



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:44 PM BST

PDB ID : 3IYD
EMDB ID: : EMD-5127
Title : Three-dimensional EM structure of an intact activator-dependent transcription initiation complex
Authors : Hudson, B.P.; Quispe, J.; Lara, S.; Kim, Y.; Berman, H.; Arnold, E.; Ebright, R.H.; Lawson, C.L.
Deposited on : 2009-08-01
Resolution : 19.80 Å(reported)
Based on PDB ID : 2AUK, 1SIG, 1LB2, 3DXJ, 1BDF

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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) : trunk27241

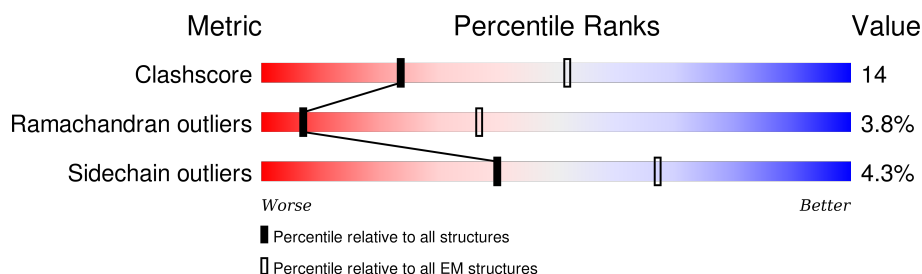
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 19.80 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 ≥ 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	329	67% 28% . .
1	B	329	47% 22% . 29%
2	C	1342	53% 25% . 19%
3	D	1413	63% 29% 5% .
4	E	90	57% 33% 9% .
5	F	613	57% 18% . 22%
6	G	209	77% 19% .
6	H	209	72% 23% .
7	I	98	44% 56%

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Mol	Chain	Length	Quality of chain
8	J	98	<div><div></div><div>45%</div><div>55%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 35254 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	322	Total	C	N	O	S	0	0
			2496	1563	438	487	8		
1	B	235	Total	C	N	O	S	0	0
			1814	1129	320	358	7		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1089	Total	C	N	O	S	0	0
			8524	5351	1481	1655	37		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1368	Total	C	N	O	S	0	0
			10606	6657	1893	2006	50		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	HIS	-	EXPRESSION TAG	UNP P0A8T7
D	1409	HIS	-	EXPRESSION TAG	UNP P0A8T7
D	1410	HIS	-	EXPRESSION TAG	UNP P0A8T7
D	1411	HIS	-	EXPRESSION TAG	UNP P0A8T7
D	1412	HIS	-	EXPRESSION TAG	UNP P0A8T7
D	1413	HIS	-	EXPRESSION TAG	UNP P0A8T7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	479	Total	C	N	O	S	0	0
			3877	2423	693	740	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	CONFLICT	UNP P00579
F	571	HIS	TYR	CONFLICT	UNP P00579

- Molecule 6 is a protein called Catabolite gene activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	201	Total	C	N	O	S	0	0
			1591	1007	280	295	9		
6	H	201	Total	C	N	O	S	0	0
			1591	1007	280	295	9		

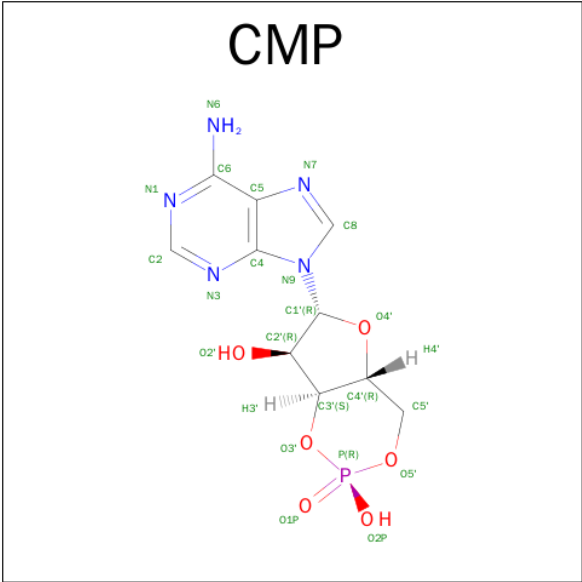
- Molecule 7 is a DNA chain called DNA (98-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	98	Total	C	N	O	P	0	0
			2006	960	366	583	97		

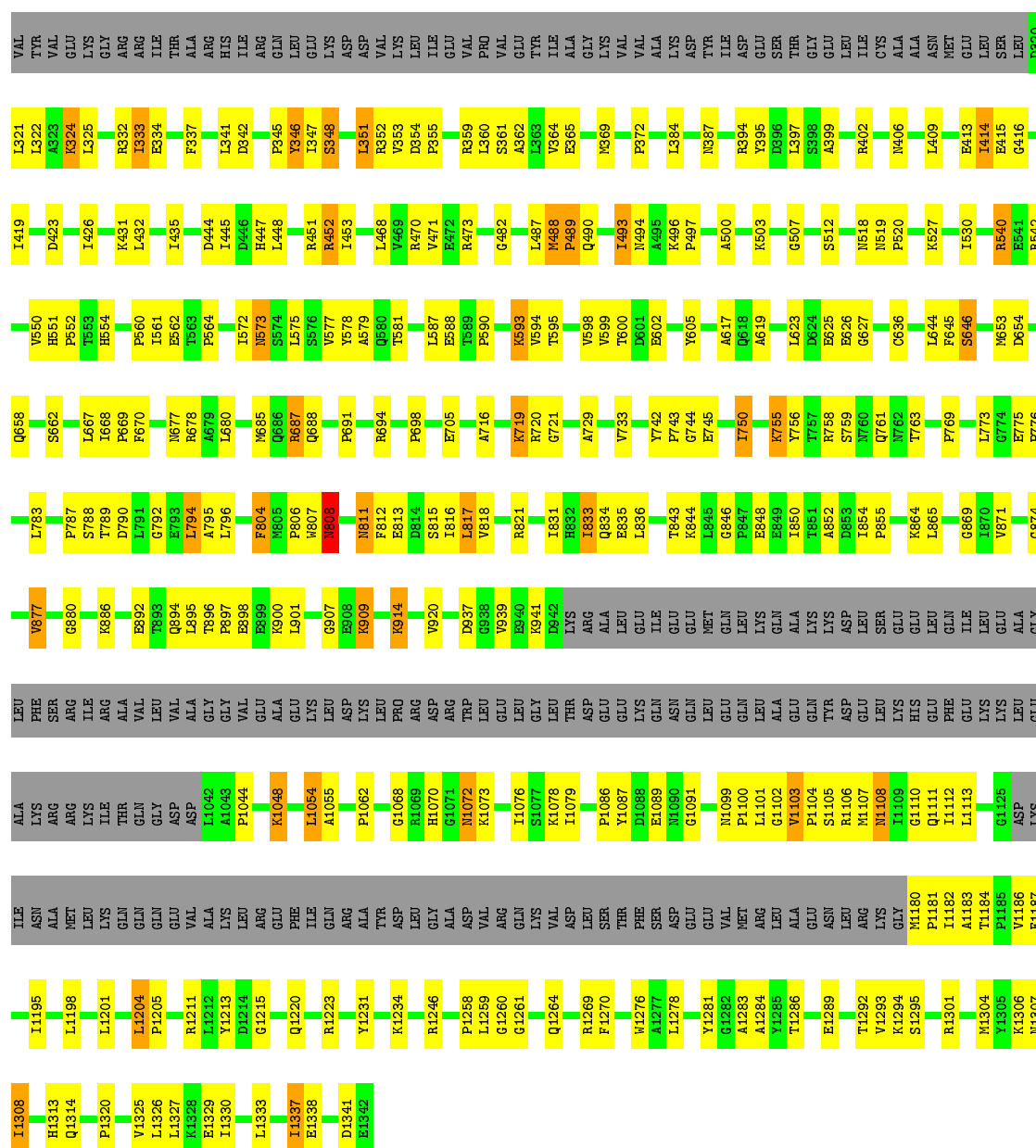
- Molecule 8 is a DNA chain called DNA (98-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	98	Total	C	N	O	P	0	0
			1996	958	353	588	97		

- Molecule 9 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C₁₀H₁₂N₅O₆P).

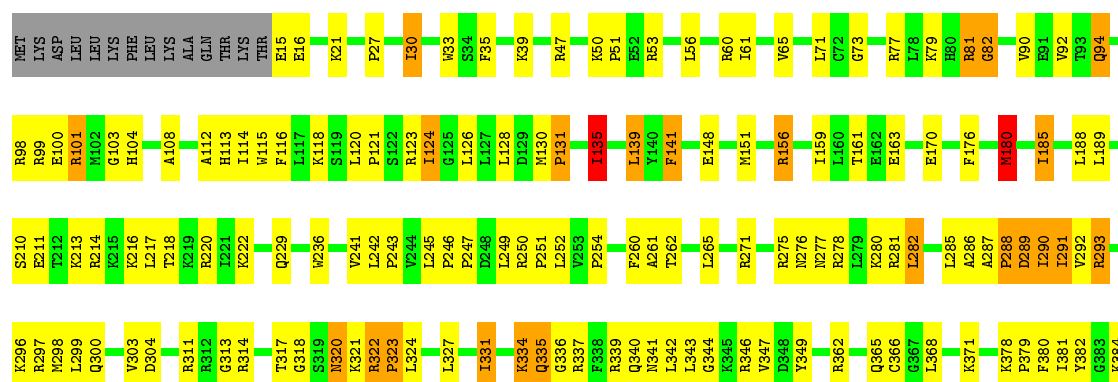


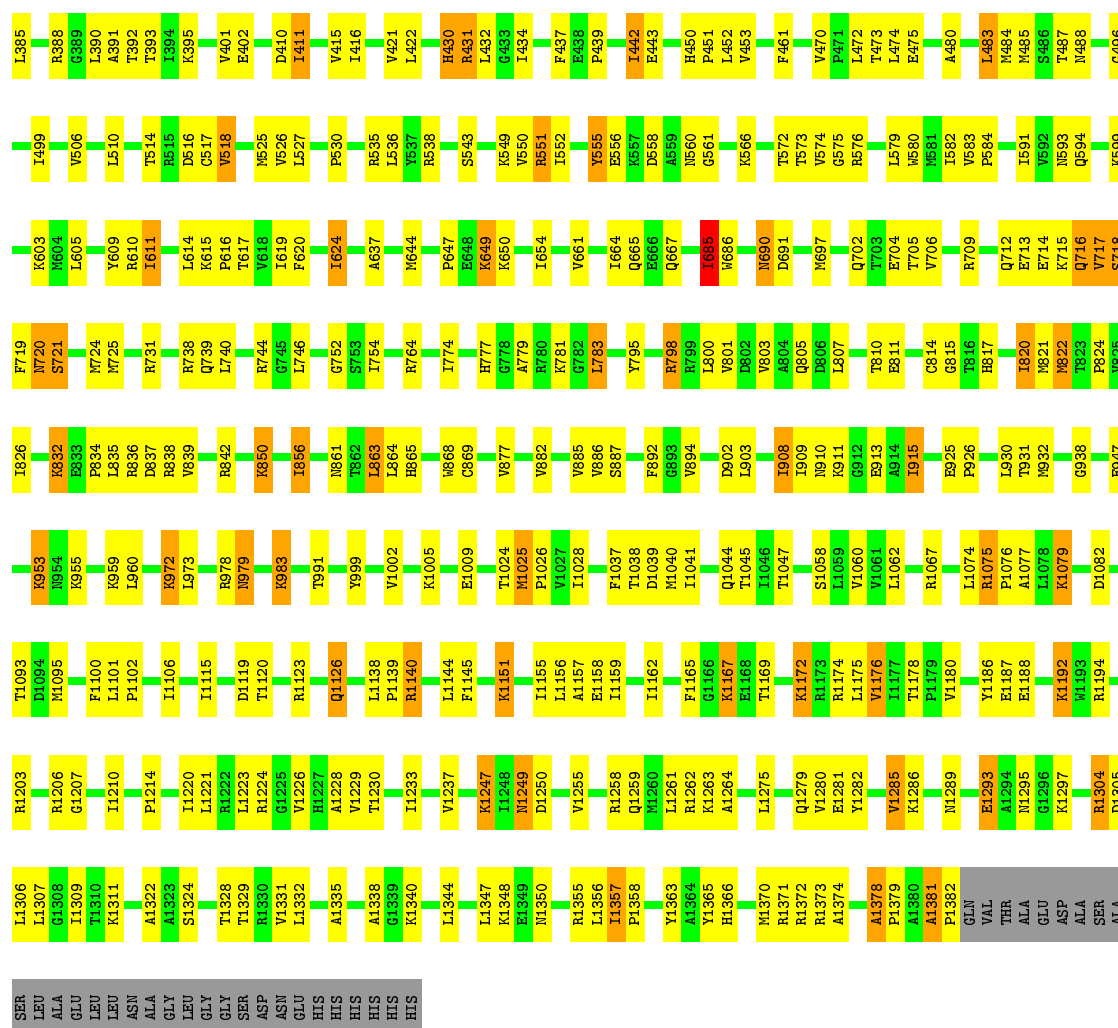
Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total	C	N	O	P	0
			22	10	5	6	1	
9	H	1	Total	C	N	O	P	0
			22	10	5	6	1	



• Molecule 3: DNA-directed RNA polymerase subunit beta

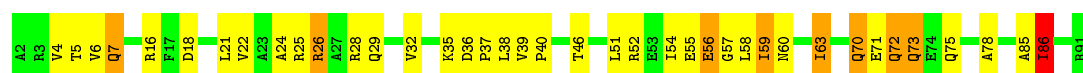
Chain D:  63%  29%  5% •





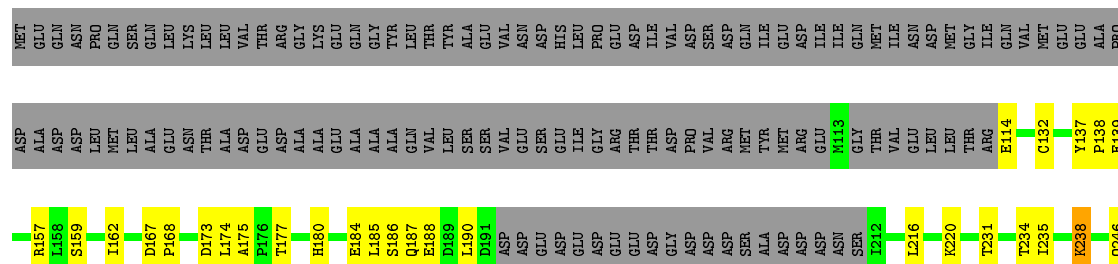
- Molecule 4: DNA-directed RNA polymerase subunit omega

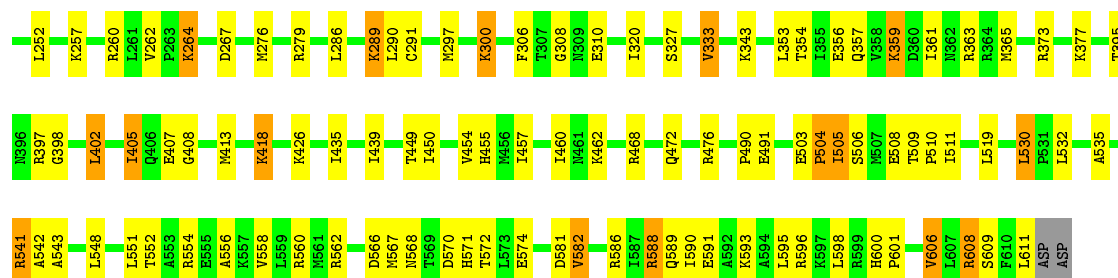
Chain E: 57% 33% 9%



- Molecule 5: RNA polymerase sigma factor rpoD

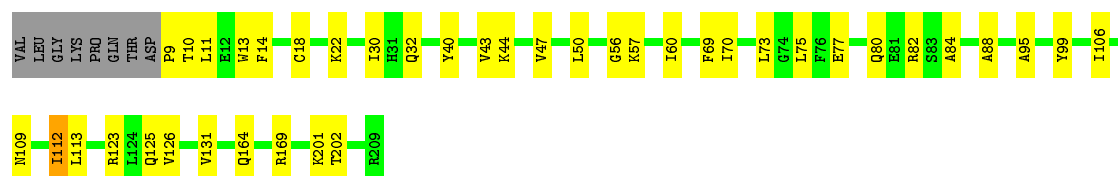
Chain F: 57% 18% 22%





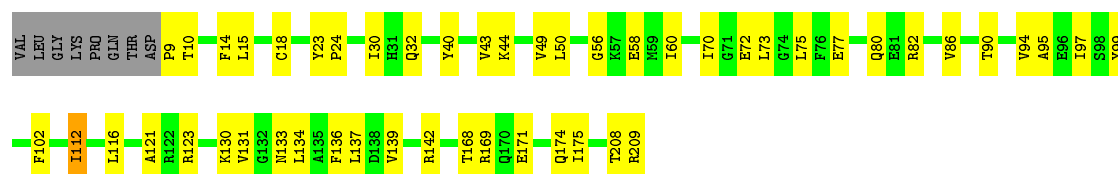
- Molecule 6: Catabolite gene activator

Chain G: 77% 19% .



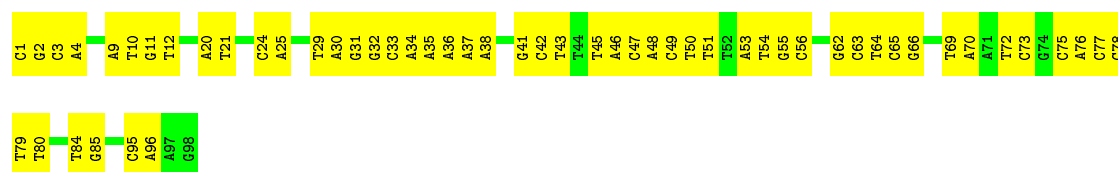
- Molecule 6: Catabolite gene activator

Chain H: 72% 23% .



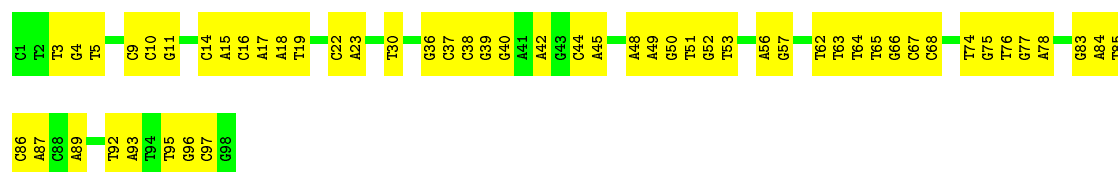
- Molecule 7: DNA (98-MER)

Chain I: 44% 56%



- Molecule 8: DNA (98-MER)

Chain J: 45% 55%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	14097	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	ACE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	50000	Depositor
Image detector	Teitz F415 4k x 4k pixel CCD camera	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: CMP

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	0.19	0/2528	0.36	0/3427
1	B	0.19	0/1836	0.35	0/2488
2	C	0.20	0/8672	0.35	0/11722
3	D	0.19	0/10769	0.35	0/14544
4	E	0.19	0/711	0.34	0/956
5	F	0.20	0/3931	0.34	0/5288
6	G	0.20	0/1616	0.33	0/2174
6	H	0.20	0/1616	0.33	0/2174
7	I	0.45	0/2251	0.93	0/3472
8	J	0.44	0/2236	0.93	0/3447
All	All	0.24	0/36166	0.47	0/49692

There are no bond length outliers.

There are no bond angle outliers.

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	2496	0	2554	74	0
1	B	1814	0	1839	60	0
2	C	8524	0	8491	275	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10606	0	10822	387	0
4	E	709	0	719	37	0
5	F	3877	0	3929	89	0
6	G	1591	0	1632	28	0
6	H	1591	0	1632	34	0
7	I	2006	0	1108	45	0
8	J	1996	0	1111	45	0
9	G	22	0	11	3	0
9	H	22	0	11	2	0
All	All	35254	0	33859	996	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 14.

All (996) 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)
9:G:679:CMP:H2	9:G:679:CMP:C2	0.97	1.49
9:H:680:CMP:C2	9:H:680:CMP:H2	0.97	1.49
4:E:59:ILE:HG12	4:E:60:ASN:H	1.45	0.81
3:D:1378:ALA:H	3:D:1379:PRO:HD3	1.45	0.81
1:A:235:ARG:HD2	1:A:235:ARG:H	1.45	0.80
3:D:550:VAL:HA	3:D:551:ARG:HH21	1.46	0.80
4:E:46:THR:HG21	4:E:58:LEU:HD23	1.64	0.79
2:C:1329:GLU:HB3	3:D:331:ILE:HD12	1.64	0.79
3:D:56:LEU:HD21	3:D:250:ARG:HH22	1.47	0.78
2:C:414:ILE:HG23	2:C:416:GLY:H	1.47	0.78
3:D:863:LEU:HD13	3:D:863:LEU:H	1.50	0.77
2:C:1269:ARG:HA	3:D:346:ARG:HA	1.67	0.76
3:D:210:SER:HA	3:D:214:ARG:HB3	1.68	0.76
1:B:192:VAL:HG13	1:B:194:GLN:H	1.49	0.75
1:A:283:GLN:HG3	1:A:284:ARG:HD2	1.67	0.75
3:D:611:ILE:HD13	3:D:611:ILE:H	1.49	0.74
1:A:297:LYS:HD3	1:A:297:LYS:H	1.51	0.74
1:B:92:VAL:HB	1:B:148:ARG:HH22	1.53	0.74
5:F:184:GLU:HG2	5:F:373:ARG:HG3	1.70	0.74
2:C:1068:GLY:H	2:C:1072:ASN:HD21	1.33	0.74
2:C:220:ILE:H	2:C:220:ILE:HD13	1.55	0.72
2:C:1330:ILE:HD12	2:C:1333:LEU:HD12	1.71	0.72
2:C:806:PRO:HD3	2:C:1100:PRO:HG2	1.72	0.72
3:D:1378:ALA:H	3:D:1379:PRO:CD	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:354:THR:HB	5:F:357:GLN:HG2	1.72	0.71
2:C:880:GLY:H	2:C:920:VAL:HB	1.56	0.71
3:D:254:PRO:HA	3:D:260:PHE:HA	1.73	0.70
1:A:104:LYS:HD3	1:A:110:VAL:HG22	1.73	0.70
2:C:789:THR:HA	2:C:795:ALA:HB3	1.74	0.70
3:D:719:PHE:HB3	3:D:725:MET:HG3	1.73	0.70
6:H:123:ARG:HD3	9:H:680:CMP:H2	1.73	0.70
2:C:755:LYS:HD2	2:C:756:TYR:H	1.57	0.69
3:D:1279:GLN:HG3	3:D:1281:GLU:H	1.55	0.69
5:F:167:ASP:HB3	5:F:168:PRO:HD3	1.75	0.69
3:D:415:VAL:HG13	3:D:416:ILE:HG13	1.73	0.69
1:A:317:ARG:HD3	1:A:317:ARG:H	1.56	0.69
1:B:11:PRO:HB2	1:B:28:LEU:HD11	1.75	0.68
2:C:598:VAL:HG12	2:C:627:GLY:HA2	1.75	0.68
1:A:62:ASP:HB2	1:A:143:ARG:HH12	1.59	0.68
1:A:195:ARG:HD2	1:A:198:LEU:HG	1.75	0.68
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.74	0.68
3:D:1366:HIS:HE1	4:E:18:ASP:HA	1.59	0.68
2:C:194:LEU:HD13	2:C:206:ALA:HB3	1.77	0.67
3:D:774:ILE:HA	3:D:777:HIS:HD2	1.59	0.67
2:C:352:ARG:HG3	2:C:359:ARG:HD3	1.74	0.67
2:C:351:LEU:HD12	2:C:353:VAL:HG22	1.76	0.67
3:D:337:ARG:HB3	8:J:16:DC:H2"	1.77	0.67
3:D:320:ASN:HD22	3:D:322:ARG:HH12	1.42	0.67
2:C:1102:GLY:HA2	3:D:718:SER:HB2	1.77	0.67
7:I:42:DC:H2"	7:I:43:DT:O5'	1.95	0.67
1:A:100:LEU:HD11	1:A:121:VAL:HG21	1.75	0.66
1:B:66:HIS:CD2	1:B:67:GLU:H	2.13	0.66
3:D:216:LYS:HE2	3:D:220:ARG:HH21	1.60	0.66
3:D:834:PRO:HB3	3:D:838:ARG:HH22	1.59	0.66
3:D:430:HIS:HD2	3:D:432:LEU:H	1.43	0.66
5:F:530:LEU:HD13	5:F:532:LEU:HB3	1.77	0.66
3:D:1115:ILE:HG23	3:D:1119:ASP:HB2	1.78	0.66
3:D:1221:LEU:HD13	3:D:1306:LEU:HD23	1.77	0.66
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	1.78	0.66
5:F:354:THR:H	5:F:357:GLN:HE21	1.43	0.66
3:D:334:LYS:HA	3:D:334:LYS:HE3	1.78	0.65
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.77	0.65
2:C:170:VAL:HG22	2:C:435:ILE:HG12	1.78	0.65
3:D:1151:LYS:H	3:D:1151:LYS:HD3	1.61	0.65
2:C:813:GLU:HB3	3:D:461:PHE:HD1	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:262:VAL:HG12	5:F:264:LYS:H	1.61	0.65
1:B:140:ILE:HD13	1:B:140:ILE:H	1.62	0.65
5:F:541:ARG:HA	5:F:606:VAL:HA	1.77	0.65
6:G:125:GLN:HE21	6:H:73:LEU:HD13	1.62	0.64
5:F:397:ARG:HH22	8:J:30:DT:H2'	1.61	0.64
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.79	0.64
3:D:925:GLU:HG3	3:D:926:PRO:HD3	1.78	0.64
3:D:100:GLU:O	3:D:101:ARG:HG2	1.97	0.64
4:E:85:ALA:O	4:E:86:ILE:HG12	1.97	0.64
1:B:65:LEU:HD23	1:B:65:LEU:H	1.61	0.64
3:D:480:ALA:HA	3:D:484:MET:HB2	1.78	0.64
3:D:1378:ALA:N	3:D:1379:PRO:CD	2.60	0.64
1:B:53:GLY:HA2	1:B:210:THR:HG21	1.79	0.64
2:C:817:LEU:H	2:C:817:LEU:HD13	1.63	0.64
3:D:864:LEU:HD11	3:D:869:CYS:HB2	1.78	0.64
5:F:455:HIS:HB3	7:I:63:DC:H41	1.62	0.64
3:D:518:VAL:HG12	3:D:536:LEU:HD13	1.79	0.64
6:H:50:LEU:HB3	6:H:60:ILE:HG12	1.80	0.64
1:B:200:LYS:HD3	1:B:200:LYS:H	1.63	0.64
3:D:475:GLU:HG2	4:E:24:ALA:HB1	1.78	0.64
3:D:82:GLY:HA2	3:D:92:VAL:HB	1.80	0.64
3:D:911:LYS:HE3	3:D:1365:TYR:HB3	1.80	0.64
3:D:573:THR:HG23	3:D:575:GLY:H	1.63	0.64
3:D:908:ILE:HD13	3:D:909:ILE:N	2.13	0.64
2:C:909:LYS:HE2	2:C:909:LYS:HA	1.81	0.63
1:B:187:VAL:HG13	1:B:188:GLU:H	1.63	0.63
1:B:6:THR:HG23	1:B:7:GLU:H	1.63	0.63
3:D:71:LEU:HD23	3:D:71:LEU:H	1.62	0.63
3:D:339:ARG:HH21	8:J:17:DA:H4'	1.64	0.63
3:D:1289:ASN:HA	3:D:1293:GLU:HB3	1.79	0.63
2:C:74:ARG:HB3	2:C:97:ARG:HB2	1.79	0.63
6:H:168:THR:HG21	7:I:9:DA:H5"	1.80	0.63
2:C:1108:ASN:H	2:C:1108:ASN:HD22	1.45	0.63
2:C:360:LEU:HA	2:C:365:GLU:HG3	1.80	0.63
3:D:1366:HIS:CE1	4:E:18:ASP:HA	2.34	0.62
3:D:573:THR:HG22	3:D:576:ARG:HG2	1.81	0.62
3:D:664:ILE:HD12	3:D:667:GLN:HE21	1.65	0.62
5:F:505:ILE:HD13	5:F:506:SER:N	2.14	0.62
2:C:342:ASP:HA	2:C:351:LEU:HD23	1.80	0.62
2:C:151:ARG:HA	2:C:451:ARG:HG2	1.80	0.62
3:D:113:HIS:CD2	3:D:115:TRP:H	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:720:ARG:HE	2:C:721:GLY:H	1.47	0.62
3:D:347:VAL:HG12	3:D:349:TYR:H	1.65	0.62
3:D:510:LEU:HD11	3:D:624:ILE:HG12	1.80	0.62
2:C:180:ARG:HD3	2:C:180:ARG:O	1.99	0.62
2:C:742:TYR:HB3	2:C:745:GLU:HB2	1.82	0.62
1:A:296:GLY:HA3	8:J:64:DT:H5'	1.82	0.61
6:H:32:GLN:HA	6:H:82:ARG:HB2	1.82	0.61
2:C:850:ILE:HD13	2:C:1048:LYS:HE2	1.81	0.61
3:D:1024:THR:HG21	3:D:1123:ARG:HD3	1.81	0.61
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.36	0.61
5:F:600:HIS:HB3	5:F:601:PRO:HD3	1.81	0.61
5:F:586:ARG:HB3	5:F:590:ILE:HG13	1.81	0.61
3:D:1060:VAL:HG22	3:D:1106:ILE:HG22	1.82	0.61
2:C:617:ALA:HB3	2:C:653:MET:HG2	1.82	0.61
3:D:550:VAL:HG22	3:D:552:ILE:H	1.63	0.61
2:C:773:LEU:H	2:C:773:LEU:HD23	1.65	0.61
3:D:1247:LYS:HE3	3:D:1247:LYS:HA	1.82	0.61
3:D:1075:ARG:H	3:D:1075:ARG:HD2	1.65	0.61
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.82	0.61
2:C:719:LYS:H	2:C:719:LYS:HD2	1.65	0.61
2:C:831:ILE:HG22	2:C:833:ILE:HG13	1.82	0.61
5:F:373:ARG:HG2	5:F:377:LYS:HE3	1.83	0.61
8:J:75:DG:H2''	8:J:76:DT:H5'	1.82	0.61
3:D:1140:ARG:HH12	3:D:1214:PRO:HG3	1.65	0.61
3:D:290:ILE:H	3:D:290:ILE:HD13	1.66	0.60
5:F:138:PRO:HD2	5:F:353:LEU:HD11	1.82	0.60
5:F:174:LEU:HD13	5:F:175:ALA:N	2.15	0.60
6:G:164:GLN:HG3	6:G:202:THR:HG23	1.83	0.60
7:I:50:DT:H1'	7:I:51:DT:H5'	1.82	0.60
2:C:1327:LEU:HD22	2:C:1337:ILE:HD12	1.84	0.60
8:J:86:DC:H2'	8:J:87:DA:H8	1.66	0.60
2:C:848:GLU:HG3	2:C:886:LYS:HZ1	1.67	0.60
3:D:411:ILE:HD13	3:D:411:ILE:O	2.02	0.60
3:D:551:ARG:HE	3:D:551:ARG:N	1.99	0.60
1:A:251:PRO:HG2	3:D:391:ALA:HA	1.84	0.60
5:F:449:THR:HG23	5:F:450:ILE:HG13	1.82	0.60
3:D:15:GLU:HG2	3:D:16:GLU:HG3	1.82	0.60
3:D:124:ILE:H	3:D:124:ILE:HD13	1.67	0.60
3:D:81:ARG:HD3	3:D:81:ARG:H	1.65	0.60
3:D:865:HIS:HB3	3:D:868:TRP:HD1	1.67	0.59
2:C:895:LEU:HD22	2:C:900:LYS:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:HA	1:A:95:LYS:HE2	1.82	0.59
2:C:579:ALA:HB1	2:C:587:LEU:HD11	1.84	0.59
3:D:98:ARG:HD2	3:D:247:PRO:HG2	1.84	0.59
2:C:26:TYR:HB2	2:C:29:SER:HB2	1.84	0.59
3:D:1067:ARG:HH22	3:D:1076:PRO:HG3	1.67	0.59
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.83	0.59
3:D:1039:ASP:HB2	3:D:1074:LEU:HD23	1.84	0.59
3:D:1307:LEU:H	3:D:1307:LEU:HD23	1.67	0.59
2:C:180:ARG:HG3	7:I:79:DT:N3	2.16	0.59
2:C:1102:GLY:HA3	3:D:716:GLN:HB3	1.84	0.59
2:C:518:ASN:HD21	2:C:761:GLN:HB2	1.68	0.59
1:A:190:ALA:H	1:A:199:ASP:HA	1.67	0.59
3:D:1005:LYS:HB3	3:D:1009:GLU:HG3	1.84	0.59
3:D:1192:LYS:N	3:D:1192:LYS:HE2	2.18	0.59
2:C:807:TRP:C	2:C:808:ASN:HD22	2.06	0.59
1:B:212:ASP:HB2	1:B:215:GLU:HG2	1.84	0.59
8:J:62:DT:H1'	8:J:63:DT:H5'	1.85	0.59
2:C:600:THR:HG22	2:C:602:GLU:H	1.68	0.58
2:C:833:ILE:HA	2:C:1055:ALA:HA	1.85	0.58
1:B:82:LEU:HD11	1:B:171:LEU:HB3	1.84	0.58
2:C:228:VAL:HG22	2:C:321:LEU:H	1.66	0.58
8:J:84:DA:H2''	8:J:85:DT:H5'	1.84	0.58
2:C:1308:ILE:H	2:C:1308:ILE:HD13	1.67	0.58
3:D:1167:LYS:HD2	3:D:1167:LYS:H	1.68	0.58
4:E:4:VAL:HG12	4:E:5:THR:HG22	1.86	0.58
2:C:143:ARG:HD2	2:C:512:SER:HB2	1.85	0.58
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.85	0.58
3:D:1370:MET:HE1	4:E:71:GLU:HB3	1.85	0.58
8:J:89:DA:H8	8:J:89:DA:H5'	1.68	0.58
3:D:1372:ARG:HD2	4:E:29:GLN:HE22	1.66	0.58
2:C:644:LEU:HD22	2:C:645:PHE:H	1.69	0.58
5:F:503:GLU:N	5:F:504:PRO:HA	2.19	0.58
2:C:619:ALA:HB2	2:C:654:ASP:HB2	1.85	0.58
3:D:388:ARG:HH22	4:E:51:LEU:HD21	1.67	0.58
2:C:65:ASN:HB3	2:C:105:TYR:HA	1.86	0.58
3:D:555:TYR:HD1	3:D:574:VAL:HG21	1.69	0.58
5:F:320:ILE:HA	5:F:327:SER:HB2	1.86	0.58
3:D:1322:ALA:HB3	3:D:1331:VAL:HG11	1.86	0.58
3:D:1335:ALA:HA	3:D:1340:LYS:HD3	1.86	0.58
3:D:1373:ARG:HH11	4:E:70:GLN:HG2	1.68	0.58
3:D:287:ALA:HB1	3:D:291:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD23	1:A:228:LEU:O	2.04	0.57
3:D:915:ILE:HD13	3:D:915:ILE:H	1.69	0.57
2:C:593:LYS:HD2	2:C:593:LYS:H	1.69	0.57
2:C:221:LEU:H	2:C:221:LEU:HD13	1.68	0.57
6:H:30:ILE:HB	6:H:86:VAL:HB	1.86	0.57
5:F:503:GLU:H	5:F:504:PRO:HA	1.69	0.57
1:B:51:MET:HB3	1:B:179:PRO:HD2	1.85	0.57
6:G:43:VAL:HG12	6:G:44:LYS:HG3	1.87	0.57
2:C:1307:ASN:HD22	2:C:1314:GLN:HA	1.69	0.57
2:C:333:ILE:HD13	2:C:334:GLU:N	2.20	0.57
2:C:843:THR:HG23	2:C:846:GLY:H	1.69	0.57
4:E:59:ILE:HG12	4:E:60:ASN:N	2.15	0.57
5:F:354:THR:HG22	5:F:356:GLU:H	1.69	0.57
1:B:211:ILE:HD13	1:B:216:ALA:HB2	1.85	0.57
2:C:1204:LEU:HB3	2:C:1205:PRO:HD3	1.85	0.57
8:J:50:DG:H2'	8:J:51:DT:C6	2.40	0.57
2:C:114:VAL:HG22	2:C:115:LYS:HD3	1.85	0.57
3:D:783:LEU:H	3:D:783:LEU:HD13	1.69	0.57
6:H:75:LEU:HD13	6:H:99:TYR:HD2	1.69	0.57
8:J:10:DC:H2'	8:J:11:DG:C8	2.40	0.57
6:H:169:ARG:HH21	7:I:10:DT:H5''	1.68	0.57
7:I:69:DT:H2'	7:I:70:DA:C8	2.39	0.57
1:A:192:VAL:HG21	1:A:198:LEU:HD12	1.87	0.57
3:D:113:HIS:HD2	3:D:115:TRP:H	1.51	0.57
2:C:518:ASN:HA	2:C:763:THR:HG21	1.87	0.57
3:D:835:LEU:HG	3:D:837:ASP:H	1.69	0.57
3:D:583:VAL:N	3:D:584:PRO:HD2	2.20	0.57
2:C:137:VAL:HA	2:C:142:GLU:HA	1.87	0.57
3:D:1249:ASN:HD22	3:D:1250:ASP:N	2.03	0.57
6:G:47:VAL:HG23	6:G:88:ALA:HA	1.86	0.57
3:D:108:ALA:H	3:D:276:ASN:HD21	1.53	0.57
2:C:224:PHE:HD2	2:C:322:LEU:HD21	1.68	0.57
2:C:10:ARG:HE	2:C:1180:MET:HA	1.69	0.57
3:D:1262:ARG:HG3	3:D:1263:LYS:HG3	1.87	0.57
3:D:327:LEU:O	3:D:331:ILE:HG12	2.05	0.56
3:D:77:ARG:HE	3:D:79:LYS:HE2	1.70	0.56
2:C:808:ASN:N	2:C:808:ASN:HD22	2.02	0.56
3:D:885:VAL:HG13	3:D:894:VAL:HG21	1.85	0.56
1:A:234:LEU:HD13	1:A:235:ARG:N	2.20	0.56
3:D:1371:ARG:HG2	4:E:22:VAL:HG13	1.86	0.56
1:A:250:ASP:HB3	1:A:253:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:803:VAL:HG21	3:D:1309:ILE:HG22	1.86	0.56
2:C:200:ARG:HE	2:C:200:ARG:HA	1.71	0.56
2:C:834:GLN:HB2	2:C:1054:LEU:HB3	1.87	0.56
8:J:18:DA:H2''	8:J:19:DT:H5'	1.88	0.56
3:D:1350:ASN:HD22	3:D:1358:PRO:HD3	1.70	0.56
2:C:161:LYS:H	2:C:161:LYS:HD3	1.69	0.56
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.88	0.56
3:D:114:ILE:HD12	3:D:304:ASP:HB2	1.87	0.56
2:C:176:ILE:H	2:C:176:ILE:HD13	1.71	0.56
1:A:251:PRO:HA	1:A:254:LEU:HD13	1.88	0.56
3:D:1175:LEU:HB3	3:D:1178:THR:HB	1.86	0.56
1:A:180:VAL:HG22	1:A:182:ARG:H	1.71	0.56
1:A:66:HIS:CD2	1:A:67:GLU:HG3	2.40	0.56
3:D:798:ARG:HA	3:D:798:ARG:HE	1.71	0.56
2:C:46:GLN:HB3	2:C:50:GLU:HG2	1.86	0.56
3:D:1221:LEU:HD21	3:D:1305:ASP:HA	1.86	0.56
3:D:288:PRO:HD2	3:D:291:ILE:HD11	1.87	0.56
5:F:291:CYS:HB2	5:F:297:MET:HE3	1.88	0.56
2:C:1101:LEU:HA	3:D:719:PHE:HA	1.86	0.56
3:D:518:VAL:HA	3:D:536:LEU:HB3	1.88	0.56
3:D:810:THR:HG23	3:D:811:GLU:HG2	1.86	0.56
3:D:1344:LEU:HD12	3:D:1355:ARG:HH11	1.71	0.55
5:F:186:SER:O	5:F:190:LEU:HD13	2.05	0.55
6:G:30:ILE:HG21	9:G:679:CMP:H5'2	1.88	0.55
3:D:388:ARG:HD2	3:D:411:ILE:HG13	1.89	0.55
3:D:1355:ARG:HG2	3:D:1356:LEU:H	1.72	0.55
3:D:141:PHE:HA	3:D:297:ARG:HD3	1.88	0.55
1:B:17:GLU:HB3	1:B:25:LYS:HB2	1.87	0.55
2:C:755:LYS:CD	2:C:756:TYR:H	2.18	0.55
3:D:839:VAL:HA	3:D:842:ARG:HD2	1.89	0.55
3:D:1249:ASN:HD22	3:D:1250:ASP:H	1.52	0.55
2:C:550:VAL:HG11	2:C:560:PRO:HB3	1.87	0.55
3:D:1381:ALA:H	3:D:1382:PRO:CD	2.20	0.55
1:A:253:LEU:HA	1:A:278:ILE:HD11	1.89	0.55
2:C:668:ILE:HD12	2:C:668:ILE:O	2.07	0.55
8:J:83:DG:H2'	8:J:84:DA:C8	2.41	0.55
2:C:1293:VAL:HG13	2:C:1301:ARG:HA	1.88	0.55
1:A:159:ILE:HD13	1:A:172:LEU:HD12	1.88	0.55
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.41	0.55
2:C:110:PRO:HB3	2:C:118:LYS:HD2	1.88	0.55
3:D:450:HIS:CD2	3:D:452:LEU:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:551:LEU:HD13	5:F:552:THR:N	2.22	0.55
2:C:40:GLU:HG3	2:C:44:GLU:HB2	1.89	0.55
2:C:1314:GLN:HE21	3:D:473:THR:HA	1.70	0.55
1:A:64:VAL:HG21	1:A:78:ILE:HD13	1.89	0.55
2:C:687:ARG:HD3	2:C:688:GLN:HG3	1.89	0.55
3:D:1025:MET:HB2	3:D:1126:GLN:HE21	1.72	0.55
3:D:1158:GLU:HG3	3:D:1159:ILE:HG12	1.89	0.55
2:C:1068:GLY:H	2:C:1072:ASN:ND2	2.03	0.54
8:J:14:DC:H2'	8:J:15:DA:C8	2.42	0.54
3:D:1206:ARG:HB3	3:D:1223:LEU:HG	1.89	0.54
2:C:1112:ILE:HG12	3:D:712:GLN:HE21	1.72	0.54
1:A:251:PRO:HB2	3:D:392:THR:HG22	1.88	0.54
3:D:1207:GLY:HA3	3:D:1224:ARG:HD3	1.89	0.54
3:D:27:PRO:HD2	3:D:236:TRP:CZ3	2.42	0.54
5:F:187:GLN:HE22	5:F:267:ASP:HB3	1.72	0.54
1:A:78:ILE:HD12	1:A:81:ILE:HD11	1.90	0.54
6:G:50:LEU:HB3	6:G:60:ILE:HA	1.90	0.54
2:C:152:SER:HB3	2:C:452:ARG:HG3	1.89	0.54
3:D:271:ARG:O	3:D:275:ARG:HG2	2.07	0.54
2:C:12:ARG:HH21	2:C:1183:ALA:HB2	1.72	0.54
2:C:202:ARG:HA	2:C:202:ARG:HH11	1.72	0.54
3:D:1126:GLN:H	3:D:1126:GLN:NE2	2.05	0.54
6:H:133:ASN:HA	6:H:137:LEU:HD13	1.90	0.54
3:D:1295:ASN:HD21	3:D:1297:LYS:HE2	1.72	0.54
7:I:84:DT:H2'	7:I:85:DG:C8	2.43	0.54
1:A:260:LEU:HB2	1:A:262:LEU:HD21	1.90	0.54
2:C:194:LEU:HD22	2:C:196:VAL:HG23	1.90	0.54
3:D:452:LEU:HD11	3:D:506:VAL:HG21	1.90	0.54
2:C:758:ARG:NH1	2:C:835:GLU:HB2	2.23	0.54
5:F:405:ILE:H	5:F:405:ILE:HD13	1.73	0.54
3:D:290:ILE:HG12	3:D:291:ILE:HG23	1.89	0.53
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.90	0.53
5:F:548:LEU:HD22	5:F:560:ARG:HD3	1.90	0.53
3:D:953:LYS:NZ	3:D:953:LYS:HB2	2.23	0.53
3:D:1282:TYR:HB3	3:D:1286:LYS:HD3	1.89	0.53
8:J:3:DT:H2'	8:J:4:DG:C8	2.44	0.53
7:I:95:DC:H2'	7:I:96:DA:C8	2.43	0.53
5:F:508:GLU:H	5:F:508:GLU:CD	2.11	0.53
2:C:1269:ARG:HE	3:D:344:GLY:HA3	1.73	0.53
3:D:572:THR:HB	3:D:576:ARG:HB2	1.91	0.53
2:C:644:LEU:HD13	2:C:645:PHE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1355:ARG:HG2	3:D:1356:LEU:N	2.23	0.53
2:C:691:PRO:HA	2:C:788:SER:HB2	1.90	0.53
5:F:177:THR:HG23	5:F:260:ARG:HD2	1.91	0.53
2:C:519:ASN:ND2	2:C:520:PRO:HD2	2.23	0.53
1:B:61:ILE:HA	1:B:142:MET:HB3	1.90	0.53
1:A:145:LYS:HG3	1:A:147:GLN:HE22	1.74	0.53
6:H:18:CYS:HB3	6:H:95:ALA:HB1	1.91	0.53
3:D:421:VAL:HG12	3:D:470:VAL:HG12	1.91	0.53
6:G:32:GLN:HA	6:G:82:ARG:HB2	1.91	0.53
2:C:599:VAL:HG11	2:C:623:LEU:HD21	1.90	0.53
1:B:195:ARG:HH21	1:B:198:LEU:HD23	1.73	0.53
3:D:1047:THR:HG22	3:D:1062:LEU:HD21	1.90	0.53
5:F:588:ARG:HH11	5:F:589:GLN:HA	1.73	0.53
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.90	0.53
4:E:39:VAL:N	4:E:40:PRO:CD	2.71	0.53
3:D:1038:THR:O	3:D:1040:MET:HG3	2.08	0.53
1:A:35:PHE:HA	1:A:38:THR:HG22	1.91	0.53
4:E:59:ILE:HG23	4:E:60:ASN:N	2.24	0.53
2:C:413:GLU:O	2:C:414:ILE:HG22	2.07	0.53
1:B:101:THR:HG22	1:B:143:ARG:HD2	1.90	0.53
6:H:112:ILE:O	6:H:112:ILE:HD13	2.09	0.53
7:I:10:DT:H2'	7:I:11:DG:C8	2.44	0.52
2:C:453:ILE:HD11	2:C:581:THR:HG21	1.91	0.52
2:C:496:LYS:N	2:C:497:PRO:HD2	2.24	0.52
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.45	0.52
6:G:57:LYS:HD2	6:H:136:PHE:HE2	1.74	0.52
5:F:132:CYS:HA	5:F:257:LYS:HE2	1.91	0.52
3:D:649:LYS:HE2	3:D:649:LYS:N	2.23	0.52
2:C:88:ARG:HH12	2:C:941:LYS:HA	1.74	0.52
8:J:42:DA:OP2	8:J:42:DA:H3'	2.10	0.52
7:I:54:DT:H2''	7:I:55:DG:H5'	1.91	0.52
5:F:582:VAL:HG11	5:F:586:ARG:HD3	1.91	0.52
2:C:817:LEU:H	2:C:817:LEU:CD1	2.23	0.52
8:J:49:DA:H2''	8:J:50:DG:C8	2.45	0.52
7:I:53:DA:H1'	7:I:54:DT:H5'	1.92	0.52
2:C:716:ALA:HB3	2:C:783:LEU:HB2	1.90	0.52
1:A:13:LEU:HD11	1:A:16:ILE:HG23	1.91	0.52
2:C:1107:MET:SD	3:D:739:GLN:HG3	2.50	0.52
2:C:488:MET:HB3	2:C:489:PRO:HD3	1.92	0.52
2:C:865:LEU:HD13	2:C:871:VAL:HB	1.91	0.52
8:J:92:DT:H2'	8:J:93:DA:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:40:TYR:HB2	6:G:70:ILE:HB	1.90	0.52
2:C:1276:TRP:CD1	3:D:801:VAL:HG11	2.44	0.52
3:D:335:GLN:NE2	3:D:335:GLN:H	2.08	0.52
1:A:166:ARG:NE	1:A:166:ARG:H	2.07	0.52
6:G:13:TRP:HD1	6:G:109:ASN:HD22	1.56	0.52
2:C:1099:ASN:HB3	3:D:715:LYS:HG2	1.91	0.52
2:C:1293:VAL:HG11	2:C:1304:MET:HE3	1.91	0.52
2:C:729:ALA:HA	2:C:769:PRO:HG2	1.90	0.52
8:J:65:DT:H2'	8:J:66:DG:C8	2.45	0.52
3:D:393:THR:HG22	3:D:395:LYS:H	1.74	0.52
2:C:705:GLU:HG2	2:C:794:LEU:HB2	1.91	0.52
5:F:231:THR:HA	5:F:234:THR:HG22	1.92	0.51
3:D:983:LYS:HD3	3:D:983:LYS:H	1.75	0.51
2:C:811:ASN:H	2:C:811:ASN:ND2	2.08	0.51
2:C:1105:SER:HB3	3:D:716:GLN:OE1	2.11	0.51
3:D:30:ILE:HD13	3:D:30:ILE:O	2.08	0.51
3:D:543:SER:HA	3:D:561:GLY:HA2	1.90	0.51
8:J:67:DC:H2''	8:J:68:DC:H5'	1.91	0.51
3:D:1226:VAL:HG23	3:D:1304:ARG:HG2	1.90	0.51
2:C:811:ASN:H	2:C:811:ASN:HD22	1.57	0.51
3:D:1106:ILE:HD11	3:D:1123:ARG:HD2	1.93	0.51
8:J:84:DA:C2'	8:J:85:DT:H5'	2.40	0.51
1:B:133:LEU:HD12	1:B:138:ALA:HB1	1.92	0.51
5:F:511:ILE:HD11	5:F:519:LEU:HA	1.92	0.51
3:D:822:MET:HB2	3:D:887:SER:HG	1.75	0.51
3:D:126:LEU:HG	3:D:216:LYS:HE3	1.91	0.51
6:G:77:GLU:HB3	6:G:80:GLN:NE2	2.25	0.51
3:D:714:GLU:HG2	3:D:715:LYS:H	1.75	0.51
2:C:1103:VAL:HG11	3:D:712:GLN:N	2.25	0.51
3:D:1258:ARG:O	3:D:1258:ARG:HD2	2.11	0.51
2:C:1111:GLN:HG3	3:D:712:GLN:HE22	1.75	0.51
3:D:856:ILE:HD13	3:D:856:ILE:O	2.10	0.51
1:A:58:GLU:HA	1:A:172:LEU:HD22	1.92	0.51
8:J:86:DC:H2'	8:J:87:DA:C8	2.46	0.51
3:D:362:ARG:H	3:D:365:GLN:HB2	1.76	0.51
8:J:39:DG:H2'	8:J:40:DG:C8	2.46	0.51
8:J:44:DC:H2'	8:J:45:DA:C8	2.46	0.51
5:F:503:GLU:HB2	5:F:504:PRO:O	2.11	0.51
3:D:1155:ILE:HB	3:D:1176:VAL:HG11	1.93	0.51
3:D:1224:ARG:HB3	3:D:1228:ALA:HB3	1.93	0.51
3:D:1156:LEU:HD23	3:D:1157:ALA:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:112:ILE:O	6:G:112:ILE:HD13	2.11	0.51
3:D:610:ARG:HE	3:D:865:HIS:CE1	2.29	0.50
8:J:89:DA:C8	8:J:89:DA:H5'	2.45	0.50
2:C:901:LEU:HD11	5:F:598:LEU:HB3	1.93	0.50
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.93	0.50
3:D:104:HIS:HB2	3:D:241:VAL:HB	1.91	0.50
4:E:59:ILE:CG1	4:E:60:ASN:H	2.19	0.50
4:E:21:LEU:HA	4:E:24:ALA:HB3	1.93	0.50
3:D:289:ASP:HA	3:D:292:VAL:HG12	1.93	0.50
6:G:50:LEU:HD23	6:G:60:ILE:HG12	1.93	0.50
3:D:442:ILE:HD13	3:D:443:GLU:N	2.25	0.50
5:F:408:GLY:HA2	5:F:435:ILE:HG23	1.93	0.50
3:D:834:PRO:HA	3:D:838:ARG:HH12	1.76	0.50
5:F:397:ARG:NH2	8:J:30:DT:H2'	2.27	0.50
7:I:11:DG:H2'	7:I:12:DT:C6	2.46	0.50
3:D:805:GLN:HB2	3:D:1347:LEU:HB3	1.92	0.50
3:D:161:THR:HG22	3:D:163:GLU:H	1.76	0.50
1:A:207:THR:HG22	1:A:209:GLY:H	1.77	0.50
6:H:49:VAL:HG22	6:H:86:VAL:HG22	1.94	0.50
1:A:253:LEU:HD11	1:A:312:LEU:HD11	1.92	0.50
1:A:99:ILE:HG13	1:A:145:LYS:HE2	1.93	0.50
3:D:60:ARG:HA	3:D:90:VAL:HG22	1.93	0.50
3:D:35:PHE:HB2	3:D:61:ILE:HG23	1.92	0.50
2:C:577:VAL:HG11	2:C:658:GLN:HG2	1.93	0.50
2:C:1211:ARG:HE	2:C:1220:GLN:HB3	1.76	0.50
5:F:185:LEU:HD12	5:F:185:LEU:H	1.76	0.50
2:C:1281:TYR:CE2	3:D:431:ARG:HB3	2.47	0.50
3:D:485:MET:HG2	3:D:487:THR:HG22	1.94	0.50
3:D:1138:LEU:HB2	3:D:1139:PRO:HD3	1.94	0.50
1:B:32:GLU:HB2	1:B:35:PHE:HD2	1.77	0.50
6:G:75:LEU:HD13	6:G:99:TYR:HD2	1.77	0.50
2:C:384:LEU:HD23	2:C:384:LEU:H	1.76	0.50
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.93	0.49
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.94	0.49
5:F:582:VAL:HG21	5:F:586:ARG:HD3	1.94	0.49
3:D:925:GLU:N	3:D:926:PRO:CD	2.74	0.49
2:C:395:TYR:CD2	2:C:399:ALA:HB3	2.47	0.49
2:C:211:ARG:HH12	2:C:216:THR:HG22	1.78	0.49
5:F:286:LEU:HA	5:F:289:LYS:HE3	1.95	0.49
1:A:47:LEU:HD21	1:A:220:ALA:HB2	1.93	0.49
8:J:52:DG:H8	8:J:52:DG:OP2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:759:SER:HB3	2:C:763:THR:H	1.78	0.49
2:C:667:LEU:HD23	2:C:705:GLU:HG3	1.94	0.49
3:D:368:LEU:HD21	3:D:439:PRO:HB3	1.93	0.49
2:C:42:ASP:HB3	2:C:43:PRO:HD3	1.95	0.49
2:C:1113:LEU:HD22	2:C:1195:ILE:HD12	1.93	0.49
3:D:135:ILE:HD13	3:D:135:ILE:O	2.12	0.49
6:G:69:PHE:H	6:G:123:ARG:HH22	1.61	0.49
3:D:579:LEU:HD21	3:D:620:PHE:HZ	1.77	0.49
7:I:56:DC:OP2	7:I:56:DC:H6	1.96	0.49
1:B:192:VAL:HG22	1:B:193:GLU:H	1.78	0.49
2:C:202:ARG:HH22	2:C:369:MET:HG3	1.77	0.49
3:D:120:LEU:HG	3:D:121:PRO:HA	1.94	0.49
3:D:822:MET:O	3:D:824:PRO:HD3	2.12	0.49
2:C:211:ARG:HD3	2:C:347:ILE:HA	1.95	0.49
6:H:130:LYS:HE3	6:H:134:LEU:HD21	1.94	0.49
2:C:169:LYS:HA	2:C:432:LEU:HA	1.95	0.49
6:G:131:VAL:HG22	6:H:131:VAL:HG22	1.94	0.49
2:C:178:PRO:HA	2:C:394:ARG:HD3	1.95	0.49
3:D:148:GLU:HB2	3:D:188:LEU:HD11	1.94	0.49
2:C:540:ARG:H	2:C:540:ARG:HD3	1.76	0.49
1:A:195:ARG:NH2	1:A:197:ASP:HB3	2.27	0.49
2:C:157:PHE:HD2	2:C:169:LYS:HD2	1.77	0.49
2:C:93:SER:HB2	2:C:126:GLU:HG2	1.95	0.49
4:E:72:GLN:H	4:E:72:GLN:CD	2.16	0.49
3:D:112:ALA:HB2	3:D:185:ILE:HD13	1.94	0.49
3:D:826:ILE:HD13	3:D:877:VAL:HG13	1.95	0.49
4:E:36:ASP:N	4:E:37:PRO:CD	2.76	0.48
2:C:431:LYS:O	2:C:435:ILE:HG22	2.14	0.48
5:F:264:LYS:N	5:F:264:LYS:HE3	2.28	0.48
3:D:262:THR:HG21	5:F:449:THR:HG21	1.95	0.48
3:D:1165:PHE:HA	3:D:1174:ARG:NH1	2.28	0.48
3:D:275:ARG:NH2	3:D:298:MET:HB3	2.28	0.48
7:I:77:DC:H2'	7:I:78:DC:C6	2.48	0.48
7:I:29:DT:H2'	7:I:30:DA:C8	2.47	0.48
2:C:542:ARG:HH11	2:C:542:ARG:HA	1.78	0.48
2:C:414:ILE:HG12	2:C:415:GLU:H	1.77	0.48
3:D:953:LYS:N	3:D:953:LYS:HD3	2.28	0.48
2:C:1306:LYS:HG2	5:F:535:ALA:HB2	1.96	0.48
3:D:118:LYS:HB2	3:D:311:ARG:HH21	1.78	0.48
2:C:423:ASP:HA	2:C:426:ILE:HG22	1.95	0.48
6:H:43:VAL:HG12	6:H:44:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:18:CYS:HB3	6:G:95:ALA:HB1	1.94	0.48
1:A:91:ARG:HB3	1:A:210:THR:HG23	1.94	0.48
1:A:240:PRO:HB3	1:B:30:PRO:HG3	1.96	0.48
3:D:265:LEU:HD11	3:D:327:LEU:HD23	1.94	0.48
3:D:836:ARG:HG3	3:D:869:CYS:SG	2.54	0.48
2:C:1108:ASN:N	2:C:1108:ASN:HD22	2.07	0.48
1:A:30:PRO:C	1:A:31:LEU:HD22	2.34	0.48
3:D:885:VAL:HG11	3:D:1255:VAL:HG12	1.96	0.48
2:C:1103:VAL:HB	2:C:1104:PRO:HD3	1.96	0.48
2:C:144:VAL:HG21	2:C:527:LYS:HG2	1.95	0.48
6:H:40:TYR:HB2	6:H:70:ILE:HB	1.95	0.48
5:F:598:LEU:O	5:F:601:PRO:HD2	2.13	0.48
2:C:1086:PRO:HG3	2:C:1215:GLY:H	1.79	0.48
2:C:698:PRO:HG3	2:C:1231:TYR:CE1	2.48	0.48
3:D:832:LYS:NZ	3:D:832:LYS:HB2	2.29	0.48
2:C:811:ASN:HD22	2:C:811:ASN:N	2.11	0.48
3:D:838:ARG:HG3	3:D:839:VAL:HG23	1.96	0.48
3:D:245:LEU:HD11	3:D:249:LEU:HD22	1.94	0.48
3:D:1174:ARG:HB3	3:D:1178:THR:HG22	1.94	0.48
3:D:452:LEU:HD21	3:D:506:VAL:HG11	1.96	0.48
2:C:1186:VAL:HG22	2:C:1187:PHE:CD1	2.49	0.48
3:D:1285:VAL:HG13	3:D:1286:LYS:HD2	1.96	0.48
3:D:337:ARG:HB2	8:J:17:DA:H8	1.79	0.48
3:D:1058:SER:HB3	3:D:1106:ILE:HB	1.96	0.48
2:C:1337:ILE:HD13	2:C:1338:GLU:N	2.29	0.48
1:A:81:ILE:HG13	1:A:82:LEU:HD22	1.95	0.48
2:C:395:TYR:HD2	2:C:399:ALA:HB3	1.79	0.48
3:D:27:PRO:HA	3:D:30:ILE:HG22	1.94	0.47
4:E:18:ASP:O	4:E:22:VAL:HG23	2.14	0.47
5:F:588:ARG:HG3	8:J:53:DT:H2'	1.96	0.47
2:C:453:ILE:HG21	2:C:530:ILE:HD13	1.97	0.47
6:H:90:THR:HG22	8:J:95:DT:H5'	1.96	0.47
3:D:341:ASN:ND2	3:D:342:LEU:H	2.12	0.47
2:C:500:ALA:HA	2:C:503:LYS:HE2	1.97	0.47
3:D:807:LEU:HB2	3:D:1259:GLN:HE21	1.80	0.47
2:C:10:ARG:NE	2:C:1181:PRO:HD3	2.29	0.47
1:A:58:GLU:HB3	1:A:145:LYS:HD2	1.96	0.47
1:A:78:ILE:O	1:A:82:LEU:HD23	2.14	0.47
2:C:157:PHE:HA	2:C:169:LYS:NZ	2.29	0.47
6:G:201:LYS:HE3	7:I:29:DT:H5''	1.95	0.47
3:D:314:ARG:NH2	3:D:323:PRO:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:PRO:HB2	1:A:241:GLU:H	1.57	0.47
3:D:1175:LEU:HD13	3:D:1188:GLU:HB2	1.96	0.47
3:D:1044:GLN:NE2	3:D:1045:THR:HG23	2.29	0.47
1:A:2:GLN:HE22	1:A:4:SER:HB2	1.79	0.47
2:C:1269:ARG:HB2	3:D:346:ARG:HG2	1.96	0.47
1:B:195:ARG:NH2	1:B:198:LEU:HD23	2.30	0.47
8:J:48:DA:H2'	8:J:49:DA:C8	2.50	0.47
5:F:180:HIS:CD2	5:F:190:LEU:HG	2.49	0.47
6:H:15:LEU:HA	6:H:18:CYS:SG	2.54	0.47
3:D:53:ARG:CZ	3:D:60:ARG:HH21	2.27	0.47
3:D:474:LEU:HD23	3:D:474:LEU:O	2.14	0.47
8:J:96:DG:H2''	8:J:97:DC:H5'	1.97	0.47
2:C:817:LEU:O	2:C:817:LEU:HD22	2.14	0.47
2:C:180:ARG:HG3	7:I:79:DT:C2	2.49	0.47
2:C:831:ILE:HD12	2:C:831:ILE:N	2.30	0.47
2:C:482:GLY:HA3	2:C:487:LEU:HD22	1.96	0.47
8:J:56:DA:H4'	8:J:57:DG:OP1	2.15	0.47
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.97	0.47
3:D:580:TRP:HD1	3:D:591:ILE:HD12	1.80	0.47
1:A:219:ARG:O	1:A:219:ARG:HD3	2.15	0.47
3:D:1324:SER:HB2	3:D:1348:LYS:NZ	2.30	0.47
3:D:850:LYS:HB3	3:D:850:LYS:NZ	2.29	0.47
3:D:432:LEU:HD21	3:D:499:ILE:HG21	1.97	0.47
3:D:483:LEU:HD23	4:E:16:ARG:HH12	1.78	0.47
3:D:909:ILE:HG23	3:D:913:GLU:HG3	1.97	0.47
2:C:157:PHE:HA	2:C:169:LYS:HZ2	1.80	0.47
2:C:1313:HIS:HE1	3:D:474:LEU:H	1.62	0.47
2:C:1078:LYS:HD2	2:C:1079:ILE:N	2.30	0.47
3:D:979:ASN:HD22	3:D:979:ASN:H	1.63	0.47
7:I:49:DC:H2'	7:I:50:DT:C6	2.50	0.47
3:D:983:LYS:HB2	3:D:991:THR:HG23	1.96	0.47
3:D:380:PHE:HZ	3:D:472:LEU:HG	1.80	0.47
2:C:886:LYS:HB3	2:C:886:LYS:NZ	2.30	0.47
3:D:1175:LEU:HD22	3:D:1186:TYR:HD2	1.80	0.47
5:F:551:LEU:HD12	5:F:556:ALA:HB2	1.95	0.47
7:I:65:DC:H2'	7:I:66:DG:C8	2.50	0.47
3:D:605:LEU:O	3:D:605:LEU:HD23	2.15	0.47
3:D:281:ARG:NH1	5:F:188:GLU:HG3	2.30	0.46
2:C:818:VAL:HG23	2:C:1076:ILE:HD13	1.97	0.46
3:D:1172:LYS:HD3	3:D:1172:LYS:O	2.16	0.46
3:D:865:HIS:HB3	3:D:868:TRP:CD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1289:GLU:HB2	2:C:1294:LYS:HE2	1.96	0.46
2:C:218:GLU:HG3	2:C:222:ASP:OD2	2.15	0.46
5:F:276:MET:HA	5:F:279:ARG:HH21	1.81	0.46
6:G:106:ILE:HD13	6:G:113:LEU:HD22	1.96	0.46
3:D:265:LEU:O	3:D:265:LEU:HD23	2.16	0.46
3:D:719:PHE:CG	3:D:720:ASN:N	2.83	0.46
3:D:1381:ALA:N	3:D:1382:PRO:CD	2.78	0.46
5:F:234:THR:HG23	5:F:235:ILE:HD12	1.97	0.46
3:D:431:ARG:HB2	3:D:431:ARG:NH1	2.30	0.46
7:I:64:DT:H2'	7:I:65:DC:C6	2.49	0.46
3:D:902:ASP:O	3:D:903:LEU:HB2	2.16	0.46
3:D:560:ASN:HB2	3:D:573:THR:HA	1.96	0.46
3:D:1328:THR:O	3:D:1332:LEU:HD23	2.16	0.46
4:E:36:ASP:CG	4:E:37:PRO:HD3	2.35	0.46
6:H:139:VAL:HG22	6:H:142:ARG:HH21	1.80	0.46
7:I:37:DA:H1'	7:I:38:DA:H5''	1.98	0.46
7:I:47:DC:H4'	7:I:48:DA:OP1	2.16	0.46
3:D:579:LEU:HD21	3:D:620:PHE:CZ	2.50	0.46
3:D:293:ARG:HH21	3:D:296:LYS:HB2	1.81	0.46
5:F:591:GLU:O	5:F:595:LEU:HG	2.16	0.46
2:C:361:SER:OG	2:C:364:VAL:HG23	2.16	0.46
1:B:33:ARG:HE	1:B:33:ARG:HA	1.81	0.46
7:I:48:DA:H4'	7:I:49:DC:OP1	2.16	0.46
3:D:1381:ALA:H	3:D:1382:PRO:HD2	1.81	0.46
3:D:450:HIS:NE2	3:D:452:LEU:HB2	2.31	0.46
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.98	0.46
3:D:953:LYS:HZ2	3:D:953:LYS:HB2	1.80	0.46
3:D:525:MET:HG2	3:D:527:LEU:HG	1.97	0.46
5:F:359:LYS:HB2	5:F:359:LYS:NZ	2.31	0.46
7:I:1:DC:H2'	7:I:2:DG:C8	2.51	0.46
3:D:516:ASP:HB3	3:D:536:LEU:HB2	1.98	0.46
3:D:450:HIS:CG	3:D:451:PRO:HD2	2.51	0.46
3:D:739:GLN:C	3:D:740:LEU:HD22	2.36	0.46
2:C:473:ARG:N	2:C:473:ARG:HD2	2.31	0.46
1:B:191:ARG:N	1:B:191:ARG:HD2	2.31	0.46
3:D:339:ARG:HB3	8:J:17:DA:H5'	1.98	0.46
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.86	0.46
3:D:609:TYR:CE2	3:D:614:LEU:HG	2.51	0.46
3:D:1028:ILE:HG12	3:D:1120:THR:HG22	1.98	0.46
3:D:222:LYS:HE2	3:D:1275:LEU:HD23	1.96	0.46
5:F:582:VAL:HG12	7:I:42:DC:H3'	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:483:LEU:HB3	4:E:16:ARG:NH1	2.31	0.45
3:D:1075:ARG:N	3:D:1075:ARG:HD2	2.30	0.45
3:D:81:ARG:N	3:D:81:ARG:HD3	2.30	0.45
1:A:252:ILE:HG23	1:A:253:LEU:HD12	1.98	0.45
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.51	0.45
5:F:457:ILE:HD12	5:F:460:ILE:HD12	1.97	0.45
1:B:164:ASP:H	1:B:167:PRO:HG3	1.80	0.45
6:H:208:THR:HG22	6:H:209:ARG:HG3	1.99	0.45
5:F:426:LYS:HB2	5:F:426:LYS:NZ	2.31	0.45
3:D:371:LYS:HB2	3:D:371:LYS:NZ	2.31	0.45
2:C:1325:VAL:HG11	3:D:99:ARG:HH21	1.81	0.45
6:H:23:TYR:HA	6:H:24:PRO:HD2	1.83	0.45
3:D:514:THR:HG23	3:D:576:ARG:HD2	1.98	0.45
6:H:169:ARG:NH2	7:I:10:DT:H5"	2.32	0.45
6:H:72:GLU:HB2	6:H:116:LEU:HD21	1.97	0.45
3:D:65:VAL:HG22	3:D:98:ARG:HH22	1.81	0.45
5:F:571:HIS:HB3	5:F:574:GLU:HB3	1.99	0.45
3:D:1144:LEU:HB3	3:D:1233:ILE:HG13	1.98	0.45
5:F:593:LYS:HD2	5:F:596:ARG:NH2	2.32	0.45
3:D:637:ALA:HA	3:D:709:ARG:HD3	1.98	0.45
3:D:685:ILE:O	3:D:685:ILE:HD13	2.16	0.45
2:C:414:ILE:HG12	2:C:415:GLU:OE1	2.17	0.45
3:D:277:ASN:HA	3:D:280:LYS:HD2	1.97	0.45
3:D:1357:ILE:HA	3:D:1358:PRO:HD3	1.77	0.45
2:C:854:ILE:HA	2:C:855:PRO:HD3	1.82	0.45
7:I:75:DC:H2"	7:I:76:DA:C8	2.52	0.45
5:F:306:PHE:O	5:F:310:GLU:HB3	2.16	0.45
5:F:300:LYS:HB3	5:F:300:LYS:NZ	2.31	0.45
2:C:811:ASN:HB2	2:C:1099:ASN:HD22	1.81	0.45
2:C:354:ASP:OD2	2:C:359:ARG:HA	2.17	0.45
3:D:430:HIS:HD2	3:D:432:LEU:N	2.12	0.45
3:D:555:TYR:CD1	3:D:574:VAL:HG21	2.49	0.45
6:H:77:GLU:HB3	6:H:80:GLN:NE2	2.32	0.45
3:D:551:ARG:HE	3:D:551:ARG:H	1.63	0.45
4:E:46:THR:O	4:E:54:ILE:HD11	2.16	0.45
1:A:118:ASP:HB3	1:A:121:VAL:HB	1.98	0.45
2:C:742:TYR:HD2	2:C:744:GLY:H	1.61	0.45
1:B:61:ILE:HG12	1:B:142:MET:HB3	1.97	0.45
3:D:1037:PHE:HD2	3:D:1040:MET:HE3	1.81	0.45
2:C:775:GLU:HA	2:C:776:PRO:HD2	1.83	0.45
5:F:343:LYS:HB2	5:F:343:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG11	1:A:183:ILE:HD11	1.98	0.45
2:C:1070:HIS:NE2	2:C:1111:GLN:HB3	2.32	0.45
2:C:117:ILE:HG23	2:C:488:MET:HG2	1.98	0.45
2:C:488:MET:H	2:C:489:PRO:CD	2.29	0.45
7:I:45:DT:H2"	7:I:46:DA:C8	2.52	0.45
5:F:566:ASP:CG	5:F:567:MET:H	2.20	0.45
1:A:298:LYS:HA	1:A:301:THR:HG22	1.99	0.45
3:D:340:GLN:HB3	8:J:18:DA:H5'	1.99	0.45
2:C:1103:VAL:H	2:C:1104:PRO:CD	2.29	0.45
5:F:402:LEU:O	5:F:402:LEU:HD13	2.16	0.45
5:F:185:LEU:HD11	5:F:413:MET:HB3	1.99	0.45
3:D:609:TYR:HE2	3:D:614:LEU:HG	1.82	0.45
3:D:930:LEU:HB3	3:D:931:THR:H	1.60	0.45
3:D:21:LYS:NZ	3:D:21:LYS:HB3	2.32	0.45
2:C:1307:ASN:ND2	2:C:1314:GLN:HA	2.30	0.45
5:F:551:LEU:HD22	5:F:552:THR:H	1.82	0.45
3:D:579:LEU:O	3:D:582:ILE:HG12	2.17	0.45
4:E:36:ASP:OD1	4:E:37:PRO:HD3	2.16	0.45
5:F:418:LYS:NZ	5:F:418:LYS:HB3	2.31	0.45
1:A:226:GLU:HA	1:A:229:GLU:HG3	1.98	0.45
4:E:56:GLU:OE1	4:E:58:LEU:HD22	2.17	0.44
3:D:483:LEU:HD12	3:D:484:MET:N	2.32	0.44
3:D:911:LYS:HG2	3:D:1365:TYR:HD2	1.82	0.44
3:D:291:ILE:H	3:D:291:ILE:HD13	1.81	0.44
2:C:1314:GLN:CD	2:C:1314:GLN:H	2.20	0.44
3:D:1145:PHE:O	3:D:1309:ILE:HG12	2.17	0.44
3:D:1101:LEU:HA	3:D:1102:PRO:HD2	1.86	0.44
2:C:470:ARG:HA	2:C:470:ARG:HH11	1.81	0.44
3:D:1366:HIS:CD2	4:E:21:LEU:HD12	2.53	0.44
2:C:1204:LEU:H	2:C:1205:PRO:CD	2.29	0.44
3:D:1350:ASN:ND2	3:D:1358:PRO:HD3	2.32	0.44
3:D:1224:ARG:HE	3:D:1228:ALA:HB1	1.82	0.44
2:C:1259:LEU:HB3	2:C:1260:GLY:H	1.67	0.44
3:D:820:ILE:O	3:D:820:ILE:HG23	2.17	0.44
3:D:955:LYS:NZ	3:D:955:LYS:HB3	2.32	0.44
2:C:1099:ASN:OD1	2:C:1101:LEU:HB2	2.17	0.44
3:D:979:ASN:N	3:D:979:ASN:HD22	2.15	0.44
7:I:41:DG:H8	7:I:41:DG:OP2	2.00	0.44
2:C:1292:THR:HG22	2:C:1320:PRO:HG3	1.99	0.44
8:J:77:DG:H2"	8:J:78:DA:C8	2.52	0.44
2:C:540:ARG:N	2:C:540:ARG:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:914:LYS:HB2	2:C:914:LYS:NZ	2.32	0.44
3:D:624:ILE:O	3:D:624:ILE:HD13	2.18	0.44
1:B:82:LEU:HA	1:B:85:LEU:HD12	1.98	0.44
1:B:51:MET:HA	1:B:52:PRO:HD2	1.84	0.44
3:D:108:ALA:HB2	3:D:280:LYS:HE2	2.00	0.44
2:C:599:VAL:HG13	2:C:626:GLU:HG3	1.99	0.44
5:F:185:LEU:HD12	5:F:185:LEU:N	2.32	0.44
3:D:135:ILE:O	3:D:139:LEU:HD12	2.16	0.44
5:F:454:VAL:HG11	7:I:64:DT:H72	1.99	0.44
1:B:164:ASP:CG	1:B:165:GLU:H	2.21	0.44
6:G:169:ARG:HH21	8:J:74:DT:H5''	1.83	0.44
5:F:216:LEU:HD21	5:F:220:LYS:HE3	1.99	0.44
3:D:910:ASN:ND2	3:D:911:LYS:H	2.15	0.44
3:D:1075:ARG:HH11	3:D:1075:ARG:N	2.16	0.44
2:C:110:PRO:HB3	2:C:118:LYS:HB2	2.00	0.44
3:D:644:MET:HG3	3:D:764:ARG:NH1	2.32	0.44
3:D:702:GLN:HA	3:D:706:VAL:HG22	1.99	0.44
2:C:564:PRO:HG2	2:C:572:ILE:HB	2.00	0.44
2:C:831:ILE:HD12	2:C:831:ILE:H	1.83	0.44
3:D:609:TYR:HD2	3:D:617:THR:HG21	1.83	0.44
2:C:471:VAL:HG21	2:C:493:ILE:HG12	1.99	0.44
2:C:1089:GLU:HG3	2:C:1213:TYR:HE2	1.83	0.44
4:E:6:VAL:HG13	4:E:7:GLN:CD	2.38	0.44
3:D:317:THR:HB	3:D:324:LEU:HD13	2.00	0.44
3:D:1079:LYS:HB3	3:D:1079:LYS:NZ	2.32	0.44
2:C:57:PHE:HA	2:C:59:ILE:N	2.32	0.44
3:D:1279:GLN:HB3	3:D:1282:TYR:HE1	1.82	0.44
3:D:566:LYS:NZ	3:D:584:PRO:HB3	2.33	0.44
2:C:11:ILE:HD13	2:C:12:ARG:N	2.32	0.44
1:A:243:LYS:HB3	1:A:245:GLU:OE2	2.18	0.44
3:D:690:ASN:HB2	3:D:738:ARG:HD3	1.98	0.44
2:C:844:LYS:HD3	2:C:844:LYS:O	2.18	0.44
8:J:37:DC:H2'	8:J:38:DC:C6	2.52	0.44
3:D:298:MET:HE2	5:F:402:LEU:HG	2.00	0.43
2:C:448:LEU:HD21	2:C:554:HIS:NE2	2.32	0.43
3:D:94:GLN:H	3:D:94:GLN:NE2	2.16	0.43
3:D:661:VAL:O	3:D:664:ILE:HG22	2.18	0.43
2:C:587:LEU:HD23	2:C:588:GLU:N	2.33	0.43
2:C:169:LYS:HZ3	2:C:175:ARG:H	1.65	0.43
7:I:34:DA:H2''	7:I:35:DA:H8	1.82	0.43
2:C:1182:ILE:HG22	2:C:1184:THR:HG23	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1041:ILE:N	3:D:1041:ILE:HD12	2.32	0.43
3:D:381:ILE:O	3:D:385:LEU:HG	2.19	0.43
1:A:224:LEU:HD12	1:B:228:LEU:HD11	2.00	0.43
7:I:54:DT:H2'	7:I:55:DG:C8	2.53	0.43
2:C:865:LEU:HD22	2:C:865:LEU:H	1.82	0.43
5:F:361:ILE:O	5:F:365:MET:HG3	2.18	0.43
2:C:1278:LEU:HD11	2:C:1286:THR:HG23	2.00	0.43
1:B:13:LEU:HD11	1:B:16:ILE:HD11	2.01	0.43
3:D:842:ARG:HD3	3:D:882:VAL:HG21	2.01	0.43
2:C:1270:PHE:HB2	3:D:347:VAL:HG23	2.00	0.43
2:C:645:PHE:O	2:C:646:SER:HB2	2.19	0.43
3:D:615:LYS:O	3:D:619:ILE:HG12	2.18	0.43
3:D:131:PRO:HD2	3:D:135:ILE:HG21	2.00	0.43
2:C:1294:LYS:HZ1	3:D:472:LEU:HD13	1.83	0.43
2:C:892:GLU:O	2:C:894:GLN:HG3	2.18	0.43
1:B:28:LEU:HB3	1:B:201:LEU:HB3	2.00	0.43
3:D:291:ILE:N	3:D:291:ILE:HD13	2.33	0.43
3:D:1372:ARG:HG2	3:D:1374:ALA:H	1.83	0.43
1:B:23:HIS:HE1	1:B:25:LYS:NZ	2.17	0.43
3:D:739:GLN:OE1	3:D:744:ARG:HD2	2.17	0.43
3:D:103:GLY:O	3:D:243:PRO:HA	2.18	0.43
1:B:219:ARG:O	1:B:223:ILE:HG13	2.19	0.43
5:F:407:GLU:HB2	5:F:439:ILE:HG22	2.01	0.43
3:D:721:SER:OG	3:D:724:MET:HB3	2.19	0.43
2:C:864:LYS:N	2:C:864:LYS:HD2	2.32	0.43
2:C:1073:LYS:NZ	2:C:1073:LYS:HB3	2.33	0.43
2:C:200:ARG:HA	2:C:200:ARG:NE	2.33	0.43
6:G:77:GLU:HB3	6:G:80:GLN:HE21	1.83	0.43
3:D:579:LEU:O	3:D:579:LEU:HD23	2.18	0.43
1:A:71:LYS:HZ3	1:A:140:ILE:HA	1.84	0.43
1:B:152:TYR:HE1	1:B:176:CYS:HG	1.65	0.43
2:C:49:LEU:HG	2:C:53:PHE:HE2	1.83	0.43
2:C:39:ILE:HD12	2:C:39:ILE:N	2.33	0.43
3:D:1194:ARG:HH21	3:D:1210:ILE:HG22	1.83	0.43
1:A:66:HIS:CG	1:A:67:GLU:H	2.37	0.43
2:C:493:ILE:HD13	2:C:494:ASN:N	2.34	0.43
2:C:189:ASP:HA	2:C:190:PRO:HD2	1.83	0.43
2:C:1198:LEU:O	2:C:1198:LEU:HD13	2.19	0.43
1:B:192:VAL:HG12	1:B:195:ARG:O	2.19	0.43
3:D:822:MET:HB2	3:D:887:SER:OG	2.19	0.43
2:C:790:ASP:C	2:C:792:GLY:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1261:GLY:H	2:C:1264:GLN:HG3	1.84	0.43
7:I:31:DG:H2'	7:I:32:DG:C8	2.53	0.43
2:C:204:LEU:O	2:C:204:LEU:HD12	2.18	0.43
1:A:246:LYS:O	1:A:246:LYS:HG2	2.19	0.43
2:C:685:MET:HA	2:C:685:MET:HE2	2.00	0.43
3:D:250:ARG:N	3:D:251:PRO:HD3	2.32	0.43
5:F:373:ARG:O	5:F:377:LYS:HG3	2.19	0.43
1:A:239:GLN:HA	1:A:240:PRO:HD3	1.91	0.43
2:C:180:ARG:HG3	7:I:79:DT:H3	1.84	0.43
3:D:1338:ALA:HB3	3:D:1340:LYS:HE3	2.01	0.43
4:E:24:ALA:O	4:E:28:ARG:HG2	2.19	0.43
3:D:336:GLY:O	3:D:340:GLN:HG2	2.18	0.43
3:D:450:HIS:O	3:D:453:VAL:HG12	2.19	0.43
2:C:1103:VAL:HG21	3:D:712:GLN:H	1.84	0.43
3:D:395:LYS:O	3:D:395:LYS:HD3	2.19	0.43
1:B:95:LYS:HD2	1:B:98:VAL:HB	2.00	0.43
2:C:677:ASN:HD21	3:D:779:ALA:HB1	1.83	0.43
2:C:804:PHE:CE1	3:D:713:GLU:HG3	2.53	0.43
3:D:717:VAL:HG13	3:D:731:ARG:HG2	2.00	0.43
5:F:353:LEU:HD12	5:F:353:LEU:N	2.34	0.42
3:D:1145:PHE:HE1	3:D:1237:VAL:HG21	1.84	0.42
3:D:1258:ARG:HA	3:D:1261:LEU:HD12	2.01	0.42
3:D:650:LYS:O	3:D:654:ILE:HG12	2.19	0.42
3:D:1162:ILE:HG22	3:D:1180:VAL:HB	2.00	0.42
4:E:63:ILE:O	4:E:63:ILE:HG23	2.18	0.42
3:D:1024:THR:O	3:D:1026:PRO:HD3	2.19	0.42
4:E:29:GLN:HA	4:E:32:VAL:HG22	2.01	0.42
2:C:836:LEU:HD13	2:C:1054:LEU:HB2	2.01	0.42
6:H:130:LYS:O	6:H:134:LEU:HG	2.19	0.42
1:A:246:LYS:N	1:A:246:LYS:HD3	2.34	0.42
3:D:746:LEU:HD13	3:D:754:ILE:HD11	2.01	0.42
1:B:86:LYS:HG3	1:B:174:ASP:HB2	2.01	0.42
1:A:317:ARG:N	1:A:317:ARG:HD3	2.29	0.42
3:D:1331:VAL:HG23	3:D:1332:LEU:HD22	2.01	0.42
8:J:9:DC:H2'	8:J:10:DC:C6	2.55	0.42
2:C:109:ALA:HA	2:C:110:PRO:HD3	1.92	0.42
2:C:152:SER:HA	2:C:153:PRO:HD3	1.92	0.42
6:G:57:LYS:HD2	6:H:136:PHE:CE2	2.54	0.42
1:B:32:GLU:HB2	1:B:35:PHE:CD2	2.53	0.42
3:D:131:PRO:HD2	3:D:135:ILE:CG2	2.49	0.42
3:D:282:LEU:O	3:D:286:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1264:ALA:HB2	3:D:1280:VAL:HG12	2.01	0.42
2:C:755:LYS:HD2	2:C:756:TYR:N	2.32	0.42
3:D:378:LYS:HE2	3:D:382:TYR:CE1	2.54	0.42
2:C:617:ALA:HA	2:C:636:CYS:HB3	2.01	0.42
3:D:1175:LEU:HB2	3:D:1187:GLU:HA	2.01	0.42
2:C:225:PHE:HD1	2:C:322:LEU:HB2	1.84	0.42
4:E:38:LEU:HD22	4:E:40:PRO:HD2	2.01	0.42
7:I:72:DT:H5''	7:I:73:DC:OP2	2.18	0.42
2:C:937:ASP:HB3	2:C:939:VAL:HG22	2.00	0.42
2:C:169:LYS:HE2	2:C:174:ALA:HA	2.02	0.42
3:D:116:PHE:HD1	3:D:123:ARG:HD2	1.83	0.42
3:D:422:LEU:HD12	3:D:434:ILE:HG22	2.01	0.42
3:D:384:LYS:HE3	3:D:415:VAL:HA	2.01	0.42
2:C:142:GLU:H	2:C:142:GLU:CD	2.23	0.42
3:D:30:ILE:HA	3:D:33:TRP:CE3	2.54	0.42
1:B:118:ASP:HB3	1:B:121:VAL:HG12	2.02	0.42
1:A:165:GLU:HB2	1:A:166:ARG:CZ	2.49	0.42
7:I:35:DA:H2''	7:I:36:DA:H8	1.85	0.42
2:C:1087:TYR:CD1	2:C:1091:GLY:HA2	2.55	0.42
1:A:265:ARG:C	1:A:265:ARG:HD3	2.40	0.42
8:J:76:DT:C2'	8:J:77:DG:H5'	2.50	0.42
2:C:1294:LYS:NZ	3:D:472:LEU:HD13	2.34	0.42
3:D:614:LEU:HD12	3:D:614:LEU:N	2.34	0.42
1:A:237:VAL:C	1:A:238:ARG:HD3	2.39	0.42
2:C:694:ARG:HA	2:C:694:ARG:HH11	1.83	0.42
2:C:1326:LEU:O	2:C:1326:LEU:HD23	2.20	0.42
3:D:972:LYS:HD2	3:D:972:LYS:N	2.35	0.42
1:A:79:LEU:O	1:A:83:LEU:HD13	2.19	0.42
3:D:278:ARG:HH22	5:F:402:LEU:HD12	1.85	0.42
2:C:530:ILE:HG13	2:C:575:LEU:HD21	2.02	0.42
3:D:128:LEU:HD23	3:D:188:LEU:HD22	2.01	0.42
3:D:252:LEU:HA	3:D:261:ALA:O	2.20	0.42
2:C:490:GLN:HE21	5:F:472:GLN:HA	1.83	0.42
2:C:562:GLU:HA	2:C:680:LEU:HD23	2.00	0.42
5:F:462:LYS:HD3	5:F:462:LYS:O	2.20	0.42
3:D:1307:LEU:CD2	3:D:1307:LEU:H	2.33	0.42
1:B:64:VAL:HG11	1:B:171:LEU:HD11	2.01	0.42
2:C:217:THR:HA	2:C:221:LEU:HD11	2.01	0.42
2:C:42:ASP:H	2:C:43:PRO:CD	2.33	0.42
8:J:4:DG:H2'	8:J:5:DT:C6	2.55	0.42
7:I:32:DG:H2'	7:I:33:DC:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:573:ASN:C	2:C:573:ASN:HD22	2.23	0.42
5:F:252:LEU:O	5:F:252:LEU:HD23	2.20	0.42
3:D:932:MET:HE2	3:D:932:MET:HB2	1.92	0.42
2:C:145:ILE:HD12	2:C:145:ILE:N	2.35	0.42
2:C:678:ARG:HE	2:C:1106:ARG:HG3	1.85	0.42
3:D:551:ARG:NE	3:D:551:ARG:H	2.17	0.42
2:C:794:LEU:HD13	2:C:796:LEU:HG	2.01	0.42
4:E:72:GLN:HG2	4:E:73:GLN:H	1.85	0.42
1:B:13:LEU:HD13	1:B:14:VAL:N	2.35	0.42
3:D:973:LEU:O	3:D:1002:VAL:HA	2.19	0.42
2:C:816:ILE:O	2:C:1076:ILE:HA	2.19	0.41
7:I:24:DC:H2"	7:I:25:DA:C8	2.54	0.41
3:D:1373:ARG:HB3	3:D:1379:PRO:HG3	2.02	0.41
4:E:55:GLU:HB3	4:E:56:GLU:H	1.74	0.41
2:C:811:ASN:HA	2:C:815:SER:HB2	2.02	0.41
2:C:194:LEU:HG	2:C:324:LYS:HD3	2.03	0.41
3:D:1151:LYS:CD	3:D:1151:LYS:H	2.31	0.41
3:D:576:ARG:HH22	3:D:594:GLN:N	2.17	0.41
3:D:783:LEU:N	3:D:783:LEU:HD13	2.35	0.41
2:C:178:PRO:HB2	2:C:179:TYR:H	1.68	0.41
3:D:781:LYS:N	3:D:781:LYS:HD2	2.35	0.41
1:A:235:ARG:CD	1:A:235:ARG:H	2.22	0.41
3:D:288:PRO:HB2	3:D:289:ASP:H	1.76	0.41
6:H:40:TYR:HB3	6:H:94:VAL:HG11	2.02	0.41
1:A:225:ALA:O	1:A:229:GLU:HG3	2.21	0.41
3:D:690:ASN:H	3:D:690:ASN:ND2	2.18	0.41
3:D:50:LYS:HA	3:D:51:PRO:HD3	1.95	0.41
2:C:852:ALA:HB2	2:C:869:GLY:H	1.86	0.41
2:C:402:ARG:HE	2:C:406:ASN:ND2	2.18	0.41
6:H:58:GLU:HB2	6:H:174:GLN:HE22	1.85	0.41
3:D:1077:ALA:HB2	3:D:1100:PHE:CD1	2.54	0.41
2:C:561:ILE:HD12	2:C:561:ILE:N	2.36	0.41
1:B:200:LYS:N	1:B:200:LYS:HD3	2.34	0.41
2:C:668:ILE:HA	2:C:669:PRO:HD3	1.85	0.41
1:A:99:ILE:HD12	1:A:99:ILE:N	2.35	0.41
2:C:577:VAL:HG13	2:C:578:TYR:CD1	2.55	0.41
1:B:77:ASP:O	1:B:81:ILE:HG12	2.21	0.41
6:H:14:PHE:CZ	6:H:97:ILE:HD12	2.55	0.41
4:E:75:GLN:HA	4:E:78:ALA:HB3	2.02	0.41
7:I:62:DG:H22	8:J:36:DG:H22	1.66	0.41
5:F:608:ARG:HH11	5:F:611:LEU:HD11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:NZ	8:J:64:DT:H2'	2.36	0.41
1:B:10:LYS:HA	1:B:11:PRO:HD2	1.86	0.41
6:H:75:LEU:HD21	6:H:102:PHE:CE1	2.55	0.41
5:F:593:LYS:HD2	5:F:596:ARG:HH21	1.85	0.41
1:B:16:ILE:N	1:B:16:ILE:HD12	2.34	0.41
5:F:554:ARG:O	5:F:558:VAL:HG23	2.19	0.41
2:C:445:ILE:HD12	2:C:445:ILE:N	2.36	0.41
3:D:1093:THR:HB	3:D:1095:MET:CE	2.50	0.41
2:C:1325:VAL:O	2:C:1329:GLU:HG3	2.20	0.41
3:D:214:ARG:O	3:D:218:THR:HG23	2.21	0.41
1:B:194:GLN:HG2	1:B:195:ARG:H	1.85	0.41
1:A:31:LEU:HB2	1:A:199:ASP:O	2.20	0.41
3:D:1165:PHE:HE2	3:D:1167:LYS:HE2	1.85	0.41
2:C:176:ILE:HG12	2:C:178:PRO:HD3	2.03	0.41
2:C:1104:PRO:HA	3:D:740:LEU:HD21	2.03	0.41
3:D:488:ASN:HA	3:D:614:LEU:HD23	2.03	0.41
6:G:9:PRO:HB2	6:G:10:THR:H	1.55	0.41
3:D:213:LYS:O	3:D:217:LEU:HG	2.21	0.41
2:C:187:GLU:HG2	2:C:188:PHE:H	1.85	0.41
1:B:11:PRO:HA	1:B:30:PRO:HB2	2.01	0.41
2:C:108:GLU:HG3	2:C:115:LYS:O	2.21	0.41
3:D:128:LEU:HD12	3:D:128:LEU:N	2.36	0.41
2:C:1246:ARG:NH1	2:C:1258:PRO:HB3	2.36	0.41
6:G:73:LEU:HD22	6:H:121:ALA:HA	2.03	0.41
3:D:385:LEU:HD22	3:D:390:LEU:HD12	2.02	0.41
3:D:1363:TYR:HD2	3:D:1365:TYR:H	1.69	0.41
3:D:1175:LEU:O	3:D:1176:VAL:C	2.59	0.41
7:I:53:DA:H2'	7:I:53:DA:OP2	2.21	0.41
3:D:959:LYS:HD3	3:D:960:LEU:N	2.36	0.41
3:D:978:ARG:HG2	3:D:999:TYR:CD1	2.55	0.41
5:F:157:ARG:HG3	5:F:159:SER:H	1.85	0.41
3:D:216:LYS:HD3	3:D:216:LYS:C	2.41	0.41
3:D:113:HIS:CD2	3:D:115:TRP:HB2	2.56	0.41
2:C:518:ASN:ND2	2:C:761:GLN:HB2	2.34	0.41
2:C:594:VAL:HG12	2:C:599:VAL:HA	2.03	0.41
2:C:705:GLU:HB3	2:C:794:LEU:HB2	2.02	0.41
6:G:123:ARG:HA	6:G:126:VAL:HG22	2.02	0.41
3:D:128:LEU:HD11	3:D:189:LEU:HD21	2.02	0.41
2:C:468:LEU:O	2:C:471:VAL:HG12	2.21	0.41
2:C:733:VAL:HG22	2:C:750:ILE:HG12	2.03	0.41
1:A:46:ILE:O	1:A:50:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD23	1:B:224:LEU:O	2.21	0.41
5:F:509:THR:HA	5:F:510:PRO:HD2	1.88	0.41
7:I:3:DC:H2''	7:I:4:DA:H5'	2.02	0.41
3:D:299:LEU:O	3:D:303:VAL:HG23	2.21	0.41
3:D:1220:ILE:HD11	3:D:1229:VAL:HG23	2.03	0.41
3:D:647:PRO:HG3	3:D:697:MET:HG3	2.02	0.41
8:J:22:DC:H2'	8:J:23:DA:C8	2.56	0.41
2:C:138:ILE:N	2:C:138:ILE:HD12	2.36	0.41
5:F:476:ARG:N	5:F:476:ARG:HD2	2.36	0.41
3:D:115:TRP:CZ3	3:D:1329:THR:HG23	2.56	0.41
7:I:48:DA:H1'	7:I:49:DC:C6	2.56	0.41
2:C:1204:LEU:H	2:C:1205:PRO:HD2	1.86	0.41
3:D:800:LEU:HD21	3:D:1145:PHE:CD2	2.56	0.41
3:D:343:LEU:HD12	8:J:18:DA:H2	1.85	0.41
2:C:1070:HIS:CE1	2:C:1111:GLN:HB3	2.56	0.41
3:D:180:MET:HG3	3:D:296:LYS:HD3	2.03	0.41
1:B:107:ILE:HD12	1:B:107:ILE:N	2.35	0.41
6:G:11:LEU:O	6:G:11:LEU:HD23	2.21	0.41
3:D:260:PHE:HB2	5:F:504:PRO:HG2	2.03	0.40
3:D:774:ILE:HA	3:D:777:HIS:CD2	2.47	0.40
3:D:378:LYS:O	3:D:381:ILE:HG22	2.21	0.40
3:D:925:GLU:CG	3:D:926:PRO:HD3	2.50	0.40
3:D:30:ILE:HG13	3:D:243:PRO:HG3	2.03	0.40
2:C:77:GLU:HA	2:C:78:PRO:HD3	1.94	0.40
2:C:346:TYR:HE1	2:C:348:SER:OG	2.04	0.40
5:F:363:ARG:HD2	5:F:363:ARG:C	2.42	0.40
2:C:341:LEU:N	2:C:341:LEU:HD12	2.36	0.40
3:D:838:ARG:HG3	3:D:839:VAL:N	2.36	0.40
5:F:231:THR:O	5:F:235:ILE:HD13	2.21	0.40
6:G:69:PHE:N	6:G:123:ARG:HH22	2.18	0.40
4:E:25:ARG:HH22	4:E:73:GLN:HG3	1.86	0.40
2:C:56:VAL:HG11	2:C:468:LEU:HD22	2.02	0.40
3:D:686:TRP:HB2	3:D:746:LEU:HD11	2.03	0.40
6:H:9:PRO:HB2	6:H:10:THR:H	1.56	0.40
3:D:704:GLU:HG2	3:D:705:THR:HG22	2.03	0.40
3:D:366:CYS:SG	3:D:437:PHE:HB2	2.61	0.40
3:D:718:SER:O	3:D:719:PHE:HB2	2.21	0.40
3:D:320:ASN:HD22	3:D:322:ARG:NH1	2.15	0.40
3:D:573:THR:HG23	3:D:575:GLY:N	2.34	0.40
3:D:1075:ARG:HA	3:D:1076:PRO:HD2	1.82	0.40
1:A:81:ILE:HG13	1:A:82:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1304:ARG:N	3:D:1304:ARG:HD3	2.36	0.40
1:B:33:ARG:NE	1:B:33:ARG:HA	2.37	0.40
1:A:46:ILE:HG22	1:A:46:ILE:O	2.22	0.40
1:A:10:LYS:HE3	1:B:226:GLU:HB3	2.03	0.40
2:C:207:THR:HG22	2:C:325:LEU:HD12	2.03	0.40
6:H:171:GLU:O	6:H:175:ILE:HG12	2.21	0.40
7:I:20:DA:H2'	7:I:21:DT:C6	2.56	0.40
1:B:48:LEU:HD11	1:B:183:ILE:HB	2.03	0.40
2:C:208:ILE:HB	2:C:362:ALA:HA	2.02	0.40
4:E:26:ARG:HD3	4:E:26:ARG:O	2.21	0.40
6:G:84:ALA:HB3	9:G:679:CMP:H8	2.02	0.40
1:B:66:HIS:CG	1:B:67:GLU:H	2.39	0.40
3:D:1224:ARG:NE	3:D:1228:ALA:HB1	2.37	0.40
3:D:795:TYR:HB3	3:D:1138:LEU:HD23	2.03	0.40
3:D:877:VAL:HG12	3:D:877:VAL:O	2.21	0.40
2:C:82:VAL:HG22	2:C:92:TYR:CE1	2.57	0.40
1:A:86:LYS:HE3	1:A:174:ASP:HB2	2.03	0.40
2:C:896:THR:HB	2:C:898:GLU:OE2	2.22	0.40
2:C:897:PRO:HG2	2:C:898:GLU:OE1	2.22	0.40
1:B:115:ILE:N	1:B:115:ILE:HD12	2.35	0.40
7:I:80:DT:H6	7:I:80:DT:H2'	1.70	0.40
2:C:354:ASP:HA	2:C:355:PRO:HD3	1.82	0.40
2:C:742:TYR:HA	2:C:743:PRO:HD3	1.93	0.40
1:A:254:LEU:HA	1:A:321:TRP:HZ3	1.86	0.40
2:C:43:PRO:HB2	2:C:44:GLU:H	1.73	0.40
3:D:27:PRO:HD2	3:D:236:TRP:HZ3	1.85	0.40
5:F:548:LEU:O	5:F:548:LEU:HD23	2.22	0.40
3:D:690:ASN:HD22	3:D:691:ASP:N	2.20	0.40
3:D:156:ARG:N	3:D:156:ARG:HD3	2.36	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 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	318/329 (97%)	259 (81%)	46 (14%)	13 (4%)	3	35
1	B	233/329 (71%)	191 (82%)	38 (16%)	4 (2%)	11	55
2	C	1085/1342 (81%)	822 (76%)	217 (20%)	46 (4%)	3	34
3	D	1366/1413 (97%)	1075 (79%)	232 (17%)	59 (4%)	3	34
4	E	88/90 (98%)	68 (77%)	14 (16%)	6 (7%)	1	23
5	F	475/613 (78%)	401 (84%)	54 (11%)	20 (4%)	3	34
6	G	199/209 (95%)	172 (86%)	24 (12%)	3 (2%)	13	57
6	H	199/209 (95%)	182 (92%)	16 (8%)	1 (0%)	34	77
All	All	3963/4534 (87%)	3170 (80%)	641 (16%)	152 (4%)	7	37

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	240	PRO
1	B	52	PRO
2	C	180	ARG
2	C	332	ARG
2	C	414	ILE
2	C	419	ILE
2	C	808	ASN
3	D	131	PRO
3	D	320	ASN
3	D	321	LYS
3	D	526	VAL
3	D	530	PRO
4	E	59	ILE
4	E	72	GLN
4	E	86	ILE
5	F	490	PRO
2	C	43	PRO
2	C	165	HIS
2	C	178	PRO
2	C	179	TYR
2	C	181	GLY
2	C	190	PRO
2	C	409	LEU
2	C	787	PRO
2	C	833	ILE
2	C	877	VAL

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Mol	Chain	Res	Type
2	C	1284	ALA
2	C	1295	SER
3	D	141	PHE
3	D	170	GLU
3	D	180	MET
3	D	185	ILE
3	D	288	PRO
3	D	289	ASP
3	D	318	GLY
3	D	331	ILE
3	D	402	GLU
3	D	410	ASP
3	D	430	HIS
3	D	518	VAL
3	D	555	TYR
3	D	685	ILE
3	D	718	SER
3	D	1293	GLU
4	E	73	GLN
5	F	238	LYS
5	F	395	THR
5	F	491	GLU
5	F	609	SER
6	G	14	PHE
1	A	61	ILE
1	A	152	TYR
1	A	179	PRO
1	A	188	GLU
1	A	323	PRO
1	B	188	GLU
2	C	372	PRO
2	C	489	PRO
2	C	625	GLU
2	C	812	PHE
2	C	1103	VAL
2	C	1110	GLY
2	C	1201	LEU
2	C	1204	LEU
3	D	135	ILE
3	D	211	GLU
3	D	285	LEU
3	D	716	GLN

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Mol	Chain	Res	Type
3	D	717	VAL
3	D	720	ASN
3	D	814	CYS
3	D	815	GLY
3	D	817	HIS
3	D	832	LYS
4	E	35	LYS
5	F	114	GLU
5	F	398	GLY
5	F	542	ALA
5	F	543	ALA
5	F	568	ASN
6	G	22	LYS
6	G	56	GLY
1	A	158	ARG
1	B	93	GLN
2	C	84	GLU
2	C	163	LYS
2	C	169	LYS
2	C	387	ASN
2	C	507	GLY
2	C	662	SER
2	C	670	PHE
2	C	804	PHE
2	C	1283	ALA
2	C	1341	ASP
3	D	101	ARG
3	D	176	PHE
3	D	282	LEU
3	D	517	CYS
3	D	593	ASN
3	D	721	SER
3	D	752	GLY
3	D	892	PHE
3	D	947	GLU
3	D	1378	ALA
5	F	173	ASP
5	F	504	PRO
5	F	541	ARG
5	F	572	THR
5	F	581	ASP
6	H	56	GLY

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Mol	Chain	Res	Type
1	A	49	SER
1	A	187	VAL
1	A	202	VAL
1	B	167	PRO
2	C	111	GLU
2	C	337	PHE
2	C	348	SER
2	C	646	SER
2	C	1223	ARG
3	D	47	ARG
3	D	322	ARG
3	D	496	GLY
3	D	538	ARG
3	D	556	GLU
3	D	558	ASP
3	D	821	MET
5	F	570	ASP
1	A	5	VAL
2	C	488	MET
3	D	938	GLY
3	D	1082	ASP
3	D	1285	VAL
2	C	345	PRO
3	D	323	PRO
5	F	333	VAL
2	C	874	GLY
3	D	73	GLY
3	D	313	GLY
3	D	1176	VAL
5	F	308	GLY
1	A	29	GLU
2	C	42	ASP
2	C	907	GLY
2	C	1044	PRO
3	D	159	ILE
3	D	1381	ALA
5	F	582	VAL
3	D	401	VAL
4	E	57	GLY
5	F	606	VAL
3	D	82	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	278/286 (97%)	268 (96%)	10 (4%)	42	74
1	B	201/286 (70%)	193 (96%)	8 (4%)	38	71
2	C	936/1157 (81%)	896 (96%)	40 (4%)	35	70
3	D	1138/1174 (97%)	1075 (94%)	63 (6%)	27	63
4	E	74/74 (100%)	67 (90%)	7 (10%)	11	41
5	F	423/540 (78%)	407 (96%)	16 (4%)	40	73
6	G	173/180 (96%)	172 (99%)	1 (1%)	90	95
6	H	173/180 (96%)	172 (99%)	1 (1%)	90	95
All	All	3396/3877 (88%)	3250 (96%)	146 (4%)	40	70

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	166	ARG
1	A	195	ARG
1	A	219	ARG
1	A	227	GLN
1	A	235	ARG
1	A	246	LYS
1	A	265	ARG
1	A	297	LYS
1	A	317	ARG
1	B	2	GLN
1	B	6	THR
1	B	86	LYS
1	B	140	ILE
1	B	142	MET
1	B	182	ARG
1	B	200	LYS
1	B	234	LEU
2	C	11	ILE

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Mol	Chain	Res	Type
2	C	20	GLN
2	C	22	LEU
2	C	83	GLN
2	C	86	GLN
2	C	161	LYS
2	C	173	ASN
2	C	176	ILE
2	C	220	ILE
2	C	221	LEU
2	C	324	LYS
2	C	333	ILE
2	C	346	TYR
2	C	351	LEU
2	C	397	LEU
2	C	452	ARG
2	C	493	ILE
2	C	540	ARG
2	C	573	ASN
2	C	593	LYS
2	C	595	THR
2	C	687	ARG
2	C	719	LYS
2	C	750	ILE
2	C	755	LYS
2	C	794	LEU
2	C	808	ASN
2	C	811	ASN
2	C	817	LEU
2	C	821	ARG
2	C	877	VAL
2	C	909	LYS
2	C	914	LYS
2	C	1048	LYS
2	C	1054	LEU
2	C	1072	ASN
2	C	1108	ASN
2	C	1234	LYS
2	C	1308	ILE
2	C	1337	ILE
3	D	30	ILE
3	D	39	LYS
3	D	81	ARG

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Mol	Chain	Res	Type
3	D	94	GLN
3	D	124	ILE
3	D	130	MET
3	D	135	ILE
3	D	139	LEU
3	D	151	MET
3	D	156	ARG
3	D	180	MET
3	D	229	GLN
3	D	290	ILE
3	D	291	ILE
3	D	293	ARG
3	D	300	GLN
3	D	334	LYS
3	D	335	GLN
3	D	411	ILE
3	D	431	ARG
3	D	442	ILE
3	D	483	LEU
3	D	535	ARG
3	D	549	LYS
3	D	551	ARG
3	D	599	LYS
3	D	603	LYS
3	D	611	ILE
3	D	624	ILE
3	D	649	LYS
3	D	665	GLN
3	D	685	ILE
3	D	690	ASN
3	D	783	LEU
3	D	798	ARG
3	D	820	ILE
3	D	822	MET
3	D	850	LYS
3	D	856	ILE
3	D	861	ASN
3	D	863	LEU
3	D	908	ILE
3	D	915	ILE
3	D	953	LYS
3	D	972	LYS

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Mol	Chain	Res	Type
3	D	979	ASN
3	D	983	LYS
3	D	1025	MET
3	D	1075	ARG
3	D	1079	LYS
3	D	1126	GLN
3	D	1140	ARG
3	D	1151	LYS
3	D	1167	LYS
3	D	1169	THR
3	D	1172	LYS
3	D	1192	LYS
3	D	1203	ARG
3	D	1247	LYS
3	D	1249	ASN
3	D	1304	ARG
3	D	1311	LYS
3	D	1357	ILE
4	E	7	GLN
4	E	26	ARG
4	E	52	ARG
4	E	56	GLU
4	E	63	ILE
4	E	70	GLN
4	E	86	ILE
5	F	162	ILE
5	F	238	LYS
5	F	246	GLN
5	F	264	LYS
5	F	289	LYS
5	F	300	LYS
5	F	359	LYS
5	F	402	LEU
5	F	405	ILE
5	F	418	LYS
5	F	468	ARG
5	F	505	ILE
5	F	530	LEU
5	F	562	ARG
5	F	588	ARG
5	F	608	ARG
6	G	112	ILE

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Mol	Chain	Res	Type
6	H	112	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	41	ASN
1	A	66	HIS
1	A	137	ASN
1	A	186	ASN
1	A	194	GLN
1	A	227	GLN
1	A	283	GLN
1	B	2	GLN
1	B	23	HIS
1	B	41	ASN
1	B	66	HIS
1	B	137	ASN
2	C	20	GLN
2	C	36	GLN
2	C	60	GLN
2	C	83	GLN
2	C	86	GLN
2	C	120	GLN
2	C	148	GLN
2	C	339	ASN
2	C	463	GLN
2	C	517	GLN
2	C	518	ASN
2	C	519	ASN
2	C	573	ASN
2	C	618	GLN
2	C	622	ASN
2	C	659	GLN
2	C	677	ASN
2	C	686	GLN
2	C	760	ASN
2	C	762	ASN
2	C	766	ASN
2	C	798	GLN
2	C	808	ASN
2	C	832	HIS

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Mol	Chain	Res	Type
2	C	1061	GLN
2	C	1072	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1244	HIS
2	C	1264	GLN
2	C	1268	GLN
2	C	1288	GLN
2	C	1307	ASN
2	C	1313	HIS
3	D	45	ASN
3	D	94	GLN
3	D	113	HIS
3	D	158	GLN
3	D	164	GLN
3	D	229	GLN
3	D	274	ASN
3	D	300	GLN
3	D	320	ASN
3	D	335	GLN
3	D	340	GLN
3	D	341	ASN
3	D	430	HIS
3	D	435	GLN
3	D	448	GLN
3	D	458	ASN
3	D	489	ASN
3	D	495	ASN
3	D	667	GLN
3	D	669	GLN
3	D	690	ASN
3	D	708	ASN
3	D	712	GLN
3	D	777	HIS
3	D	792	ASN
3	D	817	HIS
3	D	861	ASN
3	D	865	HIS
3	D	867	GLN
3	D	875	ASN
3	D	962	ASN
3	D	979	ASN

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Mol	Chain	Res	Type
3	D	1010	GLN
3	D	1019	ASN
3	D	1044	GLN
3	D	1049	GLN
3	D	1098	GLN
3	D	1126	GLN
3	D	1195	GLN
3	D	1244	GLN
3	D	1249	ASN
3	D	1279	GLN
3	D	1295	ASN
3	D	1326	GLN
3	D	1366	HIS
4	E	7	GLN
4	E	60	ASN
5	F	128	ASN
5	F	129	GLN
5	F	131	GLN
5	F	149	ASN
5	F	180	HIS
5	F	187	GLN
5	F	258	GLN
5	F	309	ASN
5	F	357	GLN
5	F	406	GLN
5	F	437	GLN
5	F	469	GLN
5	F	579	GLN
6	G	65	ASN
6	G	66	GLN
6	G	125	GLN
6	G	133	ASN
6	H	17	HIS
6	H	21	HIS
6	H	66	GLN
6	H	133	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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	CMP	G	679	-	20,25,25	1.18	1 (5%)	18,39,39	2.19	3 (16%)
9	CMP	H	680	-	20,25,25	1.18	2 (10%)	18,39,39	2.21	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CMP	G	679	-	-	0/0/31/31	0/4/4/4
9	CMP	H	680	-	-	0/0/31/31	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	680	CMP	O4'-C1'	2.01	1.44	1.41
9	G	679	CMP	C5-C4	3.11	1.47	1.40
9	H	680	CMP	C5-C4	3.12	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	680	CMP	N3-C2-N1	-6.62	123.67	128.87
9	G	679	CMP	N3-C2-N1	-6.51	123.76	128.87
9	H	680	CMP	O3'-C3'-C4'	-4.81	106.88	110.72
9	G	679	CMP	O3'-C3'-C4'	-4.80	106.88	110.72
9	H	680	CMP	C4'-O4'-C1'	-2.03	107.49	109.64
9	G	679	CMP	C4'-O4'-C1'	-2.03	107.50	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	679	CMP	3	0
9	H	680	CMP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.