



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:07 PM UTC

PDB ID : 6CUU / pdb_00006cuu
Title : Thermus thermophiles RNA polymerase in complex with promoter DNA and antibiotic Kanglemycin A
Authors : Molodtsov, V.; Murakami, K.S.
Deposited on : 2018-03-26
Resolution : 2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

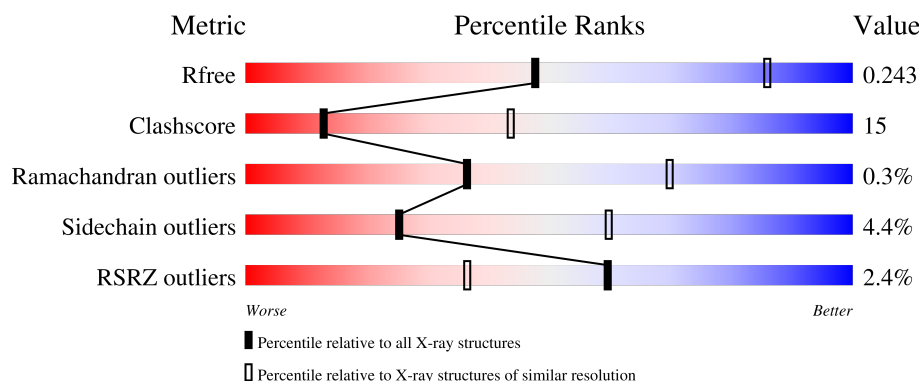
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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.



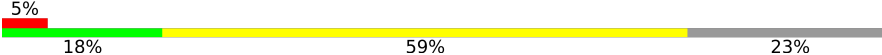
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	2% 50% 21% 28%
1	B	315	2% 48% 22% 29%
2	C	1119	3% 68% 28%
3	D	1524	2% 68% 27%
4	E	99	3% 67% 28% 5%

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Mol	Chain	Length	Quality of chain
5	F	423	
6	G	22	
7	H	27	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28403 atoms, of which 62 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1787	1141	311	333	2			
1	B	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8717	5517	1555	1622	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	958	THR	PRO	conflict	UNP Q72HM5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11652	7391	2046	2180	35			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	274	ARG	GLN	conflict	UNP Q72HM6
D	1041	LEU	MET	conflict	UNP Q72HM6
D	1313	VAL	ALA	conflict	UNP Q72HM6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2793	1763	508	518	4			

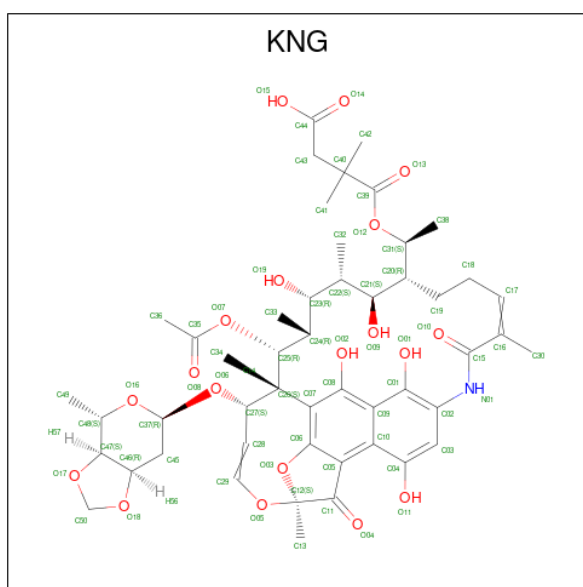
- Molecule 6 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			348	165	69	97	17			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*CP*TP*CP*TP*GP*AP*TP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	22	Total	C	N	O	P	0	0	0
			451	216	84	130	21			

- Molecule 8 is Kanglemycin A (CCD ID: KNG) (formula: C₅₀H₆₇NO₁₉).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			132	50	62	1	19		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		

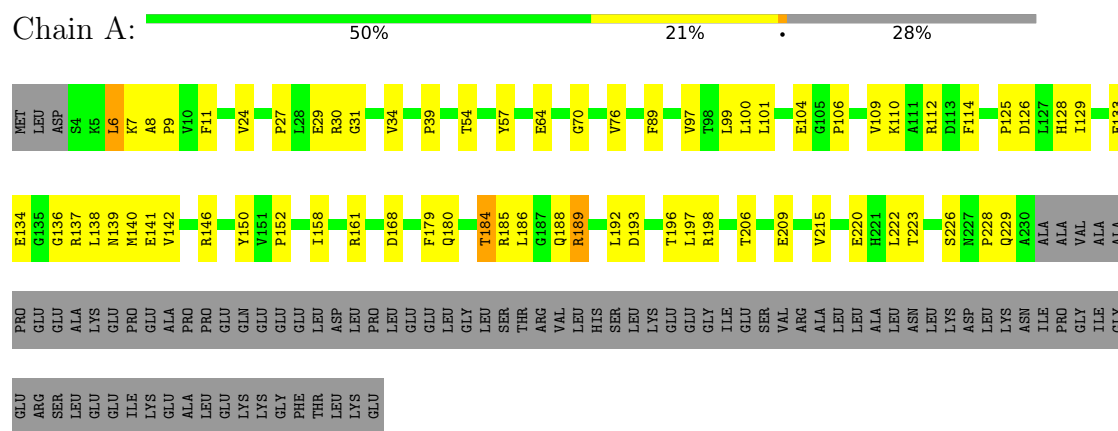
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Mg	0	0
			2	2		

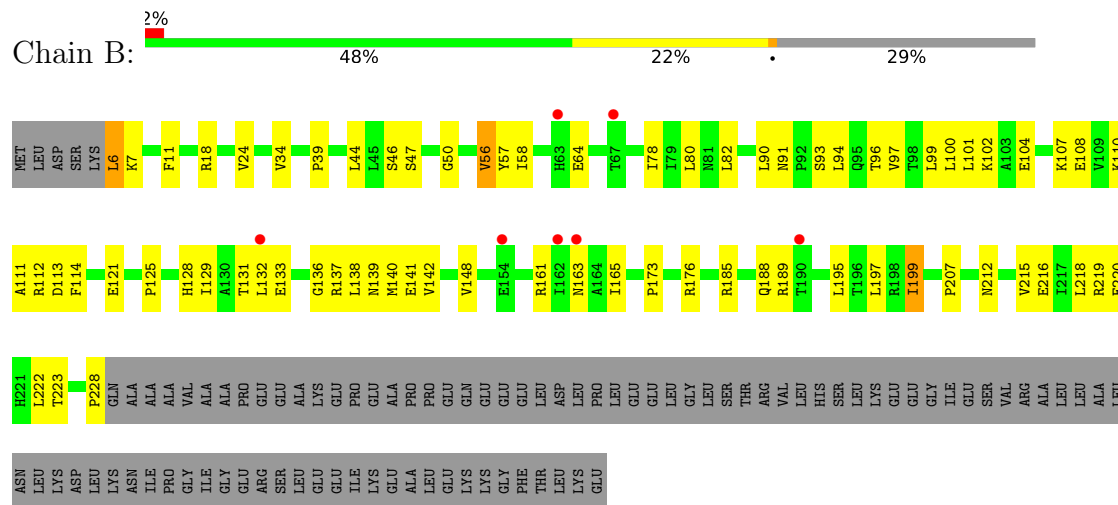
3 Residue-property plots

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

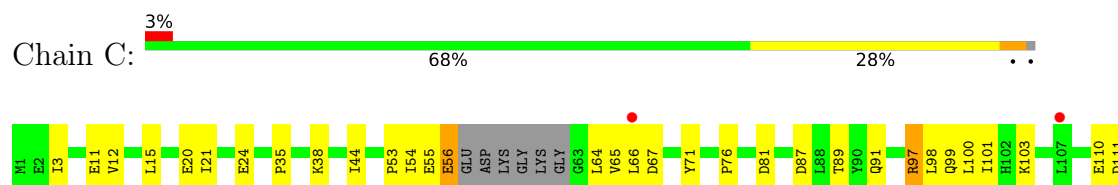
• Molecule 1: DNA-directed RNA polymerase subunit alpha

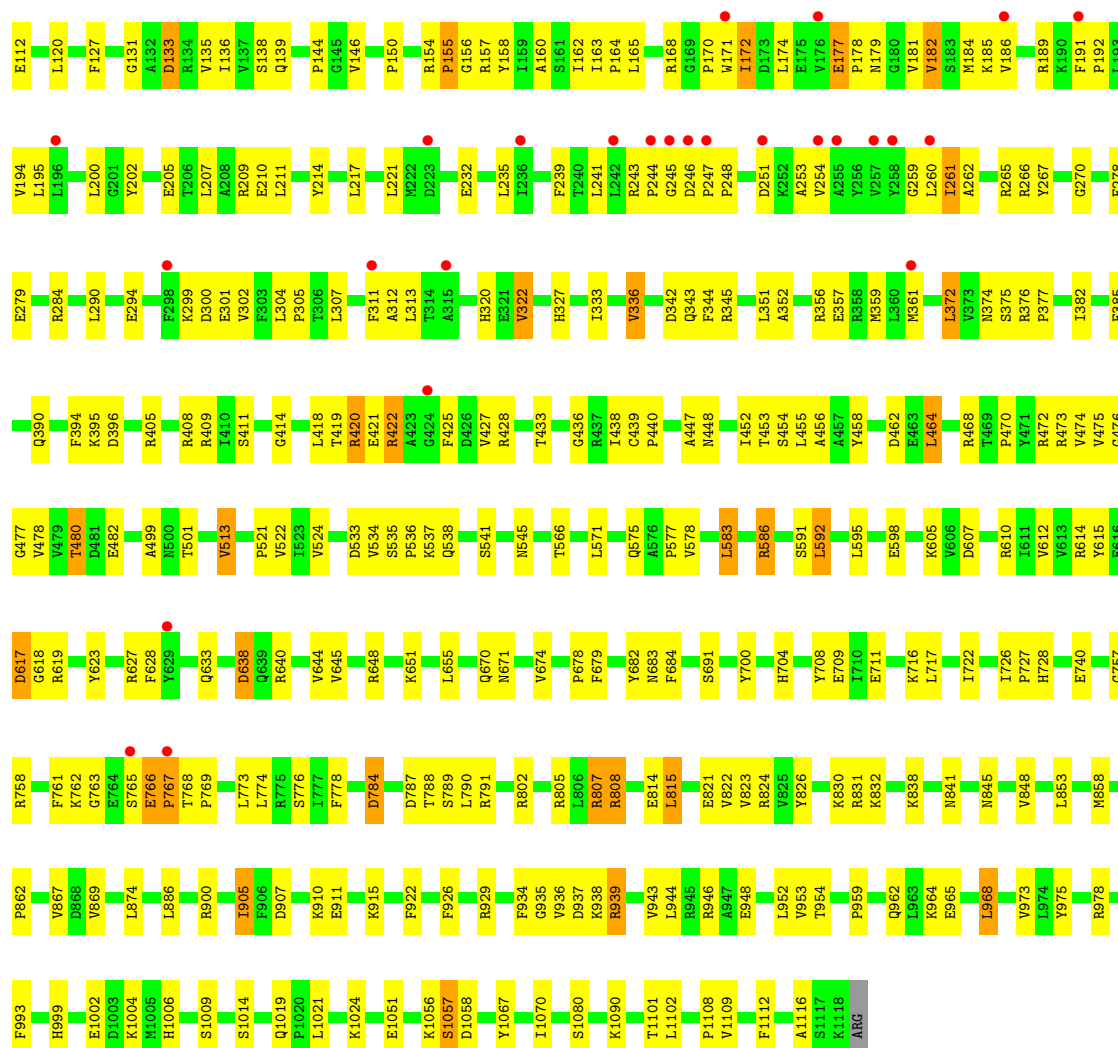


• Molecule 1: DNA-directed RNA polymerase subunit alpha

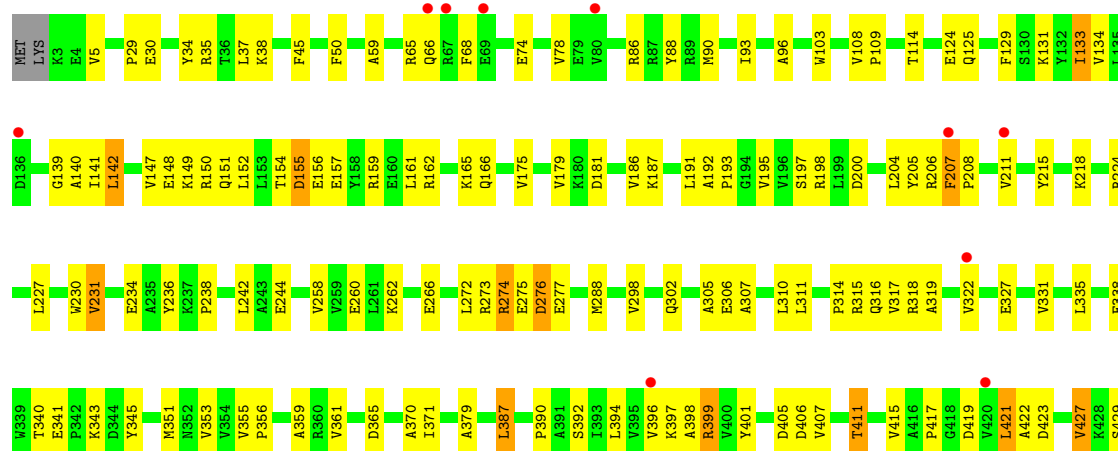


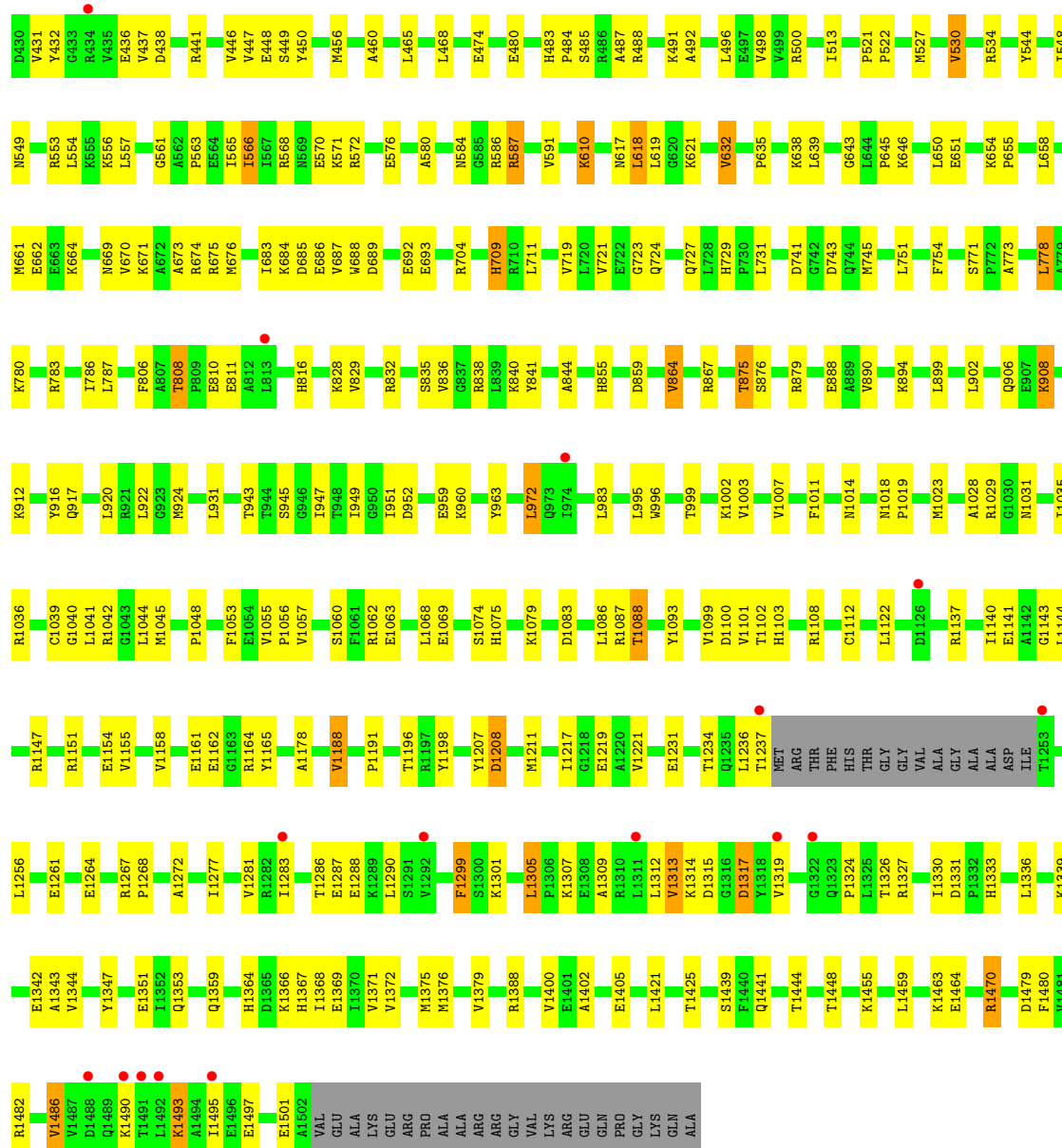
• Molecule 2: DNA-directed RNA polymerase subunit beta



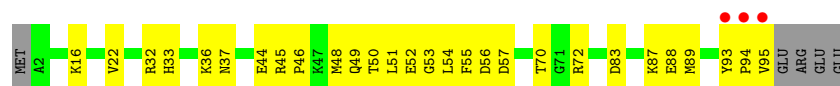


• Molecule 3: DNA-directed RNA polymerase subunit beta'



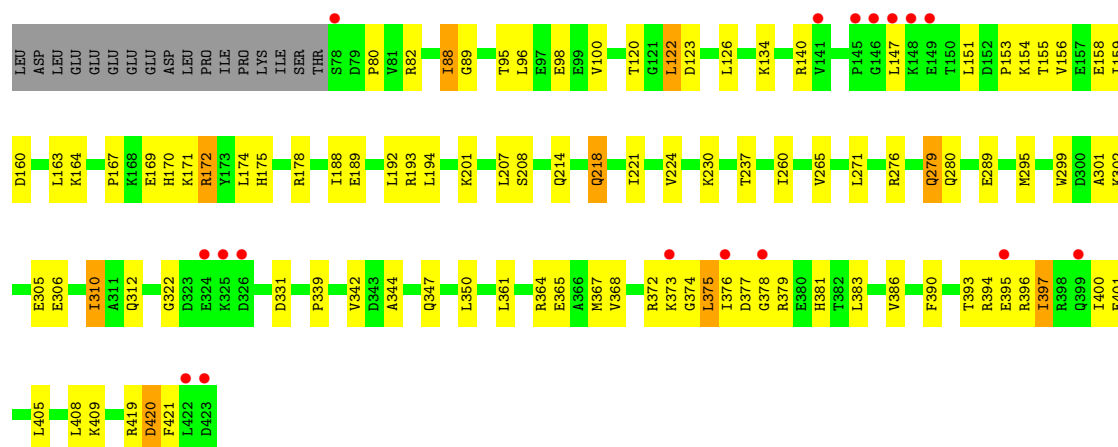


• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA

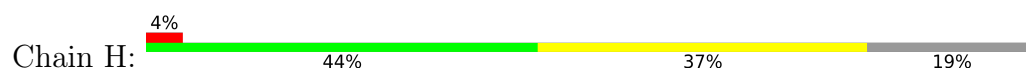




- Molecule 6: DNA (5'-D(P*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*AP*AP*A P*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*CP*TP*CP*TP *GP*AP*TP*GP*CP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.22Å 101.31Å 294.28Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	46.30 – 2.99 46.30 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.30-2.99) 98.7 (46.30-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.201 , 0.248 0.202 , 0.243	Depositor DCC
R_{free} test set	1992 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28403	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1819	0.64	0/2473
1	B	0.29	0/1790	0.72	0/2435
2	C	0.27	0/8883	0.64	4/12022 (0.0%)
3	D	0.32	2/11857 (0.0%)	0.66	3/16040 (0.0%)
4	E	0.27	0/775	0.61	0/1045
5	F	0.26	0/2838	0.62	1/3820 (0.0%)
6	G	0.45	0/391	0.82	0/600
7	H	0.39	0/505	0.78	0/776
All	All	0.30	2/28858 (0.0%)	0.66	8/39211 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	521	PRO	CA-C	-8.03	1.47	1.51
3	D	566	ILE	CA-CB	-5.29	1.48	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	274	ARG	N-CA-C	-6.91	102.12	108.75
2	C	765	SER	CA-C-N	6.88	138.60	121.80
2	C	765	SER	C-N-CA	6.88	138.60	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	521	PRO	O-C-N	-6.22	118.45	121.31
3	D	274	ARG	CB-CA-C	-6.09	107.58	116.53
5	F	419	ARG	CB-CG-CD	5.59	124.17	111.30
2	C	761	PHE	CA-C-N	5.12	127.98	120.71
2	C	761	PHE	C-N-CA	5.12	127.98	120.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	422	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1839	53	0
1	B	1758	0	1808	82	0
2	C	8717	0	8787	290	0
3	D	11652	0	11828	376	2
4	E	761	0	778	34	0
5	F	2793	0	2863	92	1
6	G	348	0	190	14	0
7	H	451	0	251	17	0
8	C	70	62	0	6	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
All	All	28341	62	28344	852	2

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 15.

All (852) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.14	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.29	1.10
3:D:1048:PRO:O	3:D:1079:LYS:NZ	1.87	1.06
3:D:669:ASN:ND2	5:F:420:ASP:OD1	1.88	1.05
6:G:6:DA:H8	6:G:6:DA:H5'	1.19	1.03
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.25	0.99
3:D:361:VAL:HG23	3:D:365:ASP:HB2	1.43	0.98
2:C:97:ARG:NH1	2:C:110:GLU:OE1	1.97	0.97
6:G:6:DA:H5'	6:G:6:DA:C8	2.00	0.97
1:B:100:LEU:HD23	1:B:141:GLU:HG2	1.45	0.97
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.48	0.96
3:D:187:LYS:N	3:D:200:ASP:OD1	1.98	0.94
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.49	0.94
2:C:420:ARG:NH1	2:C:448:ASN:OD1	2.00	0.94
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.49	0.92
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.51	0.92
2:C:615:TYR:HH	2:C:623:TYR:HH	1.09	0.91
2:C:628:PHE:H	2:C:638:ASP:HB2	1.36	0.91
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.54	0.90
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.53	0.89
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.55	0.88
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.54	0.87
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.10	0.87
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.55	0.87
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.55	0.86
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.56	0.86
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.57	0.86
2:C:420:ARG:HG3	2:C:420:ARG:HH11	1.40	0.86
1:B:188:GLN:HG3	3:D:685:ASP:OD2	1.75	0.85
3:D:274:ARG:O	3:D:276:ASP:N	2.10	0.85
3:D:1305:LEU:HD12	3:D:1309:ALA:HB3	1.59	0.85
3:D:133:ILE:HD12	3:D:152:LEU:HD23	1.59	0.84
3:D:1151:ARG:HH21	3:D:1151:ARG:HG2	1.43	0.83
2:C:294:GLU:HB3	2:C:299:LYS:HD2	1.60	0.82
3:D:65:ARG:CB	5:F:377:ASP:HA	2.10	0.81
2:C:408:ARG:NH1	2:C:456:ALA:O	2.13	0.81
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.14	0.80
1:B:100:LEU:CD2	1:B:141:GLU:HG2	2.12	0.80
3:D:485:SER:OG	6:G:3:DT:OP1	1.98	0.80
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.14	0.80
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.17	0.79
1:B:112:ARG:HG3	1:B:125:PRO:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:15:DC:H2'	6:G:16:DA:C8	2.17	0.79
2:C:211:LEU:HD23	2:C:311:PHE:CD2	2.18	0.79
2:C:614:ARG:NH2	2:C:618:GLY:O	2.17	0.78
3:D:658:LEU:HD23	3:D:661:MET:CE	2.13	0.78
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.65	0.78
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.66	0.78
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.67	0.78
2:C:978:ARG:HG3	2:C:978:ARG:HH11	1.49	0.77
5:F:147:LEU:HD23	5:F:151:LEU:HD13	1.66	0.77
2:C:182:VAL:HG11	2:C:221:LEU:HD13	1.64	0.77
4:E:37:ASN:ND2	4:E:89:MET:HE1	2.00	0.76
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.67	0.76
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.65	0.76
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.16	0.76
3:D:1288:GLU:O	3:D:1288:GLU:HG2	1.87	0.75
2:C:853:LEU:HB2	2:C:858:MET:CE	2.17	0.75
4:E:50:THR:HG22	4:E:53:GLY:O	1.86	0.75
1:A:104:GLU:OE2	1:A:137:ARG:NH1	2.20	0.74
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.70	0.74
2:C:361:MET:HE1	5:F:201:LYS:HZ1	1.54	0.73
1:B:112:ARG:CG	1:B:125:PRO:HB2	2.18	0.73
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.04	0.73
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.18	0.73
2:C:678:PRO:CA	2:C:683:ASN:HD21	1.98	0.73
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.22	0.73
1:A:29:GLU:OE1	1:A:29:GLU:HA	1.90	0.72
1:A:206:THR:OG1	1:A:209:GLU:HG3	1.89	0.72
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.69	0.72
3:D:147:VAL:HG21	3:D:161:LEU:HD21	1.71	0.72
2:C:55:GLU:O	2:C:359:MET:HE1	1.89	0.72
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.24	0.72
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.71	0.72
3:D:322:VAL:HG22	3:D:335:LEU:HD21	1.71	0.72
5:F:393:THR:HG22	5:F:395:GLU:H	1.55	0.72
3:D:205:TYR:CD2	3:D:390:PRO:HG3	2.25	0.71
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.72	0.71
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.73	0.70
3:D:1042:ARG:HG2	3:D:1045:MET:HE2	1.73	0.70
3:D:1314:LYS:H	3:D:1314:LYS:HD2	1.56	0.70
3:D:155:ASP:OD2	3:D:568:ARG:NH2	2.23	0.70
3:D:401:TYR:HB3	3:D:427:VAL:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:480:GLU:HG2	3:D:492:ALA:HB2	1.73	0.70
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.27	0.70
1:B:56:VAL:CG2	1:B:142:VAL:HG12	2.22	0.70
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.26	0.70
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.74	0.69
2:C:678:PRO:HA	2:C:683:ASN:ND2	1.99	0.69
2:C:475:VAL:O	2:C:478:VAL:HG22	1.93	0.69
3:D:658:LEU:HA	3:D:661:MET:HE3	1.74	0.69
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.25	0.69
3:D:361:VAL:CG2	3:D:365:ASP:HB2	2.23	0.68
3:D:134:VAL:HG22	3:D:151:GLN:H	1.59	0.68
3:D:322:VAL:HG22	3:D:335:LEU:CD2	2.24	0.68
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.21	0.68
3:D:258:VAL:HG12	3:D:273:ARG:O	1.94	0.68
2:C:428:ARG:NH2	2:C:447:ALA:O	2.26	0.68
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.73	0.68
2:C:352:ALA:HB1	2:C:356:ARG:HH22	1.59	0.68
2:C:1002:GLU:HA	3:D:724:GLN:OE1	1.94	0.68
3:D:156:GLU:OE1	3:D:156:GLU:N	2.24	0.67
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.24	0.67
5:F:82:ARG:HB2	7:H:8:DG:O6	1.95	0.67
1:B:80:LEU:HD13	3:D:867:ARG:HD3	1.77	0.67
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.77	0.67
2:C:361:MET:HE1	5:F:201:LYS:NZ	2.10	0.67
3:D:399:ARG:HG2	3:D:431:VAL:HG22	1.76	0.67
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.75	0.67
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.76	0.67
3:D:133:ILE:HD12	3:D:152:LEU:CD2	2.25	0.67
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.77	0.66
3:D:361:VAL:HG23	3:D:365:ASP:CB	2.23	0.66
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.77	0.66
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.77	0.66
1:A:27:PRO:HG3	1:A:186:LEU:HD13	1.77	0.66
2:C:243:ARG:NH2	7:H:10:DA:N1	2.43	0.66
2:C:948:GLU:HG3	2:C:953:VAL:HG23	1.78	0.66
2:C:278:GLU:OE1	2:C:284:ARG:NH2	2.29	0.66
3:D:806:PHE:O	3:D:829:VAL:HA	1.96	0.65
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.78	0.65
1:B:47:SER:C	1:B:148:VAL:HG21	2.22	0.65
2:C:537:LYS:HG2	2:C:905:ILE:HD11	1.79	0.65
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.78	0.65
3:D:399:ARG:HB2	3:D:401:TYR:CE1	2.32	0.65
4:E:70:THR:OG1	4:E:72:ARG:HG3	1.98	0.64
2:C:168:ARG:NH1	2:C:345:ARG:HD3	2.13	0.64
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.30	0.64
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.32	0.64
3:D:1151:ARG:HG2	3:D:1151:ARG:NH2	2.05	0.64
3:D:191:LEU:CD1	3:D:197:SER:HB2	2.28	0.64
5:F:339:PRO:HB2	5:F:344:ALA:HB2	1.78	0.64
3:D:206:ARG:HB2	3:D:392:SER:O	1.98	0.64
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.31	0.64
3:D:361:VAL:HG21	3:D:379:ALA:CB	2.27	0.64
3:D:1333:HIS:HE1	3:D:1421:LEU:O	1.81	0.63
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.13	0.63
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.80	0.63
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.31	0.63
2:C:221:LEU:HD21	2:C:307:LEU:HD21	1.80	0.63
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.81	0.63
5:F:361:LEU:HB3	5:F:365:GLU:CG	2.28	0.63
3:D:288:MET:HA	3:D:306:GLU:O	1.98	0.63
2:C:390:GLN:HA	8:C:2001:KNG:C49	2.29	0.62
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.17	0.62
3:D:191:LEU:HD13	3:D:197:SER:HB2	1.82	0.62
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.34	0.62
2:C:420:ARG:NH1	2:C:420:ARG:HG3	2.14	0.62
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.81	0.62
3:D:262:LYS:HE2	3:D:341:GLU:OE2	2.00	0.62
3:D:835:SER:OG	3:D:838:ARG:HG3	1.98	0.62
2:C:501:THR:CG2	2:C:513:VAL:HG23	2.28	0.62
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.15	0.62
3:D:266:GLU:OE2	3:D:315:ARG:N	2.33	0.62
3:D:411:THR:HG23	3:D:436:GLU:HA	1.81	0.62
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.80	0.61
4:E:50:THR:CG2	4:E:53:GLY:H	2.13	0.61
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.82	0.61
3:D:397:LYS:HD3	3:D:448:GLU:OE2	1.99	0.61
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.81	0.61
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.81	0.61
4:E:49:GLN:OE1	4:E:54:LEU:HD12	1.99	0.61
2:C:312:ALA:HB1	2:C:320:HIS:CE1	2.35	0.61
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.35	0.61
1:A:112:ARG:HG3	1:A:125:PRO:CB	2.31	0.61
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.01	0.61
3:D:134:VAL:HG23	3:D:149:LYS:HA	1.82	0.61
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.83	0.61
4:E:36:LYS:CG	4:E:93:TYR:HB3	2.29	0.61
1:B:101:LEU:HD11	1:B:113:ASP:CB	2.31	0.61
2:C:243:ARG:HH22	7:H:10:DA:N6	1.99	0.60
3:D:1267:ARG:NE	3:D:1331:ASP:OD2	2.34	0.60
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.83	0.60
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.82	0.60
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.82	0.60
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.84	0.60
1:A:6:LEU:CD1	1:A:7:LYS:H	2.14	0.60
2:C:1019:GLN:NE2	3:D:617:ASN:HB3	2.16	0.60
1:A:226:SER:O	1:A:228:PRO:HD3	2.01	0.60
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.83	0.60
1:B:128:HIS:HD2	1:B:129:ILE:N	2.00	0.60
2:C:12:VAL:HG21	2:C:472:ARG:CD	2.28	0.60
2:C:758:ARG:HH21	2:C:788:THR:HB	1.65	0.60
4:E:44:GLU:OE1	4:E:72:ARG:NH2	2.34	0.60
3:D:399:ARG:HG2	3:D:431:VAL:CG2	2.32	0.60
3:D:277:GLU:OE1	3:D:277:GLU:HA	2.02	0.59
5:F:386:VAL:HG12	5:F:397:ILE:HG12	1.84	0.59
4:E:50:THR:HG23	4:E:52:GLU:N	2.18	0.59
2:C:182:VAL:HG11	2:C:221:LEU:CD1	2.33	0.59
4:E:33:HIS:HD2	4:E:89:MET:HE2	1.67	0.59
5:F:405:LEU:O	5:F:409:LYS:HG3	2.03	0.59
1:B:58:ILE:CD1	1:B:140:MET:HE2	2.32	0.59
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.84	0.59
2:C:591:SER:O	2:C:592:LEU:HB2	2.03	0.59
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.84	0.59
3:D:1277:ILE:HD13	3:D:1301:LYS:HE3	1.84	0.59
1:B:6:LEU:HD12	1:B:189:ARG:HH11	1.68	0.59
1:B:18:ARG:O	1:B:207:PRO:HD3	2.02	0.59
1:B:104:GLU:HA	1:B:132:LEU:HD23	1.82	0.59
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.85	0.59
2:C:858:MET:HG2	2:C:867:VAL:O	2.01	0.59
3:D:165:LYS:HG2	3:D:165:LYS:O	2.02	0.59
3:D:906:GLN:OE1	3:D:906:GLN:HA	2.03	0.59
3:D:1083:ASP:OD2	3:D:1087:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:231:VAL:O	3:D:236:TYR:OH	2.21	0.58
3:D:65:ARG:CB	5:F:376:ILE:O	2.51	0.58
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.36	0.58
1:B:6:LEU:HB2	1:B:189:ARG:NH1	2.18	0.58
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.85	0.58
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.02	0.58
2:C:259:GLY:HA3	2:C:266:ARG:HD3	1.84	0.58
2:C:521:PRO:HG2	3:D:1053:PHE:CZ	2.39	0.58
5:F:89:GLY:HA3	7:H:7:DG:C6	2.38	0.58
2:C:773:LEU:HB2	5:F:375:LEU:HD11	1.85	0.58
3:D:1281:VAL:HB	3:D:1317:ASP:H	1.68	0.58
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.85	0.58
3:D:258:VAL:HG13	3:D:273:ARG:HG3	1.85	0.58
2:C:54:ILE:HG23	2:C:356:ARG:HH21	1.68	0.58
3:D:808:THR:O	3:D:811:GLU:HB2	2.04	0.58
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.84	0.58
1:B:136:GLY:C	1:B:137:ARG:HG3	2.28	0.58
3:D:456:MET:HE1	3:D:568:ARG:NE	2.19	0.58
2:C:774:LEU:HD22	5:F:350:LEU:HD11	1.86	0.57
3:D:238:PRO:CD	3:D:318:ARG:HG3	2.32	0.57
2:C:617:ASP:OD1	2:C:617:ASP:N	2.35	0.57
3:D:676:MET:CE	3:D:684:LYS:HG2	2.34	0.57
8:C:2001:KNG:C33	8:C:2001:KNG:C34	2.82	0.57
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.85	0.57
3:D:288:MET:HE2	3:D:305:ALA:HB3	1.85	0.57
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.04	0.57
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.87	0.57
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.37	0.57
1:B:46:SER:O	1:B:148:VAL:HG22	2.04	0.57
2:C:605:LYS:HE2	2:C:610:ARG:NH2	2.19	0.57
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.38	0.57
3:D:1042:ARG:CG	3:D:1045:MET:HE2	2.35	0.57
5:F:368:VAL:HG22	5:F:397:ILE:HD11	1.86	0.57
1:A:110:LYS:HD3	1:A:128:HIS:HA	1.87	0.57
2:C:259:GLY:HA3	2:C:266:ARG:HH11	1.70	0.57
3:D:401:TYR:HB3	3:D:427:VAL:CG2	2.34	0.57
1:B:58:ILE:HG12	1:B:140:MET:CB	2.34	0.57
2:C:200:LEU:HD13	2:C:300:ASP:CB	2.35	0.57
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.20	0.57
4:E:48:MET:N	4:E:55:PHE:O	2.33	0.57
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.87	0.56
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.86	0.56
3:D:684:LYS:O	3:D:687:VAL:HG12	2.04	0.56
4:E:33:HIS:CD2	4:E:89:MET:HB3	2.41	0.56
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.87	0.56
2:C:390:GLN:HE21	2:C:414:GLY:HA2	1.69	0.56
1:A:100:LEU:CD2	1:A:141:GLU:HG2	2.36	0.56
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.88	0.56
1:A:11:PHE:O	1:B:228:PRO:HA	2.06	0.56
5:F:420:ASP:OD2	5:F:420:ASP:N	2.37	0.56
4:E:50:THR:HG22	4:E:53:GLY:H	1.71	0.55
2:C:163:ILE:HG23	2:C:171:TRP:NE1	2.21	0.55
2:C:195:LEU:CD2	2:C:241:LEU:HD12	2.35	0.55
2:C:279:GLU:OE2	2:C:279:GLU:HA	2.06	0.55
3:D:181:ASP:HB2	3:D:205:TYR:HD1	1.65	0.55
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.05	0.55
3:D:238:PRO:HD3	3:D:318:ARG:CG	2.33	0.55
3:D:530:VAL:HG22	3:D:534:ARG:O	2.07	0.55
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.87	0.55
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.88	0.55
2:C:766:GLU:O	2:C:768:THR:N	2.40	0.55
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.87	0.55
2:C:452:ILE:HG21	8:C:2001:KNG:O10	2.06	0.55
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.06	0.55
3:D:689:ASP:OD2	4:E:51:LEU:HD11	2.07	0.55
5:F:156:VAL:O	5:F:160:ASP:HB2	2.06	0.55
1:B:188:GLN:CG	3:D:685:ASP:OD2	2.51	0.55
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.87	0.55
3:D:816:HIS:CG	3:D:836:VAL:HG11	2.42	0.55
2:C:905:ILE:HD12	2:C:905:ILE:O	2.07	0.55
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.89	0.55
2:C:521:PRO:HG2	3:D:1053:PHE:HZ	1.72	0.55
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.43	0.54
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.88	0.54
4:E:32:ARG:O	4:E:95:VAL:HG13	2.07	0.54
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.90	0.54
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.43	0.54
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.33	0.54
2:C:954:THR:HG23	2:C:965:GLU:OE2	2.07	0.54
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.08	0.54
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:661:MET:CE	3:D:673:ALA:HB1	2.38	0.54
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.90	0.54
5:F:167:PRO:HG2	5:F:170:HIS:HB2	1.90	0.54
1:B:80:LEU:HB3	3:D:867:ARG:NH1	2.23	0.54
2:C:261:ILE:HG22	2:C:262:ALA:N	2.23	0.54
3:D:319:ALA:HB1	3:D:335:LEU:HD22	1.90	0.54
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.07	0.54
2:C:243:ARG:HH22	7:H:10:DA:H61	1.55	0.54
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.43	0.54
3:D:175:VAL:CG1	3:D:193:PRO:HD2	2.38	0.54
5:F:374:GLY:C	5:F:376:ILE:H	2.15	0.54
1:B:47:SER:C	1:B:148:VAL:CG2	2.81	0.53
2:C:359:MET:HG2	2:C:372:LEU:HD21	1.90	0.53
2:C:440:PRO:HB2	3:D:1074:SER:OG	2.08	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.53
3:D:876:SER:OG	3:D:879:ARG:HG3	2.08	0.53
5:F:306:GLU:O	5:F:310:ILE:HG13	2.07	0.53
1:B:101:LEU:CD1	1:B:113:ASP:HB2	2.38	0.53
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.90	0.53
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.91	0.53
5:F:386:VAL:CG1	5:F:397:ILE:HG12	2.39	0.53
2:C:390:GLN:NE2	2:C:414:GLY:HA2	2.24	0.53
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.73	0.53
2:C:111:ASP:OD2	2:C:112:GLU:N	2.42	0.53
2:C:943:VAL:HG11	2:C:973:VAL:HG22	1.89	0.53
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.73	0.53
3:D:1283:ILE:HG12	3:D:1315:ASP:CG	2.32	0.53
4:E:36:LYS:HG3	4:E:93:TYR:HB3	1.90	0.53
2:C:259:GLY:CA	2:C:266:ARG:HD3	2.39	0.53
3:D:34:TYR:HD1	5:F:310:ILE:HG22	1.72	0.53
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.09	0.53
1:A:6:LEU:HD13	1:A:7:LYS:H	1.74	0.53
1:B:47:SER:HA	1:B:148:VAL:HG21	1.91	0.53
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.39	0.53
3:D:231:VAL:HG13	3:D:242:LEU:O	2.09	0.53
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.43	0.53
3:D:487:ALA:O	3:D:491:LYS:HG2	2.09	0.53
2:C:598:GLU:O	2:C:651:LYS:HG3	2.09	0.52
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.44	0.52
3:D:711:LEU:HD13	3:D:778:LEU:CD2	2.39	0.52
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:154:LYS:O	5:F:158:GLU:HG3	2.08	0.52
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.90	0.52
3:D:999:THR:O	3:D:1003:VAL:HG13	2.09	0.52
2:C:766:GLU:CB	2:C:767:PRO:CD	2.87	0.52
3:D:654:LYS:HD3	3:D:674:ARG:HH12	1.75	0.52
3:D:844:ALA:O	3:D:867:ARG:HB3	2.09	0.52
1:A:138:LEU:HD11	1:A:140:MET:HE3	1.91	0.52
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.45	0.52
1:B:58:ILE:HG12	1:B:140:MET:HB2	1.92	0.52
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.91	0.52
2:C:784:ASP:OD2	2:C:784:ASP:N	2.37	0.52
2:C:243:ARG:HH12	7:H:10:DA:H61	1.57	0.52
3:D:288:MET:HG2	3:D:307:ALA:HB2	1.90	0.52
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.44	0.52
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.37	0.52
5:F:169:GLU:O	5:F:172:ARG:HG2	2.10	0.52
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.75	0.52
3:D:485:SER:HB3	3:D:488:ARG:HB2	1.91	0.52
5:F:377:ASP:OD2	5:F:381:HIS:HE1	1.93	0.52
2:C:211:LEU:HD23	2:C:311:PHE:HD2	1.74	0.52
5:F:368:VAL:HG21	5:F:400:ILE:CD1	2.40	0.52
6:G:3:DT:H2"	6:G:4:DG:C8	2.45	0.52
3:D:134:VAL:CG2	3:D:151:GLN:H	2.21	0.52
3:D:645:PRO:HB3	3:D:723:GLY:O	2.10	0.52
3:D:1493:LYS:NZ	3:D:1493:LYS:HA	2.25	0.52
3:D:103:TRP:HB3	3:D:1448:THR:CG2	2.40	0.51
3:D:398:ALA:HA	3:D:446:VAL:O	2.10	0.51
3:D:1313:VAL:HG11	3:D:1319:VAL:HG11	1.91	0.51
2:C:172:ILE:HG13	2:C:186:VAL:HG22	1.92	0.51
2:C:405:ARG:HD2	2:C:566:THR:OG1	2.11	0.51
3:D:227:LEU:HD13	3:D:331:VAL:HG22	1.92	0.51
6:G:4:DG:H2"	6:G:5:DC:OP2	2.10	0.51
1:A:229:GLN:HB3	1:B:11:PHE:O	2.10	0.51
2:C:757:GLY:HA2	2:C:789:SER:OG	2.09	0.51
2:C:769:PRO:HB3	5:F:374:GLY:C	2.35	0.51
3:D:140:ALA:HA	3:D:450:TYR:CE2	2.46	0.51
3:D:215:TYR:O	3:D:340:THR:HA	2.11	0.51
3:D:396:VAL:HG12	3:D:397:LYS:N	2.26	0.51
3:D:474:GLU:OE2	3:D:1388:ARG:NH1	2.43	0.51
3:D:945:SER:OG	3:D:947:ILE:HG12	2.10	0.51
2:C:1058:ASP:OD2	3:D:621:LYS:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:556:LYS:HD3	5:F:218:GLN:OE1	2.10	0.51
1:B:128:HIS:CD2	1:B:129:ILE:N	2.78	0.51
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.93	0.51
2:C:501:THR:HG21	2:C:513:VAL:CG2	2.32	0.51
3:D:211:VAL:HG22	3:D:387:LEU:HD12	1.92	0.51
1:A:128:HIS:HD2	1:A:129:ILE:N	2.09	0.51
2:C:136:ILE:CB	2:C:336:VAL:HG13	2.38	0.51
3:D:288:MET:HE2	3:D:305:ALA:CB	2.40	0.51
3:D:1313:VAL:HG11	3:D:1319:VAL:CG1	2.40	0.51
5:F:364:ARG:HH22	5:F:396:ARG:NH2	2.09	0.51
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.45	0.51
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.91	0.51
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.54	0.51
1:B:104:GLU:OE1	1:B:137:ARG:NH1	2.44	0.51
3:D:275:GLU:O	3:D:276:ASP:HB3	2.11	0.51
1:B:94:LEU:HD12	1:B:96:THR:H	1.76	0.51
8:C:2001:KNG:C38	8:C:2001:KNG:O13	2.59	0.51
2:C:978:ARG:HG3	2:C:978:ARG:NH1	2.21	0.50
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.26	0.50
3:D:654:LYS:HD3	3:D:674:ARG:NH1	2.26	0.50
2:C:684:PHE:HE1	3:D:783:ARG:HB2	1.76	0.50
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.93	0.50
4:E:50:THR:HG23	4:E:52:GLU:H	1.77	0.50
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.46	0.50
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.94	0.50
2:C:926:PHE:HE1	2:C:929:ARG:HH21	1.60	0.50
4:E:54:LEU:O	4:E:55:PHE:HD1	1.93	0.50
2:C:312:ALA:CB	2:C:320:HIS:CE1	2.95	0.50
3:D:175:VAL:HG13	3:D:193:PRO:HG2	1.94	0.50
3:D:262:LYS:CE	3:D:341:GLU:OE2	2.59	0.50
3:D:343:LYS:HD3	3:D:345:TYR:OH	2.11	0.50
3:D:407:VAL:HA	3:D:422:ALA:CB	2.41	0.50
3:D:432:TYR:O	3:D:448:GLU:HA	2.12	0.50
4:E:95:VAL:HG12	4:E:95:VAL:O	2.11	0.50
1:A:133:GLU:HG2	1:A:134:GLU:N	2.27	0.50
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.93	0.50
2:C:221:LEU:CD2	2:C:307:LEU:HD21	2.41	0.50
1:A:185:ARG:HH21	1:A:188:GLN:HA	1.75	0.50
1:B:58:ILE:HG12	1:B:140:MET:HB3	1.93	0.50
2:C:352:ALA:HB1	2:C:356:ARG:NH2	2.25	0.50
3:D:134:VAL:HG21	3:D:148:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.42	0.50
5:F:372:ARG:NH2	5:F:381:HIS:O	2.45	0.50
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.75	0.50
1:B:90:LEU:N	1:B:90:LEU:HD22	2.27	0.49
1:B:57:TYR:O	1:B:140:MET:HA	2.12	0.49
3:D:1036:ARG:O	3:D:1040:GLY:N	2.45	0.49
3:D:1211:MET:SD	4:E:16:LYS:HE3	2.52	0.49
5:F:134:LYS:HG3	5:F:178:ARG:NH2	2.27	0.49
1:B:44:LEU:HD13	1:B:199:ILE:HD13	1.94	0.49
2:C:211:LEU:HD21	2:C:307:LEU:HG	1.93	0.49
3:D:236:TYR:CD2	3:D:322:VAL:HG21	2.48	0.49
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.42	0.49
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.93	0.49
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.28	0.49
3:D:1312:LEU:HD21	3:D:1327:ARG:HG2	1.95	0.49
1:A:228:PRO:HA	1:B:11:PHE:CD2	2.47	0.49
2:C:774:LEU:HD11	2:C:778:PHE:HE2	1.77	0.49
5:F:383:LEU:HD12	5:F:394:ARG:NH2	2.28	0.49
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.48	0.49
2:C:44:ILE:HD11	2:C:71:TYR:CZ	2.48	0.49
3:D:65:ARG:CB	5:F:377:ASP:CA	2.87	0.49
3:D:134:VAL:HG22	3:D:151:GLN:N	2.26	0.49
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.93	0.49
3:D:1479:ASP:OD1	3:D:1482:ARG:NE	2.38	0.49
5:F:155:THR:O	5:F:159:ILE:HG12	2.12	0.49
2:C:1019:GLN:HE22	3:D:617:ASN:CA	2.26	0.49
2:C:1051:GLU:HB3	2:C:1056:LYS:HE3	1.95	0.49
3:D:828:LYS:HA	3:D:832:ARG:O	2.12	0.49
7:H:21:DA:H5'	7:H:21:DA:C8	2.48	0.49
2:C:177:GLU:HB3	2:C:179:ASN:ND2	2.27	0.48
2:C:513:VAL:HG12	2:C:524:VAL:O	2.13	0.48
3:D:66:GLN:C	3:D:68:PHE:H	2.20	0.48
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.95	0.48
1:B:212:ASN:O	1:B:215:VAL:HG22	2.13	0.48
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.54	0.48
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.95	0.48
1:B:185:ARG:NH1	3:D:692:GLU:OE2	2.46	0.48
2:C:716:LYS:HD2	3:D:37:LEU:HD12	1.95	0.48
1:A:220:GLU:O	1:A:223:THR:HB	2.14	0.48
2:C:351:LEU:HD12	2:C:375:SER:HA	1.95	0.48
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.12	0.48
3:D:1288:GLU:O	3:D:1307:LYS:HE3	2.12	0.48
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.13	0.48
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.96	0.48
2:C:302:VAL:O	2:C:305:PRO:HD2	2.13	0.48
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.79	0.48
3:D:155:ASP:OD1	3:D:159:ARG:NH2	2.46	0.48
5:F:376:ILE:HG22	5:F:377:ASP:N	2.28	0.48
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.96	0.48
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.95	0.48
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.95	0.48
5:F:120:THR:HG21	5:F:122:LEU:HD22	1.95	0.48
5:F:368:VAL:HG21	5:F:400:ILE:HD11	1.95	0.48
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.96	0.48
1:B:101:LEU:HB2	1:B:114:PHE:CD1	2.49	0.48
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.96	0.48
2:C:769:PRO:CB	5:F:375:LEU:HA	2.43	0.48
3:D:103:TRP:HB3	3:D:1448:THR:HG21	1.96	0.48
3:D:298:VAL:HA	3:D:302:GLN:OE1	2.14	0.48
3:D:959:GLU:N	3:D:959:GLU:OE1	2.44	0.48
3:D:1493:LYS:HA	3:D:1493:LYS:HZ2	1.78	0.48
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.94	0.48
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.47	0.48
2:C:290:LEU:O	2:C:301:GLU:HB2	2.14	0.48
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.49	0.48
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.96	0.48
5:F:377:ASP:OD2	5:F:379:ARG:HG2	2.13	0.48
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.96	0.48
2:C:419:THR:HG22	2:C:420:ARG:H	1.78	0.48
2:C:910:LYS:HD3	2:C:910:LYS:HA	1.54	0.48
2:C:359:MET:CG	2:C:372:LEU:HD21	2.43	0.47
3:D:1011:PHE:CE1	3:D:1018:ASN:ND2	2.82	0.47
3:D:1217:ILE:HD12	3:D:1480:PHE:CE2	2.48	0.47
3:D:1495:ILE:CG1	4:E:88:GLU:HG3	2.42	0.47
1:B:110:LYS:C	1:B:129:ILE:HD13	2.39	0.47
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.96	0.47
2:C:769:PRO:HG3	5:F:378:GLY:HA2	1.96	0.47
2:C:76:PRO:HG3	2:C:120:LEU:CD1	2.45	0.47
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.95	0.47
2:C:464:LEU:HD12	2:C:464:LEU:HA	1.68	0.47
3:D:480:GLU:CG	3:D:492:ALA:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.97	0.47
5:F:123:ASP:HB3	5:F:126:LEU:HB3	1.96	0.47
5:F:289:GLU:HG3	5:F:301:ALA:HB2	1.96	0.47
5:F:401:GLU:HG2	5:F:405:LEU:HD13	1.94	0.47
2:C:422:ARG:HD2	7:H:16:DC:C5	2.48	0.47
3:D:319:ALA:HB1	3:D:335:LEU:CD2	2.44	0.47
2:C:144:PRO:HG2	2:C:165:LEU:HD23	1.96	0.47
2:C:202:TYR:HD2	2:C:207:LEU:HD21	1.78	0.47
1:B:94:LEU:HD11	1:B:96:THR:O	2.14	0.47
1:B:188:GLN:HE22	3:D:688:TRP:CD1	2.32	0.47
3:D:262:LYS:NZ	3:D:341:GLU:OE2	2.47	0.47
1:A:139:ASN:C	1:A:139:ASN:OD1	2.57	0.47
1:B:58:ILE:HD13	1:B:140:MET:HE2	1.96	0.47
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.50	0.47
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.96	0.47
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.45	0.47
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.96	0.47
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.29	0.47
2:C:595:LEU:HD11	2:C:623:TYR:HB3	1.97	0.47
3:D:50:PHE:CG	3:D:522:PRO:HD3	2.50	0.47
3:D:586:ARG:NH1	6:G:10:DG:OP1	2.44	0.47
3:D:1087:ARG:HD2	3:D:1236:LEU:O	2.15	0.47
3:D:1261:GLU:OE1	3:D:1268:PRO:HA	2.14	0.47
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.45	0.47
2:C:89:THR:O	2:C:91:GLN:HG2	2.15	0.47
3:D:806:PHE:HD1	3:D:811:GLU:HB3	1.79	0.47
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.97	0.47
3:D:1459:LEU:HD23	3:D:1464:GLU:HB3	1.96	0.47
2:C:1067:TYR:CZ	5:F:342:VAL:HG22	2.49	0.47
3:D:191:LEU:HD11	3:D:197:SER:HB2	1.97	0.47
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.47	0.47
3:D:483:HIS:ND1	3:D:488:ARG:HD3	2.29	0.47
3:D:816:HIS:CB	3:D:836:VAL:HG11	2.45	0.47
1:A:180:GLN:NE2	2:C:935:GLY:O	2.48	0.46
2:C:158:TYR:CE2	2:C:313:LEU:HG	2.50	0.46
3:D:5:VAL:O	3:D:1470:ARG:NH2	2.46	0.46
3:D:224:ARG:HA	3:D:331:VAL:O	2.16	0.46
3:D:316:GLN:OE1	3:D:340:THR:OG1	2.30	0.46
3:D:662:GLU:HG3	3:D:669:ASN:HA	1.96	0.46
3:D:1277:ILE:HD13	3:D:1299:PHE:CE1	2.50	0.46
2:C:922:PHE:CD2	2:C:964:LYS:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:CE2	3:D:35:ARG:HG3	2.49	0.46
2:C:170:PRO:HD2	2:C:267:TYR:CE1	2.50	0.46
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.51	0.46
3:D:576:GLU:OE2	5:F:80:PRO:HG3	2.15	0.46
7:H:22:DT:H2''	7:H:23:DG:C8	2.50	0.46
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.97	0.46
2:C:716:LYS:HE3	3:D:35:ARG:O	2.16	0.46
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.98	0.46
3:D:266:GLU:OE2	3:D:315:ARG:HG3	2.15	0.46
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.68	0.46
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.45	0.46
2:C:421:GLU:OE2	2:C:421:GLU:N	2.41	0.46
2:C:473:ARG:HG3	2:C:474:VAL:N	2.31	0.46
3:D:316:GLN:O	3:D:316:GLN:HG3	2.14	0.46
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.98	0.46
2:C:260:LEU:O	2:C:261:ILE:HD12	2.15	0.46
3:D:311:LEU:HD12	3:D:311:LEU:O	2.15	0.46
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.98	0.46
7:H:23:DG:O5'	7:H:23:DG:H2'	2.14	0.46
1:B:197:LEU:HD22	1:B:199:ILE:HD11	1.97	0.46
2:C:205:GLU:O	2:C:209:ARG:HG2	2.16	0.46
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.74	0.46
2:C:607:ASP:HB3	2:C:610:ARG:H	1.81	0.46
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.16	0.46
2:C:127:PHE:O	2:C:133:ASP:HA	2.16	0.46
2:C:682:TYR:CE1	3:D:635:PRO:HD2	2.50	0.46
2:C:838:LYS:HE3	3:D:741:ASP:O	2.16	0.46
3:D:731:LEU:CD1	3:D:931:LEU:HB3	2.45	0.46
2:C:53:PRO:HB3	2:C:67:ASP:OD1	2.15	0.46
2:C:185:LYS:HA	2:C:189:ARG:O	2.15	0.46
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.98	0.46
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.98	0.45
2:C:211:LEU:HD23	2:C:311:PHE:CE2	2.52	0.45
2:C:513:VAL:HG13	2:C:524:VAL:HG23	1.99	0.45
3:D:1161:GLU:CD	3:D:1164:ARG:HB2	2.41	0.45
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.97	0.45
3:D:90:MET:HE3	3:D:90:MET:HB3	1.85	0.45
3:D:1490:LYS:HD3	4:E:93:TYR:OH	2.17	0.45
5:F:147:LEU:CD2	5:F:151:LEU:HD22	2.46	0.45
1:B:138:LEU:HD21	1:B:140:MET:HE3	1.98	0.45
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:HD1	5:F:310:ILE:CG2	2.30	0.45
3:D:1283:ILE:HD13	3:D:1315:ASP:HB2	1.98	0.45
6:G:3:DT:H6	6:G:3:DT:O5'	1.98	0.45
1:A:104:GLU:HA	1:A:136:GLY:O	2.16	0.45
1:A:198:ARG:HD3	2:C:934:PHE:CE1	2.51	0.45
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.44	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
3:D:93:ILE:HD13	3:D:548:ILE:HG12	1.99	0.45
3:D:664:LYS:CE	3:D:693:GLU:OE1	2.65	0.45
3:D:875:THR:HG23	3:D:876:SER:N	2.31	0.45
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.52	0.45
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.99	0.45
3:D:236:TYR:HD2	3:D:322:VAL:HG21	1.82	0.45
3:D:417:PRO:HA	3:D:429:SER:O	2.17	0.45
3:D:419:ASP:O	3:D:421:LEU:HD13	2.17	0.45
3:D:1191:PRO:HD2	3:D:1369:GLU:OE1	2.17	0.45
2:C:150:PRO:HG3	2:C:322:VAL:HG11	1.99	0.45
2:C:776:SER:HB2	5:F:373:LYS:NZ	2.32	0.45
1:B:107:LYS:HE2	1:B:113:ASP:OD1	2.16	0.45
2:C:65:VAL:CG2	2:C:103:LYS:HE3	2.47	0.45
2:C:717:LEU:HD23	2:C:762:LYS:O	2.17	0.45
3:D:351:MET:HG2	3:D:370:ALA:CB	2.47	0.45
3:D:709:HIS:CD2	3:D:1231:GLU:HG3	2.52	0.45
2:C:405:ARG:CZ	2:C:409:ARG:NH1	2.79	0.45
3:D:405:ASP:CG	3:D:406:ASP:H	2.25	0.45
3:D:662:GLU:OE2	3:D:670:VAL:HG23	2.17	0.45
3:D:1353:GLN:HG2	3:D:1368:ILE:HD12	1.99	0.45
2:C:65:VAL:HG21	2:C:103:LYS:HE3	1.98	0.45
2:C:99:GLN:OE1	2:C:101:ILE:HD11	2.16	0.45
2:C:158:TYR:CD2	2:C:313:LEU:HG	2.51	0.45
2:C:774:LEU:HD21	5:F:421:PHE:HB2	1.99	0.45
3:D:396:VAL:CG1	3:D:447:VAL:HG13	2.47	0.45
5:F:279:GLN:HG3	5:F:280:GLN:N	2.31	0.45
3:D:684:LYS:HE2	3:D:684:LYS:HB3	1.61	0.44
3:D:741:ASP:OD1	3:D:743:ASP:OD1	2.35	0.44
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.42	0.44
1:A:101:LEU:HD11	1:A:109:VAL:CG1	2.47	0.44
1:A:168:ASP:OD2	2:C:832:LYS:NZ	2.36	0.44
2:C:595:LEU:HD22	2:C:655:LEU:HB2	1.99	0.44
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.99	0.44
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:771:SER:HA	3:D:778:LEU:HD22	1.97	0.44
3:D:29:PRO:HG3	3:D:549:ASN:OD1	2.17	0.44
3:D:45:PHE:O	3:D:86:ARG:NH2	2.50	0.44
1:B:220:GLU:O	1:B:223:THR:OG1	2.23	0.44
2:C:191:PHE:HB2	2:C:192:PRO:HD2	1.98	0.44
2:C:536:PRO:HB2	2:C:905:ILE:HD13	1.99	0.44
3:D:972:LEU:HD23	3:D:972:LEU:HA	1.60	0.44
1:B:24:VAL:HA	1:B:195:LEU:O	2.17	0.44
2:C:170:PRO:HD2	2:C:267:TYR:HE1	1.83	0.44
2:C:211:LEU:HD22	2:C:221:LEU:HD22	2.00	0.44
3:D:534:ARG:HD2	5:F:312:GLN:OE1	2.18	0.44
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.34	0.44
3:D:1376:MET:HE3	3:D:1376:MET:HB3	1.72	0.44
2:C:138:SER:HB3	2:C:333:ILE:CG2	2.48	0.44
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.83	0.44
2:C:807:ARG:HG3	2:C:821:GLU:HB3	1.98	0.44
3:D:204:LEU:HD22	3:D:441:ARG:NH1	2.33	0.44
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.18	0.44
4:E:54:LEU:O	4:E:55:PHE:CD1	2.69	0.44
5:F:377:ASP:OD2	5:F:381:HIS:CE1	2.71	0.44
1:B:6:LEU:HD23	1:B:7:LYS:HG3	2.00	0.44
3:D:129:PHE:CZ	3:D:571:LYS:HB3	2.53	0.44
3:D:166:GLN:HB2	3:D:396:VAL:HG22	1.98	0.44
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.99	0.44
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.99	0.44
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.25	0.44
2:C:374:ASN:OD1	2:C:376:ARG:HG2	2.18	0.44
2:C:944:LEU:HD22	2:C:962:GLN:HB3	2.00	0.44
3:D:671:LYS:HD3	5:F:420:ASP:O	2.18	0.44
3:D:1087:ARG:HG3	3:D:1256:LEU:CD2	2.47	0.44
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.83	0.44
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.43	0.44
2:C:1021:LEU:HD22	5:F:331:ASP:O	2.18	0.44
8:C:2001:KNG:C18	8:C:2001:KNG:O09	2.66	0.44
3:D:1053:PHE:CE1	3:D:1055:VAL:HG23	2.53	0.43
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.81	0.43
2:C:165:LEU:HD11	2:C:270:GLY:HA2	1.99	0.43
2:C:376:ARG:N	2:C:377:PRO:HD2	2.33	0.43
2:C:691:SER:HA	2:C:858:MET:CE	2.48	0.43
3:D:134:VAL:HG23	3:D:134:VAL:O	2.18	0.43
3:D:288:MET:CE	3:D:305:ALA:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:638:LYS:HA	3:D:638:LYS:HD3	1.82	0.43
3:D:1372:VAL:CA	3:D:1375:MET:HE3	2.39	0.43
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.73	0.43
1:A:185:ARG:HB2	1:A:189:ARG:O	2.18	0.43
1:B:99:LEU:HB2	1:B:142:VAL:CG2	2.48	0.43
2:C:97:ARG:HE	2:C:97:ARG:HB3	1.57	0.43
2:C:154:ARG:HH12	2:C:178:PRO:HB3	1.82	0.43
2:C:805:ARG:NH2	2:C:821:GLU:OE1	2.49	0.43
3:D:563:PRO:HB3	5:F:189:GLU:CG	2.48	0.43
3:D:565:ILE:HG21	5:F:88:ILE:CD1	2.47	0.43
4:E:87:LYS:HD3	4:E:87:LYS:HA	1.64	0.43
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.00	0.43
5:F:271:LEU:HD12	5:F:295:MET:SD	2.59	0.43
1:B:112:ARG:HG2	1:B:125:PRO:HB2	1.96	0.43
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.00	0.43
2:C:164:PRO:HD2	2:C:171:TRP:CD1	2.53	0.43
2:C:644:VAL:HG22	2:C:645:VAL:N	2.33	0.43
3:D:125:GLN:HB3	3:D:131:LYS:HB2	2.01	0.43
3:D:356:PRO:HG2	3:D:359:ALA:HB2	2.01	0.43
3:D:1018:ASN:OD1	3:D:1019:PRO:HD2	2.19	0.43
3:D:1068:LEU:HD12	3:D:1068:LEU:HA	1.85	0.43
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.33	0.43
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	2.00	0.43
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.27	0.43
2:C:214:TYR:CB	2:C:217:LEU:HD12	2.49	0.43
2:C:521:PRO:CG	3:D:1053:PHE:CZ	3.02	0.43
3:D:192:ALA:HB3	3:D:195:VAL:HB	2.00	0.43
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.85	0.43
3:D:632:VAL:O	3:D:727:GLN:HA	2.19	0.43
3:D:1305:LEU:HD23	3:D:1305:LEU:N	2.33	0.43
3:D:1314:LYS:HD2	3:D:1314:LYS:N	2.27	0.43
2:C:522:VAL:HG13	2:C:524:VAL:HG13	2.00	0.43
2:C:691:SER:HA	2:C:858:MET:HE3	2.01	0.43
3:D:230:TRP:CE3	3:D:331:VAL:HG21	2.54	0.43
3:D:1286:THR:HG22	3:D:1287:GLU:N	2.34	0.43
2:C:1009:SER:HB3	3:D:651:GLU:O	2.18	0.43
3:D:530:VAL:CG2	3:D:534:ARG:HB2	2.49	0.43
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.54	0.43
4:E:44:GLU:CD	4:E:72:ARG:HH22	2.26	0.43
5:F:193:ARG:HB3	7:H:7:DG:H5"	2.01	0.43
5:F:260:ILE:HG22	5:F:265:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LYS:CD	1:A:128:HIS:HA	2.48	0.43
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.01	0.43
2:C:243:ARG:NH1	7:H:9:DG:O6	2.51	0.43
2:C:679:PHE:HA	3:D:943:THR:HG23	2.01	0.43
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.54	0.43
6:G:18:DA:H2'	6:G:19:DA:C8	2.54	0.43
2:C:769:PRO:HB3	5:F:375:LEU:N	2.34	0.43
3:D:154:THR:OG1	3:D:157:GLU:HG3	2.19	0.43
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.54	0.43
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.79	0.43
6:G:8:DC:H2''	6:G:9:DA:C8	2.53	0.43
1:A:196:THR:HG21	2:C:934:PHE:CE2	2.54	0.42
2:C:139:GLN:HA	2:C:411:SER:O	2.19	0.42
2:C:327:HIS:CD2	2:C:433:THR:HG21	2.54	0.42
2:C:815:LEU:N	2:C:815:LEU:HD13	2.33	0.42
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.54	0.42
3:D:114:THR:HG21	3:D:498:VAL:HG21	2.01	0.42
3:D:787:LEU:HD21	3:D:947:ILE:HG21	2.00	0.42
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.18	0.42
1:B:102:LYS:HG2	1:B:139:ASN:CG	2.44	0.42
2:C:763:GLY:O	2:C:766:GLU:CB	2.67	0.42
3:D:205:TYR:CE2	3:D:390:PRO:HG3	2.53	0.42
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.01	0.42
3:D:610:LYS:HE2	3:D:610:LYS:HB2	1.91	0.42
3:D:780:LYS:HE3	3:D:912:LYS:HD3	2.02	0.42
4:E:83:ASP:OD1	4:E:83:ASP:N	2.52	0.42
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.01	0.42
5:F:237:THR:OG1	7:H:4:DA:H8	2.02	0.42
2:C:422:ARG:NH1	6:G:13:DC:O2	2.45	0.42
3:D:1028:ALA:O	3:D:1029:ARG:HG2	2.18	0.42
5:F:95:THR:HB	5:F:98:GLU:HG3	2.00	0.42
1:B:50:GLY:HA3	1:B:173:PRO:HD3	2.01	0.42
1:B:102:LYS:HE3	1:B:139:ASN:OD1	2.20	0.42
2:C:571:LEU:HD22	2:C:700:TYR:HA	2.00	0.42
2:C:841:ASN:ND2	2:C:845:ASN:HB3	2.34	0.42
3:D:277:GLU:OE1	3:D:277:GLU:CA	2.68	0.42
3:D:773:ALA:HA	3:D:1367:HIS:NE2	2.34	0.42
3:D:1088:THR:CG2	6:G:14:DC:C2	3.02	0.42
1:B:138:LEU:HD11	1:B:140:MET:CE	2.49	0.42
2:C:66:LEU:HD11	2:C:98:LEU:HB3	2.02	0.42
5:F:374:GLY:C	5:F:376:ILE:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLY:N	1:A:193:ASP:OD1	2.42	0.42
3:D:527:MET:HE2	3:D:527:MET:HB2	1.90	0.42
3:D:586:ARG:HH12	6:G:10:DG:H5"	1.84	0.42
2:C:15:LEU:HD23	2:C:458:TYR:CZ	2.54	0.42
2:C:44:ILE:HD11	2:C:71:TYR:CE1	2.55	0.42
2:C:245:GLY:O	2:C:246:ASP:C	2.63	0.42
2:C:421:GLU:H	2:C:421:GLU:CD	2.26	0.42
3:D:314:PRO:HD2	3:D:317:VAL:HG13	2.01	0.42
3:D:561:GLY:HA2	5:F:140:ARG:NH1	2.34	0.42
3:D:580:ALA:O	3:D:584:ASN:HB2	2.20	0.42
1:A:70:GLY:N	2:C:607:ASP:OD1	2.52	0.42
1:B:47:SER:CA	1:B:148:VAL:HG21	2.50	0.42
2:C:154:ARG:NH1	2:C:178:PRO:HB3	2.35	0.42
2:C:168:ARG:O	2:C:267:TYR:HA	2.20	0.42
2:C:356:ARG:HA	2:C:359:MET:HE2	2.02	0.42
2:C:769:PRO:HB2	5:F:375:LEU:HA	2.02	0.42
3:D:322:VAL:HG22	3:D:335:LEU:HD23	2.01	0.42
3:D:1314:LYS:O	3:D:1317:ASP:HB2	2.19	0.42
1:A:184:THR:O	1:A:192:LEU:HB2	2.20	0.42
1:A:193:ASP:OD2	2:C:938:LYS:HD2	2.19	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.75	0.42
2:C:278:GLU:CD	2:C:284:ARG:HD2	2.44	0.42
3:D:38:LYS:HA	3:D:38:LYS:HD3	1.82	0.42
3:D:155:ASP:CG	3:D:568:ARG:HH22	2.22	0.42
3:D:1444:THR:O	3:D:1448:THR:HG23	2.20	0.42
2:C:182:VAL:CG1	2:C:221:LEU:CD1	2.97	0.42
2:C:964:LYS:O	2:C:968:LEU:HD13	2.20	0.42
3:D:162:ARG:O	3:D:449:SER:HB2	2.20	0.42
3:D:361:VAL:HG21	3:D:379:ALA:HB2	2.01	0.42
2:C:344:PHE:CD2	2:C:382:ILE:HD11	2.55	0.41
2:C:1019:GLN:HE22	3:D:617:ASN:HB3	1.82	0.41
3:D:557:LEU:HD13	3:D:566:ILE:HG22	2.01	0.41
3:D:816:HIS:HB2	3:D:836:VAL:HG11	2.02	0.41
1:B:97:VAL:HG12	1:B:99:LEU:HD12	2.01	0.41
3:D:147:VAL:HG21	3:D:161:LEU:CD2	2.43	0.41
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.20	0.41
3:D:719:VAL:O	3:D:721:VAL:HG13	2.20	0.41
4:E:36:LYS:HG2	4:E:93:TYR:HB3	2.02	0.41
2:C:394:PHE:O	8:C:2001:KNG:C32	2.68	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.29	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1277:ILE:CD1	3:D:1299:PHE:CE1	3.02	0.41
2:C:376:ARG:HE	5:F:276:ARG:HD3	1.85	0.41
3:D:108:VAL:HA	3:D:109:PRO:C	2.45	0.41
3:D:175:VAL:CG1	3:D:193:PRO:HG2	2.50	0.41
4:E:50:THR:HG23	4:E:53:GLY:H	1.86	0.41
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.86	0.41
2:C:195:LEU:HD23	2:C:241:LEU:HD12	2.02	0.41
2:C:605:LYS:HB2	2:C:612:VAL:HB	2.01	0.41
2:C:20:GLU:O	2:C:24:GLU:HB2	2.21	0.41
2:C:55:GLU:O	2:C:56:GLU:C	2.62	0.41
2:C:408:ARG:HH11	2:C:456:ALA:C	2.27	0.41
2:C:886:LEU:HD21	3:D:951:ILE:HG12	2.02	0.41
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.49	0.41
3:D:405:ASP:HB3	3:D:423:ASP:OD1	2.21	0.41
2:C:422:ARG:HD2	7:H:16:DC:C6	2.56	0.41
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.89	0.41
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.56	0.41
5:F:194:LEU:HB2	7:H:6:DT:C2	2.56	0.41
5:F:295:MET:HE3	5:F:299:TRP:CE2	2.56	0.41
3:D:133:ILE:CG2	3:D:460:ALA:HB1	2.50	0.41
3:D:879:ARG:HD3	3:D:902:LEU:O	2.20	0.41
6:G:15:DC:H2'	6:G:16:DA:H8	1.79	0.41
1:A:128:HIS:CD2	1:A:129:ILE:N	2.88	0.41
1:B:56:VAL:HG21	1:B:82:LEU:CD1	2.46	0.41
2:C:211:LEU:HD12	2:C:211:LEU:N	2.35	0.41
2:C:344:PHE:HD2	2:C:382:ILE:HD11	1.86	0.41
2:C:438:ILE:CG2	2:C:453:THR:HB	2.51	0.41
3:D:139:GLY:O	3:D:141:ILE:HD12	2.20	0.41
3:D:149:LYS:O	3:D:150:ARG:HB2	2.21	0.41
3:D:474:GLU:HG3	3:D:496:LEU:HD11	2.01	0.41
3:D:561:GLY:HA2	5:F:140:ARG:HH11	1.85	0.41
3:D:1165:TYR:HB3	3:D:1207:TYR:CE1	2.56	0.41
3:D:1459:LEU:CD2	3:D:1464:GLU:HB3	2.51	0.41
5:F:96:LEU:O	5:F:100:VAL:HG23	2.20	0.41
5:F:163:LEU:HD13	5:F:174:LEU:CD1	2.48	0.41
7:H:21:DA:H5'	7:H:21:DA:H8	1.85	0.41
1:B:101:LEU:HB2	1:B:114:PHE:CE1	2.56	0.41
2:C:155:PRO:O	2:C:157:ARG:N	2.54	0.41
2:C:172:ILE:HG12	2:C:184:MET:HE3	2.02	0.41
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.03	0.41
1:A:54:THR:HB	1:A:158:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:357:GLU:O	2:C:361:MET:HG2	2.21	0.40
2:C:814:GLU:C	2:C:815:LEU:HD13	2.46	0.40
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.86	0.40
3:D:778:LEU:HD12	3:D:778:LEU:HA	1.79	0.40
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.22	0.40
3:D:1339:LYS:HB3	3:D:1343:ALA:HB3	2.02	0.40
3:D:1364:HIS:CE1	3:D:1366:LYS:HB2	2.56	0.40
5:F:193:ARG:HB3	7:H:7:DG:C5'	2.52	0.40
5:F:397:ILE:CD1	5:F:400:ILE:HD11	2.47	0.40
1:B:91:ASN:HD21	1:B:93:SER:HB2	1.85	0.40
3:D:1154:GLU:HA	3:D:1158:VAL:O	2.21	0.40
4:E:46:PRO:HB2	4:E:57:ASP:HB3	2.03	0.40
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.03	0.40
1:A:30:ARG:NH2	3:D:855:HIS:HD2	2.19	0.40
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.03	0.40
2:C:418:LEU:CD1	2:C:427:VAL:HG21	2.51	0.40
2:C:473:ARG:O	2:C:480:THR:HG23	2.21	0.40
3:D:875:THR:HG23	3:D:876:SER:O	2.20	0.40
2:C:189:ARG:NH2	2:C:244:PRO:CD	2.84	0.40
2:C:259:GLY:O	2:C:266:ARG:HB2	2.22	0.40
2:C:436:GLY:HA2	2:C:538:GLN:O	2.22	0.40
3:D:74:GLU:CD	3:D:74:GLU:H	2.29	0.40
3:D:207:PHE:HA	3:D:208:PRO:HD2	1.96	0.40
3:D:544:TYR:O	3:D:548:ILE:HG13	2.22	0.40
3:D:786:ILE:HD13	3:D:908:LYS:HB2	2.03	0.40
1:A:27:PRO:HB2	1:A:192:LEU:HD13	2.04	0.40
2:C:946:ARG:NH2	3:D:859:ASP:HB3	2.37	0.40
3:D:231:VAL:O	3:D:231:VAL:HG22	2.22	0.40
3:D:244:GLU:HG3	3:D:310:LEU:HG	2.03	0.40
3:D:1237:THR:HG23	3:D:1359:GLN:NE2	2.37	0.40
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_1359]	1.95	0.25
3:D:1287:GLU:OE1	5:F:302:LYS:NZ[3_445]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
1	B	221/315 (70%)	217 (98%)	4 (2%)	0	100	100
2	C	1108/1119 (99%)	1080 (98%)	22 (2%)	6 (0%)	24	60
3	D	1481/1524 (97%)	1444 (98%)	34 (2%)	3 (0%)	43	76
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	11	43
5	F	344/423 (81%)	337 (98%)	5 (2%)	2 (1%)	21	56
All	All	3471/3795 (92%)	3389 (98%)	70 (2%)	12 (0%)	36	70

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	766	GLU
2	C	156	GLY
5	F	322	GLY
2	C	477	GLY
3	D	276	ASP
5	F	375	LEU
2	C	767	PRO
2	C	155	PRO
4	E	94	PRO
3	D	207	PHE
2	C	476	GLY
3	D	530	VAL

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/273 (73%)	193 (97%)	6 (3%)	36	69
1	B	196/273 (72%)	191 (97%)	5 (3%)	40	72
2	C	922/941 (98%)	878 (95%)	44 (5%)	23	57
3	D	1233/1279 (96%)	1170 (95%)	63 (5%)	21	55
4	E	83/88 (94%)	83 (100%)	0	100	100
5	F	297/370 (80%)	287 (97%)	10 (3%)	32	66
All	All	2930/3224 (91%)	2802 (96%)	128 (4%)	25	60

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	126	ASP
1	A	142	VAL
1	A	184	THR
1	A	189	ARG
1	B	6	LEU
1	B	34	VAL
1	B	56	VAL
1	B	133	GLU
1	B	199	ILE
2	C	56	GLU
2	C	81	ASP
2	C	97	ARG
2	C	133	ASP
2	C	172	ILE
2	C	177	GLU
2	C	182	VAL
2	C	194	VAL
2	C	232	GLU
2	C	251	ASP
2	C	261	ILE
2	C	265	ARG
2	C	322	VAL
2	C	336	VAL
2	C	342	ASP
2	C	372	LEU
2	C	420	ARG

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Mol	Chain	Res	Type
2	C	454	SER
2	C	464	LEU
2	C	480	THR
2	C	482	GLU
2	C	513	VAL
2	C	575	GLN
2	C	583	LEU
2	C	586	ARG
2	C	592	LEU
2	C	617	ASP
2	C	638	ASP
2	C	640	ARG
2	C	648	ARG
2	C	670	GLN
2	C	784	ASP
2	C	807	ARG
2	C	808	ARG
2	C	815	LEU
2	C	830	LYS
2	C	848	VAL
2	C	905	ILE
2	C	939	ARG
2	C	952	LEU
2	C	968	LEU
2	C	1014	SER
2	C	1057	SER
2	C	1080	SER
3	D	30	GLU
3	D	133	ILE
3	D	142	LEU
3	D	155	ASP
3	D	179	VAL
3	D	186	VAL
3	D	198	ARG
3	D	231	VAL
3	D	234	GLU
3	D	272	LEU
3	D	355	VAL
3	D	387	LEU
3	D	399	ARG
3	D	411	THR
3	D	415	VAL

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Mol	Chain	Res	Type
3	D	421	LEU
3	D	427	VAL
3	D	500	ARG
3	D	572	ARG
3	D	587	ARG
3	D	591	VAL
3	D	610	LYS
3	D	618	LEU
3	D	632	VAL
3	D	646	LYS
3	D	650	LEU
3	D	675	ARG
3	D	686	GLU
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	810	GLU
3	D	864	VAL
3	D	875	THR
3	D	894	LYS
3	D	908	LYS
3	D	924	MET
3	D	972	LEU
3	D	983	LEU
3	D	995	LEU
3	D	1014	ASN
3	D	1039	CYS
3	D	1041	LEU
3	D	1062	ARG
3	D	1088	THR
3	D	1155	VAL
3	D	1162	GLU
3	D	1188	VAL
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1234	THR
3	D	1290	LEU
3	D	1299	PHE
3	D	1305	LEU
3	D	1313	VAL

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Mol	Chain	Res	Type
3	D	1317	ASP
3	D	1455	LYS
3	D	1470	ARG
3	D	1486	VAL
3	D	1493	LYS
3	D	1501	GLU
5	F	88	ILE
5	F	122	LEU
5	F	172	ARG
5	F	208	SER
5	F	218	GLN
5	F	279	GLN
5	F	310	ILE
5	F	347	GLN
5	F	397	ILE
5	F	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	B	63	HIS
1	B	91	ASN
1	B	128	HIS
2	C	91	GLN
2	C	187	ASN
2	C	390	GLN
2	C	498	GLN
2	C	609	ASN
2	C	683	ASN
2	C	728	HIS
2	C	860	HIS
2	C	991	GLN
2	C	1019	GLN
3	D	350	HIS
3	D	709	HIS
3	D	768	ASN
3	D	991	GLN
3	D	1033	GLN
3	D	1172	HIS
3	D	1184	GLN
3	D	1195	GLN

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Mol	Chain	Res	Type
3	D	1333	HIS
3	D	1359	GLN
3	D	1441	GLN
3	D	1445	HIS
5	F	185	GLN
5	F	269	ASN
5	F	381	HIS
5	F	402	ASN
5	F	411	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	KNG	C	2001	-	75,75,75	3.82	28 (37%)	107,114,114	2.38	28 (26%)

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
8	KNG	C	2001	-	-	23/76/113/113	0/5/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2001	KNG	O18-C46	-14.12	1.21	1.44
8	C	2001	KNG	O03-C06	11.12	1.58	1.37
8	C	2001	KNG	O17-C47	-10.88	1.20	1.43
8	C	2001	KNG	C04-C10	8.42	1.57	1.43
8	C	2001	KNG	O16-C37	7.74	1.62	1.42
8	C	2001	KNG	O17-C50	6.13	1.51	1.41
8	C	2001	KNG	O11-C04	-5.94	1.19	1.36
8	C	2001	KNG	C15-N01	5.82	1.47	1.35
8	C	2001	KNG	C12-C11	-5.64	1.32	1.54
8	C	2001	KNG	C01-C09	5.60	1.59	1.43
8	C	2001	KNG	C03-C02	5.54	1.48	1.39
8	C	2001	KNG	O18-C50	5.37	1.50	1.41
8	C	2001	KNG	C03-C04	5.19	1.50	1.37
8	C	2001	KNG	O01-C01	-5.13	1.19	1.35
8	C	2001	KNG	C02-C01	5.04	1.54	1.40
8	C	2001	KNG	O12-C39	4.93	1.43	1.34
8	C	2001	KNG	C19-C18	-4.90	1.37	1.53
8	C	2001	KNG	C47-C48	4.12	1.59	1.52
8	C	2001	KNG	O06-C37	-3.89	1.31	1.41
8	C	2001	KNG	O07-C25	-3.87	1.39	1.44
8	C	2001	KNG	C47-C46	3.83	1.62	1.52
8	C	2001	KNG	C02-N01	3.72	1.49	1.41
8	C	2001	KNG	O10-C15	-2.96	1.18	1.23
8	C	2001	KNG	O07-C35	2.36	1.40	1.35
8	C	2001	KNG	O16-C48	2.23	1.49	1.44
8	C	2001	KNG	C18-C17	2.12	1.56	1.50
8	C	2001	KNG	C49-C48	-2.04	1.46	1.51
8	C	2001	KNG	C45-C37	2.01	1.55	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2001	KNG	C33-C24-C23	-8.30	95.10	111.43
8	C	2001	KNG	C25-O07-C35	-7.77	105.64	117.72
8	C	2001	KNG	O03-C06-C07	7.50	133.87	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2001	KNG	C23-C24-C25	5.65	121.36	110.58
8	C	2001	KNG	C18-C19-C20	5.16	124.92	114.56
8	C	2001	KNG	C12-C11-C05	5.00	116.97	107.30
8	C	2001	KNG	O07-C35-C36	4.77	119.59	111.09
8	C	2001	KNG	O04-C11-C05	-4.62	123.12	131.63
8	C	2001	KNG	C37-O06-C27	4.41	121.19	113.84
8	C	2001	KNG	C34-C26-C27	-4.40	102.04	110.95
8	C	2001	KNG	C01-C02-N01	4.38	129.63	117.46
8	C	2001	KNG	C03-C02-N01	-3.89	111.76	121.95
8	C	2001	KNG	O07-C25-C26	3.84	116.37	107.52
8	C	2001	KNG	C45-C46-C47	-3.83	109.65	114.66
8	C	2001	KNG	C26-C25-C24	-3.42	107.78	114.68
8	C	2001	KNG	C24-C23-C22	3.23	120.80	115.41
8	C	2001	KNG	C49-C48-C47	-3.18	108.66	113.39
8	C	2001	KNG	C12-O03-C06	-3.16	102.40	107.69
8	C	2001	KNG	C31-O12-C39	2.99	121.01	117.62
8	C	2001	KNG	C19-C18-C17	2.89	119.75	112.16
8	C	2001	KNG	O10-C15-C16	-2.86	116.23	121.49
8	C	2001	KNG	O16-C48-C47	2.86	114.48	109.19
8	C	2001	KNG	O12-C39-C40	2.85	118.21	112.03
8	C	2001	KNG	O12-C31-C38	2.85	113.89	108.20
8	C	2001	KNG	C30-C16-C17	-2.65	117.92	123.64
8	C	2001	KNG	O03-C06-C05	-2.61	106.41	113.56
8	C	2001	KNG	C05-C06-C07	-2.31	119.72	125.29
8	C	2001	KNG	C23-C22-C21	-2.22	108.09	112.55

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	2001	KNG	C21-C22-C23-O19
8	C	2001	KNG	C23-C24-C25-O07
8	C	2001	KNG	C33-C24-C25-C26
8	C	2001	KNG	C33-C24-C25-O07
8	C	2001	KNG	O06-C27-C28-C29
8	C	2001	KNG	C38-C31-O12-C39
8	C	2001	KNG	C36-C35-O07-C25
8	C	2001	KNG	O08-C35-O07-C25
8	C	2001	KNG	C23-C24-C25-C26
8	C	2001	KNG	C03-C02-N01-C15
8	C	2001	KNG	C32-C22-C23-C24
8	C	2001	KNG	O09-C21-C22-C32

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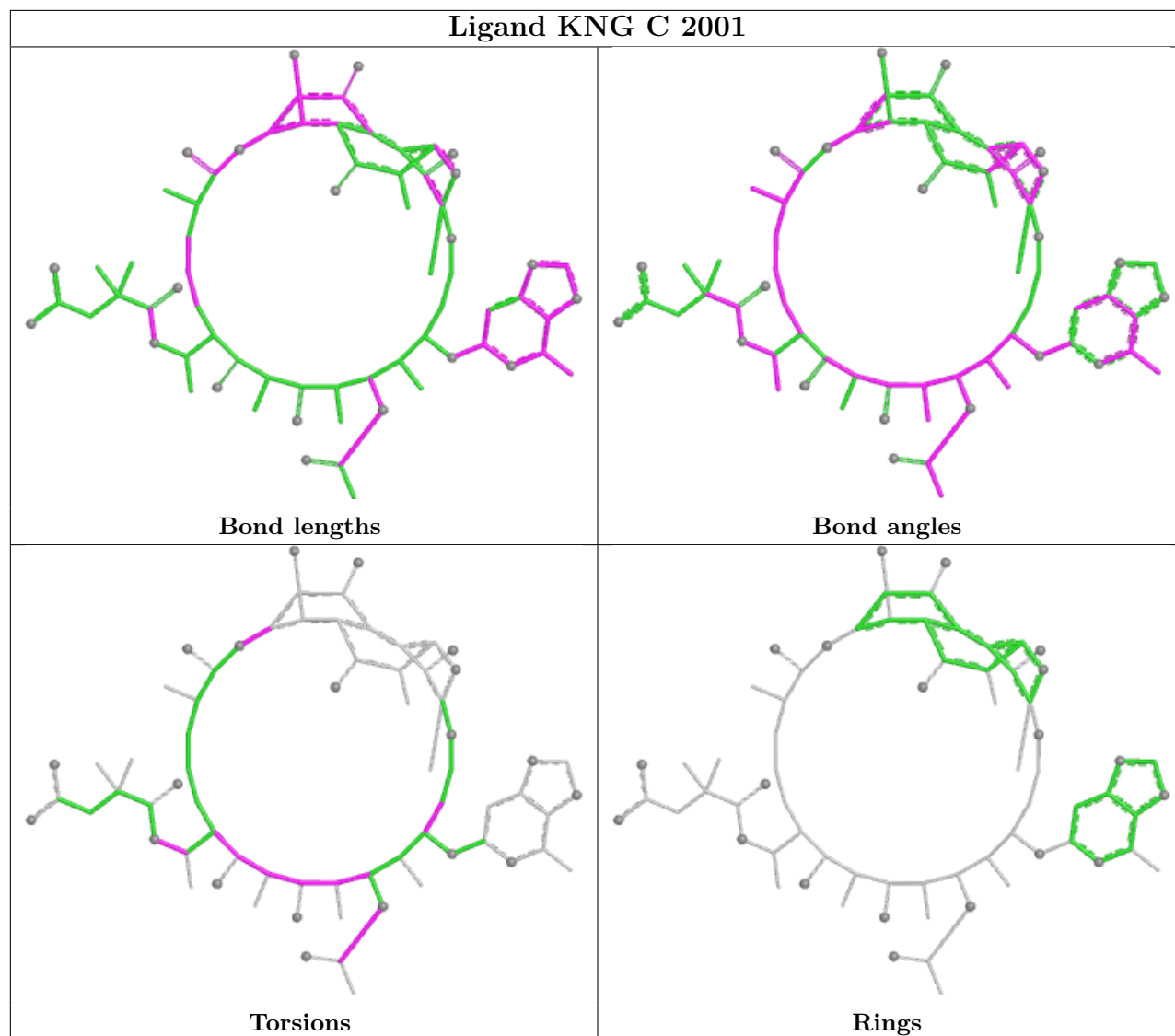
Mol	Chain	Res	Type	Atoms
8	C	2001	KNG	C32-C22-C23-O19
8	C	2001	KNG	C21-C22-C23-C24
8	C	2001	KNG	O09-C21-C22-C23
8	C	2001	KNG	O19-C23-C24-C25
8	C	2001	KNG	C26-C27-C28-C29
8	C	2001	KNG	C20-C21-C22-C23
8	C	2001	KNG	O19-C23-C24-C33
8	C	2001	KNG	C20-C21-C22-C32
8	C	2001	KNG	C01-C02-N01-C15
8	C	2001	KNG	C22-C23-C24-C33
8	C	2001	KNG	C31-C20-C21-O09

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	2001	KNG	6	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	227/315 (72%)	-0.15	0	100	100	67, 92, 127, 170	0
1	B	223/315 (70%)	0.36	7 (3%)	51	30	64, 101, 158, 189	0
2	C	1112/1119 (99%)	-0.00	28 (2%)	58	35	40, 82, 174, 268	0
3	D	1485/1524 (97%)	-0.07	26 (1%)	67	44	36, 80, 163, 253	0
4	E	94/99 (94%)	-0.03	3 (3%)	50	29	47, 83, 155, 175	0
5	F	346/423 (81%)	0.16	17 (4%)	35	18	50, 102, 172, 240	0
6	G	17/22 (77%)	-0.20	1 (5%)	28	14	75, 94, 187, 191	0
7	H	22/27 (81%)	-0.19	1 (4%)	38	20	79, 113, 202, 219	0
All	All	3526/3844 (91%)	-0.01	83 (2%)	59	36	36, 86, 167, 268	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	242	LEU	6.3
2	C	186	VAL	5.0
5	F	378	GLY	4.6
2	C	236	ILE	4.4
2	C	311	PHE	3.9
5	F	326	ASP	3.9
2	C	424	GLY	3.7
2	C	247	PRO	3.6
5	F	422	LEU	3.4
2	C	176	VAL	3.2
2	C	254	VAL	3.2
3	D	66	GLN	3.2
3	D	67	ARG	3.1
2	C	257	VAL	3.1
2	C	298	PHE	3.1
4	E	95	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
5	F	145	PRO	2.9
3	D	420	VAL	2.8
3	D	1491	THR	2.8
3	D	211	VAL	2.8
5	F	147	LEU	2.8
3	D	1292	VAL	2.8
3	D	1311	LEU	2.8
5	F	78	SER	2.7
2	C	171	TRP	2.7
4	E	94	PRO	2.7
2	C	629	TYR	2.7
5	F	399	GLN	2.6
2	C	255	ALA	2.6
5	F	149	GLU	2.6
2	C	244	PRO	2.6
2	C	767	PRO	2.6
3	D	1322	GLY	2.6
3	D	207	PHE	2.6
4	E	93	TYR	2.5
5	F	423	ASP	2.5
3	D	1495	ILE	2.5
5	F	146	GLY	2.5
2	C	191	PHE	2.5
1	B	163	ASN	2.5
1	B	162	ILE	2.4
2	C	107	LEU	2.4
3	D	69	GLU	2.4
2	C	66	LEU	2.4
2	C	245	GLY	2.4
3	D	136	ASP	2.4
2	C	258	TYR	2.4
3	D	322	VAL	2.4
5	F	148	LYS	2.4
5	F	325	LYS	2.3
3	D	1492	LEU	2.3
5	F	373	LYS	2.3
2	C	223	ASP	2.3
1	B	63	HIS	2.3
5	F	141	VAL	2.3
5	F	376	ILE	2.3
1	B	190	THR	2.3
5	F	324	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	132	LEU	2.2
2	C	315	ALA	2.2
3	D	974	ILE	2.2
3	D	1283	ILE	2.2
3	D	1126	ASP	2.2
3	D	1253	THR	2.2
3	D	1490	LYS	2.2
5	F	395	GLU	2.2
2	C	246	ASP	2.2
3	D	1319	VAL	2.2
2	C	765	SER	2.2
2	C	251	ASP	2.1
1	B	67	THR	2.1
2	C	196	LEU	2.1
3	D	813	LEU	2.1
3	D	396	VAL	2.1
2	C	260	LEU	2.1
3	D	434	ARG	2.1
3	D	1488	ASP	2.1
3	D	1237	THR	2.0
2	C	361	MET	2.0
6	G	19	DA	2.0
7	H	12	DC	2.0
1	B	154	GLU	2.0
3	D	80	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

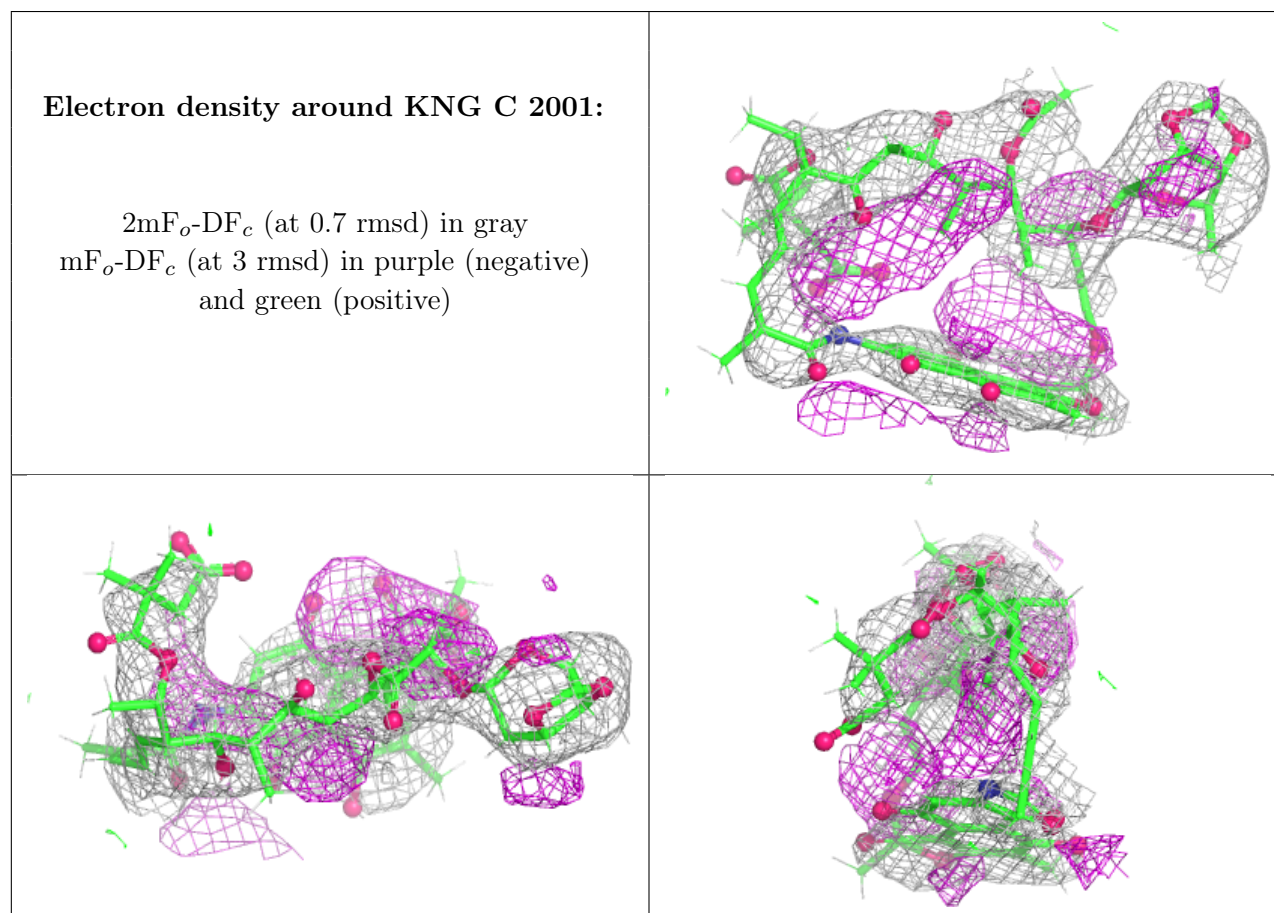
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MG	D	2003	1/1	0.65	0.31	120,120,120,120	0
8	KNG	C	2001	70/70	0.79	0.14	87,141,186,187	0
10	MG	D	2004	1/1	0.92	0.25	70,70,70,70	0
9	ZN	D	2002	1/1	0.99	0.02	91,91,91,91	0
9	ZN	D	2001	1/1	1.00	0.03	65,65,65,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.