35
5	L	61	23G	C3'-C4'	-7.15	1.32	1.52
5	L	61	23G	O3'-C3'	-6.63	1.30	1.45
5	L	61	23G	O4'-C4'	6.59	1.60	1.45
5	L	61	23G	C2-N1	6.23	1.46	1.36
5	L	61	23G	C6-N1	6.10	1.45	1.36
5	L	61	23G	P-OP1	4.32	1.51	1.46
5	L	61	23G	PC-O3'	4.31	1.62	1.58
5	L	61	23G	C3'-C2'	3.46	1.61	1.53
5	L	61	23G	O2'-C2'	3.17	1.52	1.45
5	L	61	23G	O6-C6	-3.09	1.17	1.24
5	L	61	23G	C6-C5	2.56	1.54	1.42
5	L	61	23G	C5-N7	-2.36	1.35	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	61	23G	O3'-PC-O2'	11.71	107.03	97.12
5	L	61	23G	C6-C5-N7	-11.26	132.62	134.14
5	L	61	23G	C2-N3-C4	6.13	122.65	115.30
5	L	61	23G	N2-C2-N1	5.37	123.57	117.82
5	L	61	23G	C1'-N9-C4	-5.23	117.59	126.64
5	L	61	23G	C5-C4-N3	-5.02	120.28	126.07
5	L	61	23G	N3-C4-N9	4.78	133.92	126.91
5	L	61	23G	OC1-PC-OC2	-4.47	95.58	109.46
5	L	61	23G	N1-C2-N3	-4.35	115.91	121.78
5	L	61	23G	O4'-C1'-N9	3.95	116.70	108.10
5	L	61	23G	C8-N9-C1'	3.48	132.71	126.15
5	L	61	23G	C8-N9-C4	3.34	109.67	106.96
5	L	61	23G	PC-O2'-C2'	-3.16	107.20	111.48
5	L	61	23G	C5'-C4'-C3'	-2.48	105.59	114.25
5	L	61	23G	OC1-PC-O2'	2.27	112.53	108.46
5	L	61	23G	C5-C6-N1	2.24	123.44	116.21
5	L	61	23G	O4'-C1'-C2'	-2.23	102.53	106.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	61	23G	OP2-P-O5'-C5'

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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