



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:08 PM BST

PDB ID : 6UTW  
Title : E. coli sigma-S transcription initiation complex with a 4-nt RNA ("Fresh" crystal)  
Authors : Zuo, Y.; De, S.; Steitz, T.A.  
Deposited on : 2019-10-30  
Resolution : 3.85 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

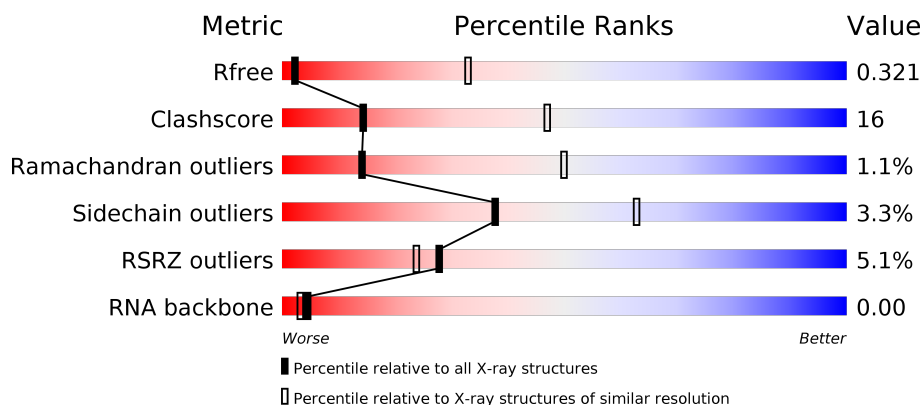
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.85 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))
$R_{free}$	130704	1048 (4.10-3.62)
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)
RNA backbone	3102	1039 (4.70-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AAA	242	<div> <div>3%</div> <div>65%</div> <div>27%</div> <div>5%</div> </div>
1	BBB	242	<div> <div>7%</div> <div>69%</div> <div>25%</div> <div>6%</div> </div>
2	CCC	1342	<div> <div>2%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
3	DDD	1407	<div> <div>7%</div> <div>68%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	EEE	90	
5	FFF	336	
6	111	50	
7	222	50	
8	333	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ZN	DDD	1501	-	-	X	-
10	ZN	DDD	1502	-	-	X	-
9	MG	CCC	1401	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29078 atoms, of which 0 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	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP P0A7Z4
AAA	-5	HIS	-	expression tag	UNP P0A7Z4
AAA	-4	HIS	-	expression tag	UNP P0A7Z4
AAA	-3	HIS	-	expression tag	UNP P0A7Z4
AAA	-2	HIS	-	expression tag	UNP P0A7Z4
AAA	-1	HIS	-	expression tag	UNP P0A7Z4
AAA	0	HIS	-	expression tag	UNP P0A7Z4
BBB	-6	ALA	-	expression tag	UNP P0A7Z4
BBB	-5	HIS	-	expression tag	UNP P0A7Z4
BBB	-4	HIS	-	expression tag	UNP P0A7Z4
BBB	-3	HIS	-	expression tag	UNP P0A7Z4
BBB	-2	HIS	-	expression tag	UNP P0A7Z4
BBB	-1	HIS	-	expression tag	UNP P0A7Z4
BBB	0	HIS	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	EEE	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	277	Total	C	N	O	S	0	0	0
			2253	1411	415	423	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	33	Total	C	N	O	P	0	0	0
			680	323	124	200	33			

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	35	Total	C	N	O	P	0	0	0
			716	342	132	208	34			

- Molecule 8 is a RNA chain called RNA 4-mer (de novo synthesized).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			

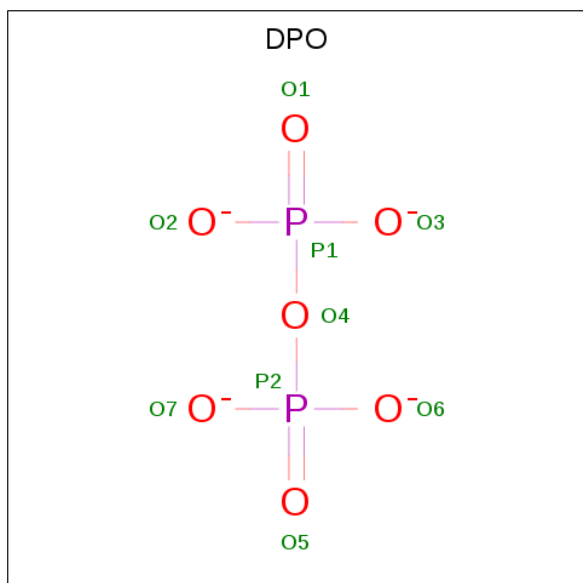
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	CCC	1	Total	Mg	0	0
			1	1		
9	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	DDD	2	Total	Zn	0	0
			2	2		

- Molecule 11 is DIPHOSPHATE (three-letter code: DPO) (formula: O<sub>7</sub>P<sub>2</sub>).

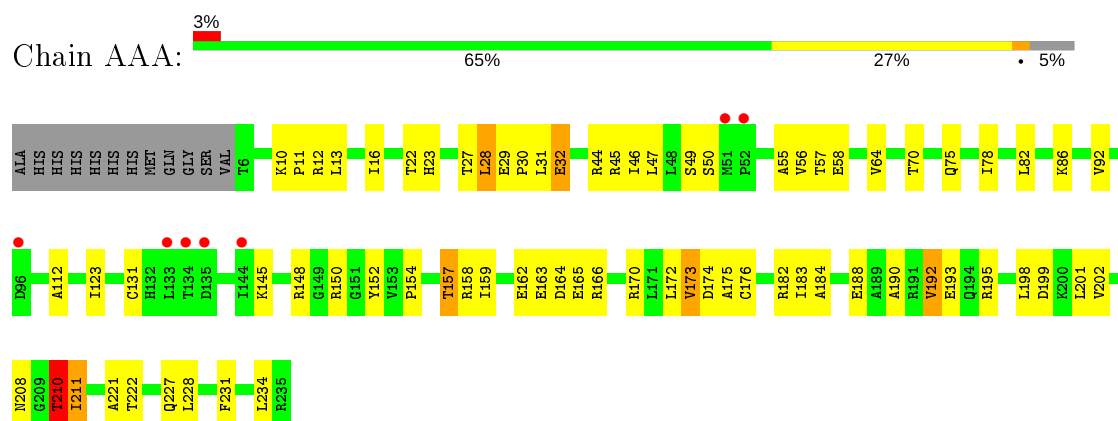


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	DDD	1	Total	O	P	0	0
			9	7	2		

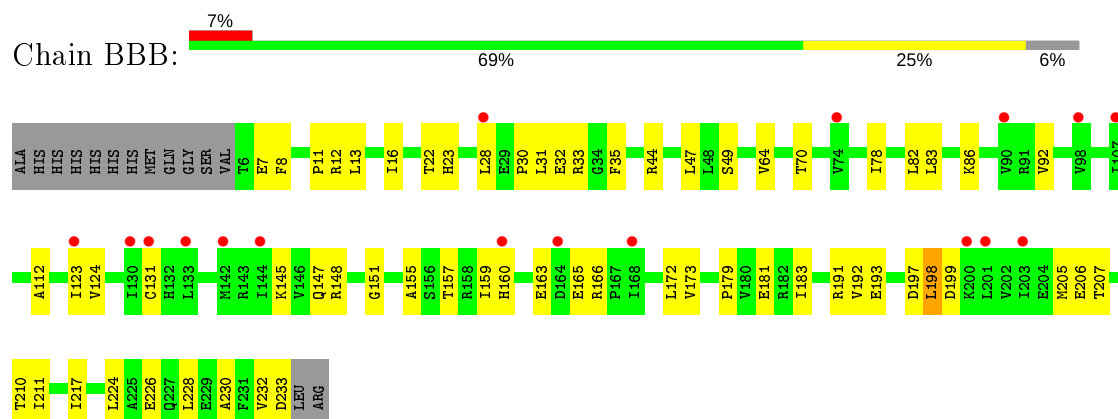
### 3 Residue-property plots [i](#)

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.

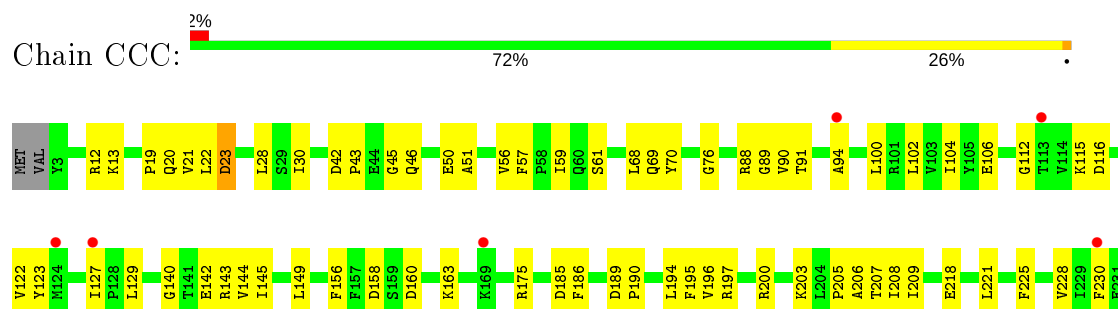
- Molecule 1: DNA-directed RNA polymerase subunit alpha

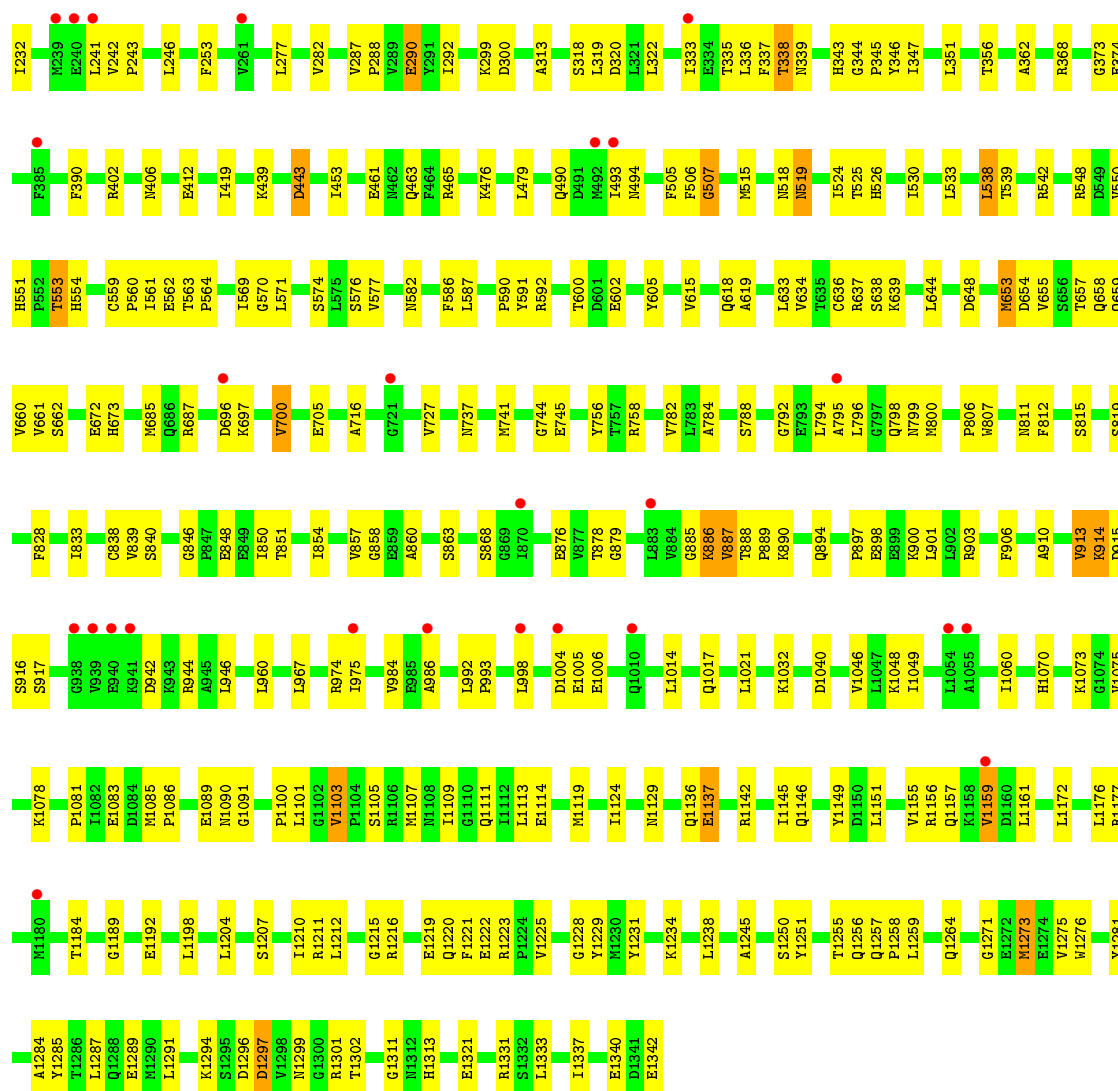


- Molecule 1: DNA-directed RNA polymerase subunit alpha

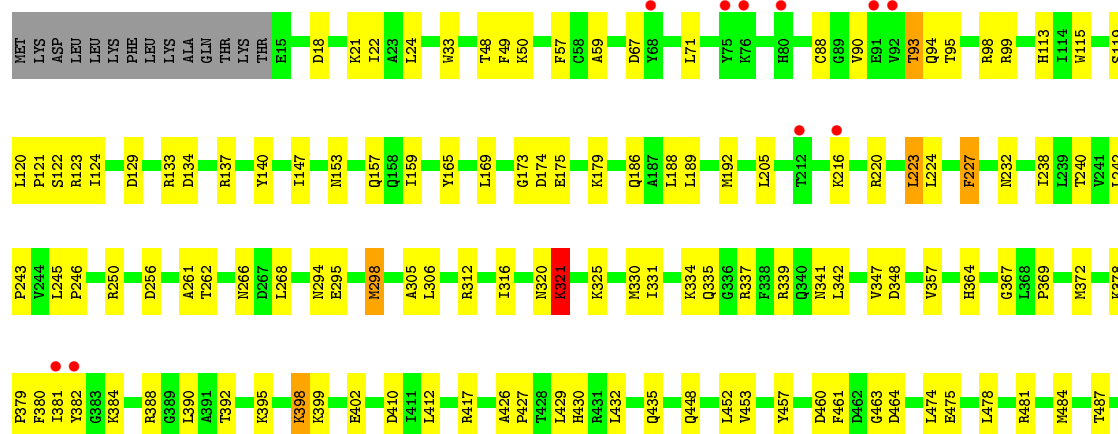
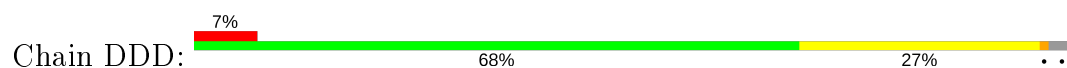


- Molecule 2: DNA-directed RNA polymerase subunit beta

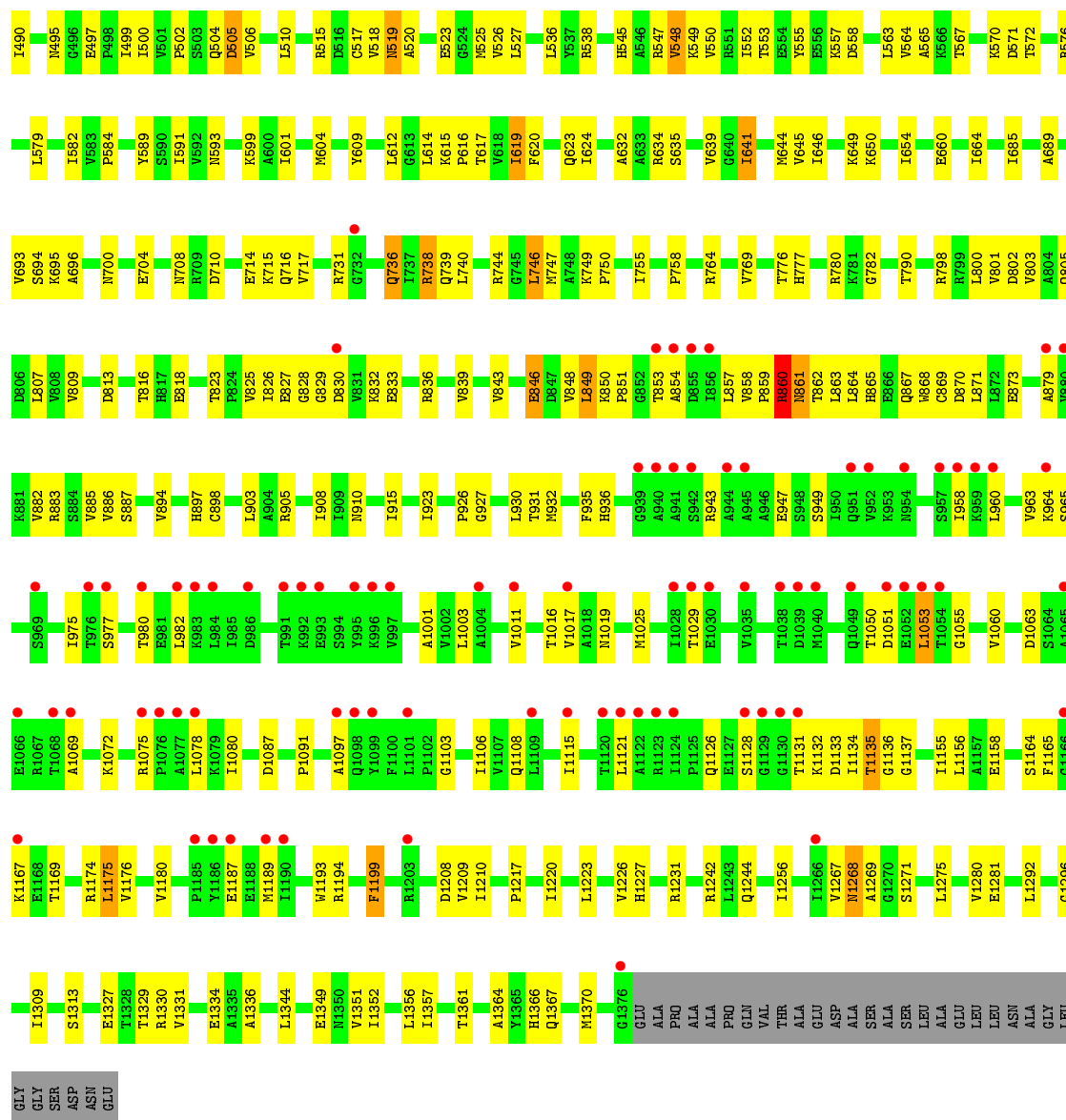




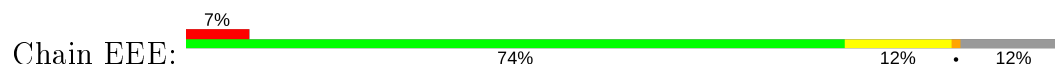
• Molecule 3: DNA-directed RNA polymerase subunit beta'



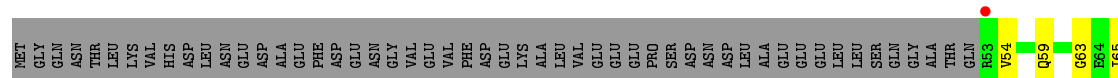


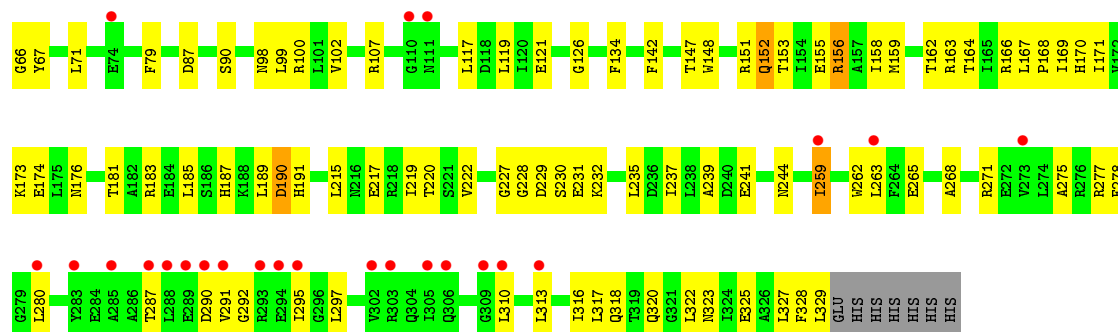


- Molecule 4: DNA-directed RNA polymerase subunit omega

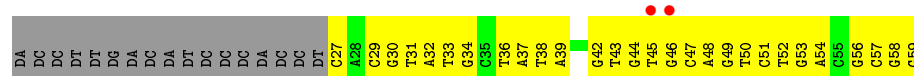
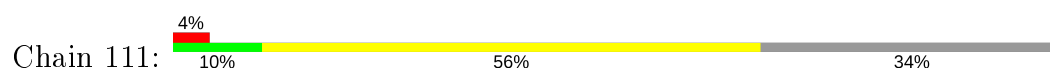


- Molecule 5: RNA polymerase sigma factor RpoS

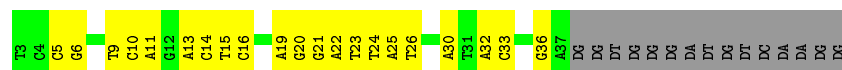




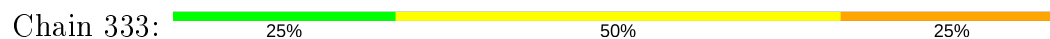
- Molecule 6: Synthetic DNA 50-MER (promoter non-template strand)



- Molecule 7: Synthetic DNA 50-MER (promoter template strand)



- Molecule 8: RNA 4-mer (de novo synthesized)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.99Å 155.45Å 234.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 3.85 49.40 – 3.85	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.40-3.85) 92.7 (49.40-3.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.268 , 0.329 0.263 , 0.321	Depositor DCC
$R_{free}$ test set	2059 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	168.6	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 176.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	29078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	257.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GTP, DPO, ZN, MG

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	AAA	0.65	0/1809	0.73	0/2450
1	BBB	0.66	0/1789	0.73	0/2425
2	CCC	0.64	0/10739	0.79	0/14489
3	DDD	0.66	0/10729	0.77	0/14487
4	EEE	0.61	0/629	0.76	0/847
5	FFF	0.67	0/2282	0.71	0/3076
6	111	0.43	0/762	0.66	0/1175
7	222	0.42	0/803	0.69	0/1238
8	333	0.40	0/71	0.73	0/106
All	All	0.64	0/29613	0.76	0/40293

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	210	THR	Peptide

## 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	AAA	1787	0	1813	76	0
1	BBB	1767	0	1789	59	1
2	CCC	10570	0	10582	349	0
3	DDD	10568	0	10783	339	1
4	EEE	627	0	634	16	0
5	FFF	2253	0	2298	110	0
6	111	680	0	373	61	0
7	222	716	0	396	37	0
8	333	97	0	45	4	0
9	CCC	1	0	0	0	0
9	DDD	1	0	0	0	0
10	DDD	2	0	0	4	0
11	DDD	9	0	0	1	0
All	All	29078	0	28713	895	1

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 16.

All (895) 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:CCC:848:GLU:OE2	2:CCC:888:THR:HG22	1.32	1.23
6:111:50:DT:H3'	6:111:51:DC:C5'	1.75	1.16
3:DDD:936:HIS:ND1	8:333:17:U:OP1	1.79	1.14
3:DDD:320:ASN:OD1	7:222:22:DA:N6	1.80	1.14
2:CCC:373:GLY:HA3	5:FFF:54:VAL:HG22	1.18	1.14
3:DDD:1133:ASP:O	3:DDD:1244:GLN:NE2	1.83	1.11
1:AAA:152:TYR:OH	1:AAA:174:ASP:OD2	1.69	1.08
2:CCC:848:GLU:CD	2:CCC:888:THR:HG22	1.72	1.08
2:CCC:373:GLY:HA3	5:FFF:54:VAL:CG2	1.84	1.06
2:CCC:848:GLU:HG2	2:CCC:888:THR:HA	1.38	1.05
2:CCC:88:ARG:NH1	2:CCC:1040:ASP:OD1	1.90	1.04
5:FFF:231:GLU:HG3	5:FFF:232:LYS:H	1.21	1.04
6:111:50:DT:H3'	6:111:51:DC:H5''	1.05	1.02
2:CCC:901:LEU:CD1	5:FFF:310:LEU:HD22	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:50:SER:HG	1:BBB:35:PHE:HZ	0.97	0.96
3:DDD:525:MET:H	3:DDD:548:VAL:CG2	1.79	0.95
3:DDD:525:MET:N	3:DDD:548:VAL:HG22	1.80	0.95
2:CCC:339:ASN:HB3	2:CCC:343:HIS:H	1.31	0.94
2:CCC:901:LEU:CD1	5:FFF:310:LEU:CD2	2.46	0.94
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.49	0.93
3:DDD:898:CYS:SG	10:DDD:1502:ZN:ZN	1.54	0.93
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD13	1.51	0.92
2:CCC:848:GLU:OE2	2:CCC:888:THR:CG2	2.18	0.92
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB2	1.68	0.92
2:CCC:1145:ILE:HG22	2:CCC:1161:LEU:HD11	1.50	0.91
2:CCC:838:CYS:SG	2:CCC:886:LYS:HB3	2.11	0.91
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	1.52	0.91
2:CCC:838:CYS:SG	2:CCC:886:LYS:HD3	2.10	0.91
3:DDD:320:ASN:O	3:DDD:321:LYS:HB3	1.68	0.91
3:DDD:936:HIS:CE1	8:333:17:U:OP1	2.23	0.90
2:CCC:123:TYR:CZ	5:FFF:190:ASP:O	2.24	0.90
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.52	0.90
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.54	0.90
1:AAA:75:GLN:HE21	2:CCC:727:VAL:HG11	1.37	0.89
2:CCC:539:THR:HB	2:CCC:542:ARG:HG3	1.54	0.88
3:DDD:898:CYS:HG	10:DDD:1502:ZN:ZN	0.76	0.88
2:CCC:241:LEU:CD2	2:CCC:277:LEU:HD21	2.03	0.88
5:FFF:227:GLY:N	7:222:20:DG:O6	2.05	0.88
2:CCC:338:THR:HG21	2:CCC:345:PRO:HB3	1.56	0.88
3:DDD:381:ILE:HD11	3:DDD:412:LEU:HD13	1.53	0.86
6:111:50:DT:C3'	6:111:51:DC:H5''	2.00	0.86
5:FFF:164:THR:HB	5:FFF:219:ILE:HD12	1.55	0.86
6:111:32:DA:C2	7:222:32:DA:C2	2.64	0.85
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	1.76	0.85
2:CCC:175:ARG:CD	6:111:50:DT:H73	2.07	0.84
3:DDD:481:ARG:NH1	4:EEE:3:ARG:O	2.09	0.84
3:DDD:525:MET:HB2	3:DDD:548:VAL:HG21	1.56	0.84
6:111:51:DC:OP1	6:111:51:DC:H2'	1.75	0.84
2:CCC:338:THR:CG2	2:CCC:345:PRO:HB3	2.07	0.84
2:CCC:175:ARG:HD3	6:111:50:DT:H73	1.60	0.83
3:DDD:649:LYS:HE3	3:DDD:696:ALA:HB1	1.60	0.83
2:CCC:123:TYR:CE2	5:FFF:190:ASP:O	2.31	0.82
3:DDD:134:ASP:HB3	3:DDD:159:ILE:HD11	1.59	0.82
5:FFF:190:ASP:OD1	5:FFF:191:HIS:N	2.13	0.82
2:CCC:228:VAL:HB	2:CCC:335:THR:OG1	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:231:GLU:CG	5:FFF:232:LYS:H	1.94	0.80
5:FFF:231:GLU:HG3	5:FFF:232:LYS:N	1.95	0.80
1:BBB:31:LEU:O	1:BBB:199:ASP:OD1	2.00	0.80
2:CCC:897:PRO:HB3	5:FFF:278:PHE:HB3	1.63	0.79
2:CCC:848:GLU:CD	2:CCC:888:THR:CG2	2.51	0.79
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CG2	2.12	0.79
3:DDD:555:TYR:CE2	3:DDD:565:ALA:HB2	2.18	0.79
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.13	0.78
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.16	0.78
3:DDD:664:ILE:HD11	3:DDD:685:ILE:HD11	1.66	0.78
2:CCC:886:LYS:HE2	2:CCC:916:SER:O	1.83	0.78
3:DDD:518:VAL:HG23	3:DDD:716:GLN:NE2	1.97	0.78
1:BBB:30:PRO:HB2	1:BBB:198:LEU:CD1	2.14	0.78
1:AAA:50:SER:OG	1:BBB:35:PHE:HZ	1.65	0.77
2:CCC:901:LEU:HD12	5:FFF:310:LEU:HD22	1.66	0.77
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.67	0.77
6:111:27:DC:H42	7:222:36:DG:H1	1.31	0.77
5:FFF:164:THR:HB	5:FFF:219:ILE:CD1	2.14	0.77
2:CCC:241:LEU:HD23	2:CCC:277:LEU:HD21	1.66	0.77
5:FFF:262:TRP:CD2	5:FFF:313:LEU:HD11	2.19	0.77
3:DDD:334:LYS:NZ	7:222:13:DA:OP1	2.12	0.76
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.65	0.76
2:CCC:741:MET:SD	2:CCC:974:ARG:NH2	2.58	0.76
1:BBB:30:PRO:HB2	1:BBB:198:LEU:HD12	1.65	0.76
3:DDD:504:GLN:HE22	3:DDD:731:ARG:HH21	1.33	0.76
3:DDD:746:LEU:H	3:DDD:746:LEU:HD12	1.51	0.76
5:FFF:189:LEU:O	5:FFF:191:HIS:N	2.20	0.75
2:CCC:186:PHE:CD2	2:CCC:196:VAL:HG22	2.22	0.75
2:CCC:1234:LYS:HE2	2:CCC:1238:LEU:HD21	1.69	0.74
2:CCC:156:PHE:CE2	2:CCC:158:ASP:HB2	2.20	0.74
6:111:47:DC:C2'	6:111:48:DA:H5'	2.16	0.74
2:CCC:838:CYS:SG	2:CCC:886:LYS:CB	2.76	0.74
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.68	0.74
2:CCC:1287:LEU:CD2	3:DDD:1357:ILE:HD11	2.17	0.74
1:AAA:32:GLU:HA	1:AAA:198:LEU:CD2	2.18	0.73
2:CCC:463:GLN:HG3	2:CCC:505:PHE:HB2	1.70	0.73
2:CCC:241:LEU:HD21	2:CCC:277:LEU:HD21	1.71	0.73
6:111:50:DT:C3'	6:111:51:DC:C5'	2.64	0.73
3:DDD:525:MET:CA	3:DDD:548:VAL:HG22	2.18	0.73
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	1.70	0.72
2:CCC:1107:MET:HE2	3:DDD:739:GLN:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	1.89	0.72
5:FFF:158:ILE:HG22	5:FFF:158:ILE:O	1.88	0.72
3:DDD:746:LEU:HG	3:DDD:758:PRO:HB3	1.71	0.72
3:DDD:525:MET:HB2	3:DDD:548:VAL:CG2	2.19	0.72
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.72	0.71
6:111:53:DG:H2"	6:111:54:DA:OP2	1.91	0.71
1:AAA:210:THR:HG22	1:AAA:211:ILE:N	2.05	0.71
2:CCC:618:GLN:HE21	3:DDD:769:VAL:HB	1.56	0.71
2:CCC:1342:GLU:HA	3:DDD:18:ASP:HB2	1.71	0.71
2:CCC:339:ASN:HB3	2:CCC:343:HIS:N	2.06	0.71
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.72	0.70
6:111:44:DG:H3'	6:111:45:DT:H5"	1.73	0.70
2:CCC:46:GLN:HB2	2:CCC:51:ALA:HA	1.72	0.70
5:FFF:166:ARG:HH12	5:FFF:168:PRO:HA	1.56	0.70
1:AAA:150:ARG:HH12	1:BBB:7:GLU:HB2	1.56	0.70
3:DDD:1217:PRO:HA	3:DDD:1220:ILE:HD12	1.73	0.70
3:DDD:746:LEU:N	3:DDD:746:LEU:HD12	2.06	0.70
1:AAA:192:VAL:HG12	1:AAA:193:GLU:N	2.07	0.69
5:FFF:268:ALA:HA	5:FFF:271:ARG:HD3	1.74	0.69
2:CCC:560:PRO:CB	3:DDD:776:THR:HG21	2.23	0.69
3:DDD:392:THR:CG2	5:FFF:320:GLN:O	2.40	0.69
5:FFF:262:TRP:CH2	5:FFF:317:LEU:HD21	2.28	0.69
7:222:13:DA:H2"	7:222:14:DC:H5'	1.74	0.69
3:DDD:572:THR:HG22	3:DDD:593:ASN:OD1	1.92	0.69
1:AAA:13:LEU:HD21	1:AAA:16:ILE:HD11	1.74	0.69
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.75	0.69
2:CCC:1113:LEU:HG	3:DDD:641:ILE:HD11	1.75	0.69
3:DDD:518:VAL:N	3:DDD:716:GLN:HE22	1.91	0.69
6:111:45:DT:O3'	6:111:46:DG:O4'	2.10	0.69
7:222:16:DC:H5"	7:222:16:DC:H6	1.57	0.69
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.74	0.69
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG22	1.72	0.69
2:CCC:143:ARG:HH12	2:CCC:507:GLY:HA2	1.57	0.69
3:DDD:846:GLU:HG3	3:DDD:860:ARG:HH22	1.58	0.69
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.23	0.68
2:CCC:838:CYS:SG	2:CCC:886:LYS:CD	2.81	0.68
5:FFF:227:GLY:O	5:FFF:229:ASP:N	2.24	0.68
2:CCC:539:THR:CB	2:CCC:542:ARG:HG3	2.24	0.68
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.76	0.68
2:CCC:577:VAL:HG23	2:CCC:661:VAL:O	1.93	0.68
3:DDD:525:MET:H	3:DDD:548:VAL:HG23	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:50:SER:OG	1:BBB:35:PHE:CZ	2.43	0.68
7:222:23:DT:H2''	7:222:24:DT:OP2	1.94	0.68
1:AAA:49:SER:HB3	2:CCC:1083:GLU:OE2	1.95	0.67
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.57	0.67
5:FFF:263:LEU:HB3	5:FFF:271:ARG:HB2	1.76	0.67
2:CCC:564:PRO:HB3	8:333:14:GTP:O2A	1.93	0.67
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HG21	1.75	0.67
3:DDD:964:LYS:NZ	3:DDD:1199:PHE:CE1	2.61	0.67
5:FFF:164:THR:CB	5:FFF:219:ILE:HD12	2.22	0.67
1:AAA:32:GLU:HA	1:AAA:198:LEU:HD21	1.76	0.67
2:CCC:494:ASN:ND2	7:222:25:DA:OP1	2.27	0.67
2:CCC:672:GLU:HG3	2:CCC:673:HIS:CD2	2.29	0.67
3:DDD:261:ALA:HA	5:FFF:220:THR:O	1.95	0.67
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.25	0.66
3:DDD:558:ASP:HB2	3:DDD:564:VAL:HG23	1.77	0.66
1:BBB:13:LEU:HD21	1:BBB:16:ILE:HD11	1.78	0.66
6:111:57:DC:H2''	6:111:58:DG:OP2	1.95	0.66
2:CCC:206:ALA:O	2:CCC:209:ILE:HG22	1.95	0.66
2:CCC:200:ARG:HD3	6:111:50:DT:O2	1.94	0.66
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	1.96	0.66
3:DDD:525:MET:N	3:DDD:548:VAL:CG2	2.44	0.66
1:AAA:31:LEU:O	1:AAA:198:LEU:HD22	1.97	0.65
2:CCC:1005:GLU:HG2	2:CCC:1006:GLU:H	1.60	0.65
3:DDD:294:ASN:O	3:DDD:298:MET:HG3	1.96	0.65
5:FFF:222:VAL:HG12	5:FFF:235:LEU:HB2	1.77	0.65
2:CCC:160:ASP:OD2	2:CCC:163:LYS:HB2	1.97	0.65
2:CCC:901:LEU:HD13	5:FFF:310:LEU:CD2	2.26	0.65
3:DDD:22:ILE:HG22	3:DDD:1336:ALA:HA	1.79	0.65
3:DDD:832:LYS:HB3	3:DDD:1242:ARG:HD3	1.77	0.65
3:DDD:88:CYS:HG	10:DDD:1501:ZN:ZN	1.11	0.65
3:DDD:71:LEU:HG	3:DDD:90:VAL:HG21	1.79	0.65
1:AAA:165:GLU:O	1:AAA:165:GLU:HG3	1.96	0.65
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	1.96	0.64
2:CCC:76:GLY:O	2:CCC:94:ALA:HB1	1.97	0.64
7:222:19:DA:H2'	7:222:20:DG:O4'	1.98	0.64
1:AAA:27:THR:HG22	1:AAA:202:VAL:HG22	1.79	0.64
2:CCC:550:VAL:HG21	3:DDD:776:THR:CG2	2.26	0.64
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.80	0.64
2:CCC:744:GLY:O	2:CCC:1014:LEU:HD23	1.98	0.64
2:CCC:1285:TYR:HD2	3:DDD:1361:THR:HG21	1.63	0.64
3:DDD:490:ILE:HD11	3:DDD:614:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:88:CYS:SG	10:DDD:1501:ZN:ZN	1.86	0.64
2:CCC:1219:GLU:OE2	3:DDD:634:ARG:NH1	2.27	0.64
1:AAA:228:LEU:HD21	1:BBB:224:LEU:HD23	1.80	0.63
1:BBB:179:PRO:HG3	1:BBB:211:ILE:HD12	1.80	0.63
2:CCC:390:PHE:HA	2:CCC:419:ILE:HG23	1.80	0.63
6:111:48:DA:OP2	6:111:48:DA:H8	1.81	0.63
2:CCC:1234:LYS:CE	2:CCC:1238:LEU:HD21	2.29	0.63
2:CCC:548:ARG:HA	2:CCC:570:GLY:HA3	1.80	0.63
3:DDD:885:VAL:HG13	3:DDD:894:VAL:HG11	1.79	0.63
3:DDD:843:VAL:CG2	3:DDD:897:HIS:O	2.47	0.63
2:CCC:848:GLU:HB3	2:CCC:887:VAL:O	1.98	0.63
3:DDD:549:LYS:HG2	3:DDD:571:ASP:OD1	1.98	0.63
6:111:27:DC:N3	7:222:36:DG:N2	2.44	0.63
3:DDD:977:SER:OG	3:DDD:980:THR:OG1	2.16	0.63
5:FFF:262:TRP:HH2	5:FFF:317:LEU:HD21	1.62	0.63
6:111:47:DC:H2''	6:111:48:DA:H5'	1.81	0.63
1:AAA:195:ARG:HG2	1:AAA:198:LEU:HG	1.79	0.63
2:CCC:100:LEU:HD22	2:CCC:493:ILE:HD11	1.80	0.63
5:FFF:147:THR:O	5:FFF:151:ARG:HG2	1.99	0.63
1:AAA:11:PRO:O	1:BBB:230:ALA:CB	2.48	0.62
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:CD1	2.29	0.62
3:DDD:518:VAL:H	3:DDD:716:GLN:HE22	1.46	0.62
2:CCC:200:ARG:CD	6:111:50:DT:O2	2.47	0.62
1:AAA:210:THR:O	1:AAA:211:ILE:C	2.36	0.62
2:CCC:638:SER:O	2:CCC:639:LYS:CG	2.46	0.62
2:CCC:1155:VAL:HG12	2:CCC:1157:GLN:O	1.99	0.62
3:DDD:818:GLU:HB3	3:DDD:887:SER:HB2	1.82	0.62
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.29	0.62
2:CCC:1271:GLY:O	2:CCC:1275:VAL:HG23	2.00	0.62
2:CCC:846:GLY:O	2:CCC:889:PRO:HG3	2.00	0.62
1:AAA:222:THR:OG1	1:BBB:233:ASP:CB	2.46	0.62
2:CCC:339:ASN:N	2:CCC:343:HIS:O	2.29	0.62
6:111:46:DG:H2''	6:111:47:DC:O4'	1.98	0.62
3:DDD:548:VAL:O	3:DDD:572:THR:O	2.18	0.62
2:CCC:562:GLU:HG2	2:CCC:574:SER:HB2	1.80	0.61
2:CCC:1245:ALA:HB2	3:DDD:372:MET:HG3	1.81	0.61
1:BBB:86:LYS:HE3	1:BBB:173:VAL:HG12	1.82	0.61
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD22	1.77	0.61
1:AAA:75:GLN:NE2	2:CCC:727:VAL:HG11	2.11	0.61
2:CCC:453:ILE:HD12	2:CCC:587:LEU:HD21	1.83	0.61
3:DDD:689:ALA:O	3:DDD:693:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:373:GLY:CA	5:FFF:54:VAL:CG2	2.70	0.61
1:BBB:181:GLU:HB3	1:BBB:206:GLU:O	2.00	0.60
2:CCC:241:LEU:HD21	2:CCC:277:LEU:CD2	2.31	0.60
3:DDD:1330:ARG:NH2	7:222:9:DT:O3'	2.34	0.60
2:CCC:175:ARG:CD	6:111:50:DT:C7	2.79	0.60
5:FFF:158:ILE:CG2	5:FFF:158:ILE:O	2.49	0.60
2:CCC:559:CYS:HB2	2:CCC:662:SER:HB3	1.84	0.60
2:CCC:563:THR:OG1	2:CCC:569:ILE:O	2.17	0.60
7:222:15:DT:H5''	7:222:15:DT:H6	1.64	0.60
1:AAA:86:LYS:HE2	1:AAA:174:ASP:N	2.17	0.60
1:AAA:188:GLU:O	1:AAA:199:ASP:HB3	2.02	0.60
3:DDD:572:THR:CG2	3:DDD:593:ASN:CG	2.69	0.60
6:111:53:DG:H1'	6:111:54:DA:H5'	1.83	0.60
2:CCC:390:PHE:HA	2:CCC:419:ILE:CG2	2.32	0.60
2:CCC:741:MET:HG2	2:CCC:974:ARG:HH22	1.66	0.60
2:CCC:292:ILE:HD12	2:CCC:322:LEU:HD22	1.83	0.60
3:DDD:843:VAL:HG21	3:DDD:897:HIS:O	2.02	0.60
3:DDD:205:LEU:O	3:DDD:205:LEU:HD23	2.02	0.59
3:DDD:294:ASN:O	3:DDD:298:MET:CG	2.50	0.59
3:DDD:620:PHE:CZ	3:DDD:624:ILE:HD11	2.37	0.59
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD2	1.82	0.59
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	1.84	0.59
2:CCC:69:GLN:O	2:CCC:100:LEU:HD12	2.01	0.59
2:CCC:1105:SER:HB2	3:DDD:731:ARG:HD2	1.84	0.59
5:FFF:100:ARG:HB3	6:111:42:DG:H5''	1.85	0.59
1:AAA:11:PRO:O	1:BBB:230:ALA:HB2	2.02	0.59
3:DDD:1075:ARG:CZ	3:DDD:1193:TRP:CG	2.85	0.59
3:DDD:609:TYR:HA	3:DDD:617:THR:HG21	1.84	0.59
2:CCC:1285:TYR:CD2	3:DDD:1361:THR:HG21	2.37	0.59
2:CCC:318:SER:OG	2:CCC:320:ASP:OD1	2.14	0.59
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.84	0.59
1:AAA:44:ARG:NH2	2:CCC:1215:GLY:O	2.35	0.59
2:CCC:560:PRO:O	3:DDD:780:ARG:NH2	2.31	0.59
3:DDD:1134:ILE:O	3:DDD:1136:GLY:N	2.35	0.59
6:111:44:DG:H4'	6:111:45:DT:OP2	2.02	0.59
2:CCC:745:GLU:HA	2:CCC:1017:GLN:OE1	2.03	0.59
6:111:32:DA:C2	7:222:32:DA:N3	2.71	0.59
2:CCC:200:ARG:O	2:CCC:200:ARG:HG2	2.02	0.58
2:CCC:443:ASP:N	2:CCC:443:ASP:OD1	2.34	0.58
6:111:49:DG:H2''	6:111:50:DT:C4'	2.32	0.58
2:CCC:889:PRO:HA	2:CCC:913:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:86:LYS:CE	1:BBB:173:VAL:HG12	2.33	0.58
1:BBB:22:THR:OG1	1:BBB:207:THR:O	2.20	0.58
2:CCC:886:LYS:O	2:CCC:917:SER:HA	2.03	0.58
5:FFF:222:VAL:CG1	5:FFF:235:LEU:HB2	2.33	0.58
2:CCC:1136:GLN:O	2:CCC:1137:GLU:HB2	2.04	0.58
3:DDD:1075:ARG:NH2	3:DDD:1193:TRP:CD2	2.71	0.58
1:AAA:31:LEU:HD11	1:AAA:201:LEU:HB2	1.85	0.58
1:AAA:75:GLN:HE21	2:CCC:727:VAL:CG1	2.13	0.58
1:AAA:11:PRO:HB3	1:AAA:31:LEU:HD23	1.85	0.58
2:CCC:560:PRO:HB2	3:DDD:776:THR:CG2	2.33	0.58
2:CCC:230:PHE:O	2:CCC:333:ILE:N	2.37	0.58
1:AAA:31:LEU:CD1	1:AAA:201:LEU:HB2	2.34	0.57
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.86	0.57
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.32	0.57
6:111:32:DA:N3	7:222:32:DA:C2	2.71	0.57
1:AAA:190:ALA:HB3	1:AAA:198:LEU:O	2.04	0.57
2:CCC:61:SER:HB3	2:CCC:479:LEU:HB3	1.84	0.57
3:DDD:515:ARG:NH2	3:DDD:717:VAL:HB	2.20	0.57
3:DDD:593:ASN:OD1	3:DDD:593:ASN:O	2.22	0.57
3:DDD:1269:ALA:HB2	3:DDD:1275:LEU:HD23	1.85	0.57
3:DDD:749:LYS:HB3	3:DDD:750:PRO:HD2	1.85	0.57
2:CCC:218:GLU:OE2	2:CCC:299:LYS:HD3	2.05	0.57
7:222:22:DA:H2''	7:222:23:DT:O5'	2.04	0.57
3:DDD:949:SER:HB3	3:DDD:1019:ASN:ND2	2.20	0.57
3:DDD:325:LYS:HE2	3:DDD:330:MET:HG2	1.86	0.57
6:111:37:DA:H4'	6:111:38:DT:OP1	2.04	0.56
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.35	0.56
7:222:22:DA:H2''	7:222:23:DT:C5'	2.36	0.56
3:DDD:1080:ILE:HB	3:DDD:1097:ALA:HB3	1.86	0.56
2:CCC:1124:ILE:HD11	2:CCC:1198:LEU:HD11	1.85	0.56
2:CCC:122:VAL:HG22	2:CCC:490:GLN:HB3	1.86	0.56
2:CCC:975:ILE:HD13	2:CCC:998:LEU:HD21	1.86	0.56
3:DDD:367:GLY:HA3	3:DDD:448:GLN:HB2	1.88	0.56
1:AAA:234:LEU:HD23	1:BBB:13:LEU:H	1.70	0.56
1:BBB:30:PRO:CB	1:BBB:198:LEU:HD12	2.35	0.56
3:DDD:553:THR:HG23	3:DDD:567:THR:OG1	2.06	0.56
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CB	2.35	0.56
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.86	0.56
2:CCC:890:LYS:HD2	2:CCC:914:LYS:HG3	1.88	0.56
1:AAA:46:ILE:HG12	1:BBB:35:PHE:CE1	2.41	0.56
3:DDD:846:GLU:HG3	3:DDD:860:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:262:TRP:CG	5:FFF:313:LEU:HD11	2.40	0.56
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.88	0.56
1:BBB:11:PRO:HB3	1:BBB:31:LEU:HD23	1.88	0.55
2:CCC:576:SER:OG	2:CCC:659:GLN:O	2.19	0.55
3:DDD:1271:SER:OG	3:DDD:1292:LEU:HD21	2.06	0.55
1:AAA:28:LEU:HB3	1:AAA:201:LEU:HB3	1.87	0.55
2:CCC:888:THR:N	2:CCC:913:VAL:HG12	2.21	0.55
3:DDD:57:PHE:O	3:DDD:98:ARG:NH2	2.39	0.55
3:DDD:1267:VAL:O	3:DDD:1268:ASN:CB	2.54	0.55
2:CCC:590:PRO:HG3	2:CCC:605:TYR:CE2	2.42	0.55
3:DDD:298:MET:SD	5:FFF:117:LEU:HB3	2.47	0.55
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG21	1.87	0.55
1:BBB:64:VAL:HG13	1:BBB:78:ILE:HD13	1.89	0.55
2:CCC:195:PHE:CG	2:CCC:203:LYS:HD3	2.42	0.55
2:CCC:253:PHE:CZ	2:CCC:287:VAL:HG12	2.42	0.55
2:CCC:828:PHE:HB3	2:CCC:1060:ILE:HG21	1.89	0.55
5:FFF:227:GLY:HA3	7:222:19:DA:H2	1.72	0.55
2:CCC:901:LEU:HD11	5:FFF:310:LEU:CD2	2.34	0.55
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.89	0.55
2:CCC:848:GLU:HG2	2:CCC:889:PRO:HD2	1.88	0.55
2:CCC:906:PHE:CE1	5:FFF:327:LEU:HD12	2.41	0.55
1:AAA:192:VAL:HG12	1:AAA:193:GLU:H	1.72	0.55
6:111:47:DC:H2'	6:111:48:DA:H5'	1.87	0.55
3:DDD:1344:LEU:HD23	3:DDD:1349:GLU:HB3	1.89	0.55
3:DDD:823:THR:OG1	3:DDD:1231:ARG:NH2	2.40	0.55
2:CCC:322:LEU:CD1	2:CCC:333:ILE:CD1	2.84	0.54
2:CCC:741:MET:HG2	2:CCC:974:ARG:NH2	2.21	0.54
3:DDD:619:ILE:O	3:DDD:623:GLN:HG2	2.07	0.54
2:CCC:1101:LEU:HD13	3:DDD:504:GLN:HG3	1.89	0.54
2:CCC:42:ASP:O	2:CCC:50:GLU:HG2	2.06	0.54
5:FFF:163:ARG:CD	5:FFF:167:LEU:HD12	2.37	0.54
6:111:44:DG:H3'	6:111:45:DT:C5'	2.37	0.54
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG11	1.88	0.54
5:FFF:152:GLN:HG3	5:FFF:153:THR:N	2.21	0.54
5:FFF:231:GLU:HG3	5:FFF:232:LYS:HG2	1.89	0.54
5:FFF:262:TRP:CE3	5:FFF:313:LEU:HD11	2.42	0.54
2:CCC:1281:TYR:CD2	3:DDD:484:MET:HE3	2.43	0.54
2:CCC:878:THR:HG22	2:CCC:879:GLY:N	2.21	0.54
3:DDD:24:LEU:HD12	3:DDD:232:ASN:HB3	1.89	0.54
3:DDD:189:LEU:O	3:DDD:192:MET:HG2	2.07	0.54
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1145:ILE:CG2	2:CCC:1161:LEU:HD11	2.33	0.54
3:DDD:165:TYR:O	3:DDD:169:LEU:HB2	2.08	0.54
2:CCC:127:ILE:O	2:CCC:127:ILE:HG13	2.06	0.54
2:CCC:189:ASP:HB2	2:CCC:190:PRO:HD2	1.90	0.54
3:DDD:122:SER:O	3:DDD:124:ILE:N	2.41	0.54
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	1.90	0.54
2:CCC:106:GLU:HG2	2:CCC:115:LYS:HD2	1.90	0.54
2:CCC:741:MET:CG	2:CCC:974:ARG:HH22	2.21	0.54
6:111:32:DA:C2	7:222:32:DA:C4	2.96	0.53
2:CCC:705:GLU:HB3	2:CCC:794:LEU:H	1.72	0.53
2:CCC:758:ARG:HG3	2:CCC:833:ILE:O	2.08	0.53
2:CCC:782:VAL:HG21	2:CCC:792:GLY:CA	2.37	0.53
3:DDD:147:ILE:HD12	3:DDD:179:LYS:HD2	1.89	0.53
3:DDD:525:MET:CB	3:DDD:548:VAL:CG2	2.86	0.53
2:CCC:185:ASP:OD2	6:111:50:DT:O4	2.26	0.53
3:DDD:572:THR:HG22	3:DDD:593:ASN:CG	2.27	0.53
2:CCC:716:ALA:HB3	2:CCC:784:ALA:HB3	1.90	0.53
2:CCC:123:TYR:O	5:FFF:187:HIS:CE1	2.61	0.53
2:CCC:228:VAL:HG23	2:CCC:337:PHE:HB2	1.89	0.53
3:DDD:1063:ASP:HB3	3:DDD:1103:GLY:HA3	1.90	0.53
3:DDD:115:TRP:CZ2	3:DDD:1329:THR:HG22	2.43	0.53
3:DDD:186:GLN:HB2	3:DDD:238:ILE:HG13	1.90	0.53
1:BBB:30:PRO:HB2	1:BBB:198:LEU:HD13	1.89	0.53
2:CCC:1100:PRO:HB3	3:DDD:639:VAL:HG23	1.90	0.53
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.73	0.53
2:CCC:1340:GLU:OE1	3:DDD:21:LYS:HB2	2.09	0.53
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	2.08	0.53
3:DDD:736:GLN:O	3:DDD:740:LEU:HG	2.08	0.53
3:DDD:859:PRO:HG2	3:DDD:862:THR:HG21	1.89	0.53
6:111:33:DT:H2''	6:111:34:DG:H5'	1.90	0.53
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.41	0.53
2:CCC:1313:HIS:HB2	3:DDD:474:LEU:HG	1.90	0.53
2:CCC:901:LEU:HD13	5:FFF:310:LEU:HD21	1.89	0.53
3:DDD:1280:VAL:HG12	3:DDD:1281:GLU:N	2.23	0.53
3:DDD:700:ASN:O	3:DDD:704:GLU:HB2	2.09	0.53
3:DDD:644:MET:O	3:DDD:764:ARG:NH1	2.42	0.53
7:222:5:DC:H1'	7:222:6:DG:H5'	1.90	0.53
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.42	0.53
2:CCC:1337:ILE:HG23	2:CCC:1337:ILE:O	2.09	0.53
3:DDD:220:ARG:O	3:DDD:224:LEU:HG	2.09	0.53
3:DDD:664:ILE:HD11	3:DDD:685:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:55:ALA:HB1	1:AAA:175:ALA:HB1	1.90	0.52
2:CCC:142:GLU:OE1	2:CCC:515:MET:HE2	2.09	0.52
3:DDD:869:CYS:O	3:DDD:873:GLU:OE1	2.27	0.52
1:BBB:124:VAL:HG21	1:BBB:210:THR:HG22	1.91	0.52
5:FFF:126:GLY:HA3	5:FFF:153:THR:HG21	1.92	0.52
2:CCC:898:GLU:OE2	5:FFF:280:LEU:HD13	2.09	0.52
3:DDD:432:LEU:HD13	3:DDD:499:ILE:HG21	1.91	0.52
3:DDD:557:LYS:HA	3:DDD:563:LEU:HD23	1.91	0.52
3:DDD:1075:ARG:NE	3:DDD:1193:TRP:HB3	2.25	0.52
3:DDD:823:THR:HG22	3:DDD:879:ALA:HB2	1.91	0.52
6:111:29:DC:H2''	6:111:30:DG:OP2	2.10	0.52
2:CCC:903:ARG:NH1	2:CCC:910:ALA:HB2	2.25	0.52
3:DDD:903:LEU:H	3:DDD:903:LEU:HD12	1.74	0.52
5:FFF:176:ASN:OD1	7:222:26:DT:H71	2.08	0.52
1:AAA:164:ASP:OD1	1:AAA:165:GLU:N	2.40	0.52
5:FFF:287:THR:H	5:FFF:290:ASP:HB2	1.75	0.52
2:CCC:186:PHE:CE2	2:CCC:196:VAL:HG22	2.44	0.52
6:111:44:DG:O3'	6:111:45:DT:O4'	2.27	0.52
2:CCC:539:THR:HB	2:CCC:542:ARG:CG	2.35	0.52
2:CCC:848:GLU:HG2	2:CCC:889:PRO:CD	2.40	0.52
3:DDD:250:ARG:HD2	3:DDD:266:ASN:OD1	2.10	0.52
3:DDD:555:TYR:CE2	3:DDD:565:ALA:CB	2.90	0.52
2:CCC:339:ASN:O	2:CCC:344:GLY:HA2	2.09	0.52
2:CCC:811:ASN:HA	2:CCC:815:SER:O	2.10	0.52
6:111:49:DG:H2''	6:111:50:DT:H4'	1.91	0.52
1:AAA:227:GLN:OE1	1:BBB:11:PRO:HD3	2.10	0.52
2:CCC:338:THR:HG21	2:CCC:345:PRO:CB	2.33	0.51
1:BBB:157:THR:HG22	1:BBB:157:THR:O	2.09	0.51
3:DDD:93:THR:HG22	3:DDD:94:GLN:H	1.75	0.51
2:CCC:1257:GLN:HB2	2:CCC:1258:PRO:HD2	1.93	0.51
2:CCC:638:SER:O	2:CCC:639:LYS:HG2	2.10	0.51
2:CCC:638:SER:O	2:CCC:639:LYS:HG3	2.10	0.51
3:DDD:519:ASN:HA	3:DDD:523:GLU:HB2	1.92	0.51
5:FFF:87:ASP:OD2	5:FFF:90:SER:OG	2.20	0.51
6:111:48:DA:OP2	6:111:48:DA:C8	2.61	0.51
2:CCC:89:GLY:HA2	2:CCC:140:GLY:HA3	1.92	0.51
2:CCC:838:CYS:HG	2:CCC:886:LYS:HB3	1.75	0.51
1:BBB:191:ARG:NH2	3:DDD:410:ASP:OD1	2.43	0.51
3:DDD:1080:ILE:HD12	3:DDD:1115:ILE:HD11	1.93	0.51
2:CCC:1192:GLU:OE2	3:DDD:764:ARG:NE	2.42	0.51
2:CCC:888:THR:C	2:CCC:913:VAL:CG1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:848:VAL:O	3:DDD:848:VAL:HG12	2.11	0.51
3:DDD:965:SER:HB3	3:DDD:975:ILE:HA	1.93	0.51
6:111:45:DT:H2"	6:111:46:DG:N9	2.25	0.51
1:AAA:195:ARG:CG	1:AAA:198:LEU:HG	2.41	0.51
3:DDD:825:VAL:HB	3:DDD:833:GLU:HB2	1.92	0.51
5:FFF:65:ILE:HG22	5:FFF:99:LEU:HD13	1.92	0.51
2:CCC:828:PHE:HB3	2:CCC:1060:ILE:CG2	2.41	0.51
2:CCC:207:THR:HG21	2:CCC:351:LEU:HG	1.91	0.51
3:DDD:1169:THR:OG1	3:DDD:1174:ARG:NH2	2.44	0.51
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.26	0.51
3:DDD:555:TYR:CD2	3:DDD:565:ALA:HB2	2.45	0.51
3:DDD:59:ALA:HB3	3:DDD:71:LEU:HD11	1.93	0.51
3:DDD:782:GLY:O	3:DDD:935:PHE:HB3	2.10	0.51
4:EEE:65:ASP:HB3	4:EEE:69:ARG:HH21	1.76	0.51
3:DDD:620:PHE:CE2	3:DDD:624:ILE:HD11	2.46	0.51
2:CCC:1070:HIS:NE2	2:CCC:1114:GLU:OE1	2.41	0.51
3:DDD:357:VAL:HG12	3:DDD:461:PHE:CE2	2.46	0.51
3:DDD:826:ILE:O	3:DDD:826:ILE:HG22	2.09	0.51
2:CCC:806:PRO:HG2	3:DDD:632:ALA:O	2.12	0.50
1:AAA:58:GLU:HB2	1:AAA:145:LYS:HB3	1.93	0.50
1:AAA:159:ILE:HD11	2:CCC:876:GLU:OE1	2.11	0.50
2:CCC:322:LEU:HD12	2:CCC:333:ILE:HD11	1.93	0.50
3:DDD:858:VAL:HG12	3:DDD:859:PRO:HD2	1.92	0.50
2:CCC:1264:GLN:CD	5:FFF:237:ILE:HG23	2.31	0.50
5:FFF:227:GLY:CA	7:222:19:DA:H2	2.24	0.50
2:CCC:1155:VAL:CG1	2:CCC:1157:GLN:O	2.60	0.50
3:DDD:334:LYS:HG2	3:DDD:339:ARG:HD2	1.94	0.50
5:FFF:230:SER:OG	5:FFF:230:SER:O	2.21	0.50
2:CCC:992:LEU:HB3	2:CCC:993:PRO:HD2	1.92	0.50
3:DDD:388:ARG:HB3	3:DDD:390:LEU:HD13	1.93	0.50
3:DDD:1175:LEU:O	3:DDD:1187:GLU:HA	2.11	0.50
3:DDD:1292:LEU:O	3:DDD:1296:GLY:N	2.45	0.50
3:DDD:478:LEU:CG	4:EEE:47:THR:HG23	2.42	0.50
2:CCC:564:PRO:O	2:CCC:569:ILE:HA	2.12	0.50
11:DDD:1504:DPO:O2	11:DDD:1504:DPO:O5	2.30	0.50
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.92	0.50
5:FFF:162:THR:HG23	5:FFF:163:ARG:HG3	1.94	0.50
2:CCC:104:ILE:HD12	2:CCC:116:ASP:HB2	1.94	0.50
2:CCC:887:VAL:HG12	2:CCC:915:ASP:HA	1.94	0.50
3:DDD:342:LEU:HG	3:DDD:1352:ILE:HG23	1.93	0.50
5:FFF:317:LEU:CD2	5:FFF:322:LEU:HD12	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:13:LYS:NZ	2:CCC:1149:TYR:O	2.45	0.49
2:CCC:782:VAL:HG21	2:CCC:792:GLY:HA3	1.94	0.49
3:DDD:157:GLN:HG2	3:DDD:188:LEU:HD21	1.94	0.49
1:BBB:86:LYS:HE3	1:BBB:173:VAL:CG1	2.41	0.49
2:CCC:142:GLU:OE1	2:CCC:515:MET:CE	2.60	0.49
2:CCC:228:VAL:CB	2:CCC:335:THR:OG1	2.58	0.49
2:CCC:860:ALA:O	2:CCC:863:SER:OG	2.19	0.49
2:CCC:90:VAL:HG12	2:CCC:91:THR:N	2.27	0.49
3:DDD:1167:LYS:HB2	3:DDD:1174:ARG:HD2	1.93	0.49
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.12	0.49
3:DDD:839:VAL:HG12	3:DDD:864:LEU:CD1	2.34	0.49
3:DDD:843:VAL:HG11	3:DDD:883:ARG:HD3	1.94	0.49
3:DDD:910:ASN:HB3	4:EEE:15:ASN:OD1	2.11	0.49
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:OE1	2.12	0.49
2:CCC:149:LEU:HB2	2:CCC:530:ILE:CG2	2.43	0.49
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CZ	2.47	0.49
3:DDD:1131:THR:O	3:DDD:1133:ASP:N	2.45	0.49
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG22	1.94	0.49
2:CCC:840:SER:OG	2:CCC:1048:LYS:HG2	2.13	0.49
3:DDD:1158:GLU:HA	3:DDD:1223:LEU:HD22	1.94	0.49
3:DDD:490:ILE:O	3:DDD:499:ILE:HG22	2.12	0.49
3:DDD:802:ASP:OD1	3:DDD:1313:SER:HB2	2.12	0.49
5:FFF:313:LEU:HA	5:FFF:316:ILE:HD12	1.95	0.49
1:AAA:82:LEU:HB3	1:AAA:173:VAL:HG11	1.95	0.49
2:CCC:1251:TYR:OH	3:DDD:348:ASP:OD2	2.31	0.49
5:FFF:148:TRP:CE3	6:111:36:DT:C2	3.01	0.49
5:FFF:171:ILE:HG21	5:FFF:215:LEU:HD13	1.94	0.49
2:CCC:897:PRO:HG3	5:FFF:278:PHE:O	2.12	0.49
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.77	0.49
1:BBB:33:ARG:O	1:BBB:33:ARG:HG2	2.13	0.49
2:CCC:1149:TYR:HB3	2:CCC:1159:VAL:CG1	2.43	0.49
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:CE2	3.01	0.49
2:CCC:1333:LEU:O	3:DDD:113:HIS:NE2	2.41	0.49
3:DDD:478:LEU:HD21	4:EEE:47:THR:CG2	2.43	0.49
3:DDD:964:LYS:NZ	3:DDD:1199:PHE:HE1	2.05	0.49
1:BBB:193:GLU:OE1	1:BBB:193:GLU:N	2.46	0.49
2:CCC:886:LYS:O	2:CCC:917:SER:CA	2.60	0.49
2:CCC:1276:TRP:CE2	3:DDD:801:VAL:HG11	2.47	0.49
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:HE2	2.31	0.49
3:DDD:1164:SER:HB2	3:DDD:1176:VAL:O	2.13	0.49
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:111:52:DT:H2''	6:111:53:DG:C8	2.48	0.49
2:CCC:916:SER:OG	2:CCC:916:SER:O	2.31	0.49
2:CCC:1294:LYS:HD3	3:DDD:347:VAL:HG13	1.94	0.49
7:222:10:DC:H2'	7:222:11:DA:C8	2.47	0.48
2:CCC:1273:MET:HG3	7:222:14:DC:H4'	1.95	0.48
5:FFF:169:ILE:HG22	5:FFF:173:LYS:HD2	1.94	0.48
3:DDD:435:GLN:HB2	3:DDD:457:TYR:OH	2.13	0.48
1:AAA:190:ALA:HB2	1:AAA:199:ASP:O	2.12	0.48
2:CCC:23:ASP:N	2:CCC:23:ASP:OD1	2.45	0.48
3:DDD:803:VAL:CG2	3:DDD:1309:ILE:O	2.62	0.48
3:DDD:335:GLN:HG3	3:DDD:335:GLN:O	2.13	0.48
3:DDD:337:ARG:NH1	3:DDD:341:ASN:ND2	2.62	0.48
2:CCC:1222:GLU:HB2	3:DDD:635:SER:O	2.13	0.48
6:111:48:DA:H2'	6:111:49:DG:C1'	2.43	0.48
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.94	0.48
2:CCC:744:GLY:O	2:CCC:1014:LEU:CD2	2.61	0.48
2:CCC:1210:ILE:CG2	2:CCC:1211:ARG:N	2.76	0.48
2:CCC:175:ARG:NH1	6:111:50:DT:H72	2.29	0.48
1:BBB:205:MET:CE	1:BBB:217:ILE:HG13	2.43	0.48
2:CCC:1311:GLY:O	4:EEE:31:GLN:NE2	2.43	0.48
2:CCC:232:ILE:HD11	2:CCC:333:ILE:HD12	1.95	0.48
7:222:16:DC:C5'	7:222:16:DC:H6	2.24	0.48
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.47	0.48
3:DDD:813:ASP:OD1	3:DDD:883:ARG:NH2	2.44	0.48
1:AAA:47:LEU:HD13	1:AAA:183:ILE:CD1	2.43	0.48
2:CCC:1255:THR:O	2:CCC:1256:GLN:HB2	2.13	0.48
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.52	0.48
2:CCC:653:MET:HG2	2:CCC:654:ASP:N	2.29	0.48
1:AAA:152:TYR:OH	1:AAA:174:ASP:CG	2.49	0.47
2:CCC:633:LEU:HD13	2:CCC:644:LEU:HD13	1.95	0.47
3:DDD:510:LEU:HD11	3:DDD:624:ILE:HG23	1.96	0.47
3:DDD:827:GLU:HB3	3:DDD:832:LYS:HG3	1.95	0.47
1:AAA:55:ALA:CB	1:AAA:175:ALA:HB1	2.45	0.47
1:BBB:155:ALA:HB1	1:BBB:172:LEU:HD23	1.95	0.47
3:DDD:572:THR:HG23	3:DDD:593:ASN:ND2	2.29	0.47
5:FFF:163:ARG:NE	5:FFF:167:LEU:HD12	2.30	0.47
2:CCC:1287:LEU:O	2:CCC:1291:LEU:HG	2.15	0.47
2:CCC:288:PRO:HB2	2:CCC:290:GLU:HG2	1.96	0.47
2:CCC:850:ILE:HA	2:CCC:885:GLY:O	2.14	0.47
3:DDD:140:TYR:OH	3:DDD:312:ARG:NH1	2.47	0.47
2:CCC:1184:THR:HG23	2:CCC:1189:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:788:SER:OG	2:CCC:795:ALA:O	2.20	0.47
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.30	0.47
2:CCC:1100:PRO:CB	3:DDD:639:VAL:HG23	2.45	0.47
2:CCC:339:ASN:O	2:CCC:343:HIS:O	2.33	0.47
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD12	1.97	0.47
5:FFF:263:LEU:HD13	5:FFF:275:ALA:HB2	1.97	0.47
3:DDD:827:GLU:OE1	3:DDD:1242:ARG:HD2	2.15	0.47
3:DDD:832:LYS:CB	3:DDD:1242:ARG:HD3	2.43	0.47
3:DDD:331:ILE:HD12	3:DDD:331:ILE:N	2.29	0.47
3:DDD:1134:ILE:HD13	3:DDD:1244:GLN:HG3	1.95	0.47
3:DDD:584:PRO:HD3	3:DDD:620:PHE:CD1	2.50	0.47
3:DDD:694:SER:OG	3:DDD:738:ARG:HG2	2.15	0.47
7:222:22:DA:H2''	7:222:23:DT:H5'	1.96	0.47
1:BBB:145:LYS:HD3	1:BBB:147:GLN:HE21	1.79	0.47
3:DDD:576:ARG:HD3	3:DDD:593:ASN:HA	1.96	0.47
5:FFF:158:ILE:HG22	7:222:26:DT:O2	2.15	0.47
2:CCC:888:THR:C	2:CCC:913:VAL:HG12	2.35	0.47
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.45	0.46
2:CCC:1103:VAL:HG22	2:CCC:1111:GLN:NE2	2.30	0.46
2:CCC:144:VAL:HB	2:CCC:526:HIS:CE1	2.50	0.46
2:CCC:160:ASP:CG	2:CCC:163:LYS:HB2	2.35	0.46
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.97	0.46
3:DDD:525:MET:C	3:DDD:548:VAL:HG22	2.35	0.46
2:CCC:123:TYR:CE1	5:FFF:190:ASP:O	2.66	0.46
6:111:38:DT:H2''	6:111:39:DA:C8	2.50	0.46
7:222:32:DA:H2''	7:222:33:DC:C6	2.50	0.46
2:CCC:200:ARG:HD2	6:111:50:DT:O2	2.15	0.46
2:CCC:551:HIS:CE1	2:CCC:553:THR:HG1	2.31	0.46
2:CCC:658:GLN:O	2:CCC:661:VAL:HG22	2.15	0.46
2:CCC:228:VAL:O	2:CCC:335:THR:N	2.33	0.46
2:CCC:461:GLU:OE2	2:CCC:465:ARG:NH2	2.48	0.46
3:DDD:846:GLU:CG	3:DDD:860:ARG:HH22	2.26	0.46
2:CCC:1157:GLN:O	2:CCC:1157:GLN:HG3	2.14	0.46
3:DDD:123:ARG:HH22	3:DDD:1334:GLU:HG2	1.79	0.46
3:DDD:849:LEU:HB3	3:DDD:857:LEU:H	1.80	0.46
5:FFF:176:ASN:ND2	7:222:26:DT:H3'	2.29	0.46
6:111:45:DT:H6	6:111:45:DT:H3'	1.80	0.46
2:CCC:850:ILE:HD11	2:CCC:1048:LYS:HG3	1.97	0.46
5:FFF:99:LEU:O	5:FFF:102:VAL:HB	2.15	0.46
1:BBB:160:HIS:CD2	1:BBB:160:HIS:C	2.89	0.46
2:CCC:300:ASP:OD1	2:CCC:313:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:123:ARG:NH2	3:DDD:1334:GLU:HG2	2.31	0.46
2:CCC:600:THR:HB	2:CCC:602:GLU:HG2	1.97	0.46
3:DDD:949:SER:HB2	3:DDD:1016:THR:HG23	1.97	0.46
3:DDD:1128:SER:OG	3:DDD:1128:SER:O	2.31	0.46
3:DDD:1176:VAL:O	3:DDD:1176:VAL:HG12	2.14	0.46
3:DDD:1356:LEU:HA	3:DDD:1356:LEU:HD23	1.79	0.46
3:DDD:849:LEU:CD1	3:DDD:853:THR:HA	2.42	0.46
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.97	0.46
1:AAA:154:PRO:HG2	1:AAA:157:THR:HB	1.98	0.46
1:AAA:221:ALA:HB1	1:BBB:228:LEU:HD22	1.97	0.46
1:BBB:163:GLU:HG3	1:BBB:163:GLU:O	2.16	0.46
2:CCC:800:MET:HE2	2:CCC:800:MET:HB3	1.86	0.46
5:FFF:183:ARG:NH2	7:222:25:DA:OP2	2.49	0.46
7:222:21:DG:H2"	7:222:22:DA:OP2	2.15	0.46
1:BBB:112:ALA:HB1	1:BBB:123:ILE:HG21	1.97	0.46
2:CCC:439:LYS:O	2:CCC:439:LYS:HG3	2.15	0.46
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	1.97	0.46
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.15	0.46
2:CCC:1257:GLN:HB3	2:CCC:1296:ASP:OD1	2.16	0.46
3:DDD:115:TRP:O	3:DDD:119:SER:HB3	2.16	0.46
3:DDD:320:ASN:O	3:DDD:321:LYS:CB	2.49	0.46
3:DDD:474:LEU:HD12	4:EEE:28:ARG:HE	1.81	0.46
2:CCC:1220:GLN:HG2	2:CCC:1221:PHE:N	2.31	0.45
3:DDD:750:PRO:HD3	3:DDD:777:HIS:ND1	2.31	0.45
2:CCC:1172:LEU:O	2:CCC:1176:LEU:HG	2.16	0.45
2:CCC:241:LEU:HD11	2:CCC:246:LEU:HD11	1.99	0.45
5:FFF:119:LEU:HD21	5:FFF:158:ILE:HD11	1.98	0.45
5:FFF:263:LEU:CD1	5:FFF:275:ALA:HB2	2.46	0.45
5:FFF:71:LEU:CD2	5:FFF:79:PHE:HE2	2.30	0.45
7:222:23:DT:C2'	7:222:24:DT:OP2	2.64	0.45
1:AAA:30:PRO:HB2	1:AAA:198:LEU:HD13	1.99	0.45
3:DDD:242:LEU:HD12	3:DDD:243:PRO:HD2	1.98	0.45
1:AAA:56:VAL:O	1:AAA:175:ALA:HB2	2.15	0.45
2:CCC:68:LEU:HD13	2:CCC:100:LEU:HD21	1.97	0.45
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	1.97	0.45
3:DDD:716:GLN:CG	3:DDD:717:VAL:N	2.79	0.45
2:CCC:1142:ARG:NH1	2:CCC:1161:LEU:O	2.49	0.45
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:HE21	1.81	0.45
3:DDD:572:THR:HG21	3:DDD:589:TYR:CE2	2.52	0.45
3:DDD:714:GLU:HG2	3:DDD:715:LYS:N	2.31	0.45
3:DDD:708:ASN:HD21	3:DDD:716:GLN:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:111:31:DT:H2''	6:111:32:DA:H5'	1.98	0.45
2:CCC:591:TYR:OH	2:CCC:637:ARG:NH2	2.50	0.45
2:CCC:889:PRO:N	2:CCC:913:VAL:HG13	2.32	0.45
3:DDD:129:ASP:HB2	3:DDD:220:ARG:NH1	2.31	0.45
3:DDD:790:THR:CG2	3:DDD:932:MET:CG	2.94	0.45
3:DDD:478:LEU:CD2	4:EEE:47:THR:CG2	2.95	0.45
1:BBB:192:VAL:HG12	1:BBB:193:GLU:H	1.82	0.45
2:CCC:1004:ASP:N	2:CCC:1004:ASP:OD1	2.49	0.45
2:CCC:967:LEU:CD2	2:CCC:1021:LEU:HD13	2.35	0.45
2:CCC:19:PRO:HA	2:CCC:1156:ARG:HD2	1.99	0.45
3:DDD:495:ASN:OD1	3:DDD:497:GLU:HB2	2.16	0.45
3:DDD:601:ILE:O	3:DDD:604:MET:HB2	2.16	0.45
3:DDD:926:PRO:O	3:DDD:930:LEU:HG	2.16	0.45
6:111:58:DG:H2''	6:111:59:DG:C8	2.51	0.45
1:BBB:44:ARG:HA	1:BBB:183:ILE:HD13	1.99	0.45
2:CCC:221:LEU:HD22	2:CCC:336:LEU:CD1	2.47	0.45
2:CCC:56:VAL:HG12	2:CCC:59:ILE:HD11	1.98	0.45
3:DDD:1134:ILE:O	3:DDD:1135:THR:C	2.55	0.45
3:DDD:369:PRO:HB2	3:DDD:372:MET:HB2	1.99	0.45
2:CCC:685:MET:SD	2:CCC:1073:LYS:HG2	2.56	0.45
2:CCC:1212:LEU:HD12	2:CCC:1225:VAL:HB	1.99	0.45
2:CCC:533:LEU:HD23	2:CCC:538:LEU:O	2.17	0.45
2:CCC:878:THR:CG2	2:CCC:879:GLY:N	2.80	0.45
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	2.17	0.45
1:AAA:86:LYS:HG2	1:AAA:174:ASP:O	2.17	0.44
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:O	2.17	0.44
3:DDD:747:MET:O	3:DDD:755:ILE:HD12	2.17	0.44
3:DDD:886:VAL:CG1	3:DDD:1226:VAL:CG1	2.95	0.44
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.99	0.44
2:CCC:356:THR:HG21	2:CCC:362:ALA:HA	1.97	0.44
2:CCC:144:VAL:HB	2:CCC:526:HIS:HE1	1.81	0.44
2:CCC:888:THR:C	2:CCC:913:VAL:HG13	2.38	0.44
2:CCC:901:LEU:CD1	5:FFF:310:LEU:HD21	2.39	0.44
2:CCC:741:MET:CG	2:CCC:974:ARG:NH2	2.79	0.44
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.37	0.44
5:FFF:164:THR:HB	5:FFF:219:ILE:HD11	1.99	0.44
5:FFF:170:HIS:NE2	6:111:31:DT:C6	2.86	0.44
2:CCC:322:LEU:HD12	2:CCC:333:ILE:CD1	2.47	0.44
2:CCC:548:ARG:HH11	2:CCC:570:GLY:H	1.66	0.44
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HG12	2.00	0.44
5:FFF:317:LEU:HD23	5:FFF:322:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:64:VAL:CG1	1:BBB:78:ILE:HD13	2.47	0.44
2:CCC:185:ASP:HB2	2:CCC:197:ARG:HG3	1.99	0.44
3:DDD:905:ARG:NH1	3:DDD:910:ASN:OD1	2.51	0.44
1:BBB:47:LEU:HD13	1:BBB:183:ILE:CD1	2.43	0.44
2:CCC:338:THR:CG2	2:CCC:345:PRO:CB	2.89	0.44
2:CCC:696:ASP:HB3	2:CCC:798:GLN:HG2	2.00	0.44
2:CCC:848:GLU:CG	2:CCC:889:PRO:HD2	2.47	0.44
2:CCC:854:ILE:HB	2:CCC:857:VAL:HG21	1.98	0.44
3:DDD:245:LEU:HG	3:DDD:246:PRO:HD2	1.99	0.44
3:DDD:714:GLU:CG	3:DDD:715:LYS:N	2.81	0.44
3:DDD:864:LEU:HD13	3:DDD:869:CYS:SG	2.57	0.44
3:DDD:475:GLU:OE2	4:EEE:28:ARG:NH2	2.50	0.44
2:CCC:374:GLU:OE2	6:111:43:DT:H72	2.18	0.44
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.99	0.44
2:CCC:1124:ILE:HD11	2:CCC:1198:LEU:CD1	2.47	0.44
2:CCC:230:PHE:HB2	2:CCC:333:ILE:HB	2.00	0.44
2:CCC:782:VAL:HG21	2:CCC:792:GLY:HA2	1.98	0.44
3:DDD:1208:ASP:O	3:DDD:1210:ILE:HD13	2.17	0.44
5:FFF:65:ILE:HG13	5:FFF:66:GLY:N	2.33	0.44
6:111:46:DG:C2'	6:111:47:DC:O4'	2.66	0.44
2:CCC:1289:GLU:HG2	2:CCC:1294:LYS:HE3	2.00	0.44
2:CCC:878:THR:HG22	2:CCC:879:GLY:H	1.82	0.44
3:DDD:615:LYS:N	3:DDD:616:PRO:CD	2.81	0.44
6:111:53:DG:C2'	6:111:54:DA:OP2	2.64	0.44
2:CCC:960:LEU:HD11	2:CCC:1032:LYS:HG3	1.99	0.44
3:DDD:325:LYS:CE	3:DDD:330:MET:HG2	2.47	0.44
3:DDD:582:ILE:HG23	3:DDD:623:GLN:CB	2.48	0.44
3:DDD:960:LEU:HB3	3:DDD:963:VAL:HG11	1.98	0.44
3:DDD:294:ASN:ND2	5:FFF:121:GLU:OE2	2.50	0.44
2:CCC:1301:ARG:HG3	2:CCC:1302:THR:N	2.33	0.44
2:CCC:858:GLY:CA	5:FFF:328:PHE:HE1	2.31	0.44
1:AAA:64:VAL:CG1	1:AAA:78:ILE:HD13	2.46	0.43
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CG1	2.48	0.43
2:CCC:225:PHE:CE2	2:CCC:347:ILE:HB	2.53	0.43
3:DDD:645:VAL:O	3:DDD:645:VAL:HG23	2.18	0.43
1:AAA:45:ARG:NH1	2:CCC:1216:ARG:HA	2.34	0.43
2:CCC:290:GLU:HA	2:CCC:319:LEU:HD21	2.00	0.43
3:DDD:1327:GLU:O	3:DDD:1331:VAL:HG23	2.18	0.43
3:DDD:525:MET:CA	3:DDD:548:VAL:CG2	2.93	0.43
5:FFF:151:ARG:HG3	5:FFF:152:GLN:N	2.33	0.43
2:CCC:402:ARG:HD2	2:CCC:406:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:615:LYS:HB2	3:DDD:616:PRO:HD3	2.00	0.43
3:DDD:863:LEU:HD22	3:DDD:908:ILE:CG1	2.48	0.43
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:CG	2.48	0.43
2:CCC:28:LEU:HD21	2:CCC:524:ILE:HG13	2.01	0.43
2:CCC:648:ASP:N	2:CCC:648:ASP:OD1	2.49	0.43
2:CCC:878:THR:CG2	2:CCC:879:GLY:H	2.32	0.43
3:DDD:1087:ASP:N	3:DDD:1087:ASP:OD1	2.51	0.43
3:DDD:262:THR:C	5:FFF:222:VAL:HG23	2.38	0.43
3:DDD:268:LEU:HD13	3:DDD:306:LEU:HA	1.99	0.43
3:DDD:860:ARG:HB3	3:DDD:861:ASN:H	1.52	0.43
3:DDD:927:GLY:O	3:DDD:931:THR:OG1	2.33	0.43
3:DDD:460:ASP:OD1	3:DDD:460:ASP:N	2.49	0.43
3:DDD:464:ASP:OD1	8:333:16:G:O2'	2.28	0.43
1:AAA:210:THR:O	1:AAA:211:ILE:O	2.36	0.43
5:FFF:181:THR:O	5:FFF:185:LEU:HG	2.17	0.43
2:CCC:1005:GLU:HG2	2:CCC:1006:GLU:N	2.29	0.43
2:CCC:20:GLN:O	2:CCC:20:GLN:HG3	2.19	0.43
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	2.01	0.43
1:AAA:31:LEU:HD11	1:AAA:201:LEU:CB	2.49	0.43
2:CCC:1129:ASN:OD1	2:CCC:1177:ARG:NH2	2.47	0.43
2:CCC:887:VAL:HG12	2:CCC:916:SER:H	1.83	0.43
3:DDD:525:MET:O	3:DDD:548:VAL:HG22	2.18	0.43
3:DDD:1011:VAL:HG11	3:DDD:1017:VAL:HG12	2.01	0.43
3:DDD:426:ALA:HA	3:DDD:427:PRO:HA	1.82	0.43
3:DDD:553:THR:CG2	3:DDD:567:THR:OG1	2.67	0.43
3:DDD:836:ARG:NH1	3:DDD:870:ASP:OD1	2.52	0.43
3:DDD:864:LEU:HD23	3:DDD:864:LEU:HA	1.84	0.43
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:HG3	2.00	0.43
2:CCC:984:VAL:O	2:CCC:984:VAL:HG13	2.18	0.43
5:FFF:134:PHE:CD1	5:FFF:142:PHE:HD1	2.37	0.43
2:CCC:900:LYS:HE2	5:FFF:277:ARG:HH12	1.82	0.42
2:CCC:1331:ARG:HD3	3:DDD:33:TRP:CZ2	2.53	0.42
3:DDD:502:PRO:HB3	3:DDD:506:VAL:HG11	2.01	0.42
5:FFF:318:GLN:HA	5:FFF:323:ASN:HB2	2.01	0.42
1:AAA:10:LYS:HG2	1:BBB:226:GLU:O	2.18	0.42
1:BBB:22:THR:HG23	1:BBB:23:HIS:N	2.34	0.42
2:CCC:145:ILE:HD11	2:CCC:506:PHE:CD2	2.54	0.42
2:CCC:22:LEU:HB3	2:CCC:655:VAL:HG11	2.01	0.42
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:HA	2.00	0.42
3:DDD:378:LYS:HE2	3:DDD:382:TYR:OH	2.19	0.42
3:DDD:478:LEU:HD21	4:EEE:47:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:228:LEU:HA	1:AAA:231:PHE:CD2	2.55	0.42
2:CCC:195:PHE:CD2	2:CCC:203:LYS:HD3	2.54	0.42
2:CCC:228:VAL:CG2	2:CCC:337:PHE:HB2	2.49	0.42
2:CCC:21:VAL:HG21	2:CCC:592:ARG:CZ	2.50	0.42
2:CCC:807:TRP:CZ3	2:CCC:1086:PRO:HG3	2.54	0.42
3:DDD:1134:ILE:O	3:DDD:1137:GLY:N	2.46	0.42
2:CCC:660:VAL:HG11	3:DDD:769:VAL:HG13	2.00	0.42
4:EEE:41:GLU:HG3	4:EEE:43:ASN:H	1.84	0.42
5:FFF:170:HIS:HE1	6:111:32:DA:N7	2.16	0.42
7:222:20:DG:H2"	7:222:21:DG:OP2	2.18	0.42
2:CCC:1109:ILE:O	2:CCC:1109:ILE:HG22	2.19	0.42
2:CCC:453:ILE:HD12	2:CCC:587:LEU:CD2	2.50	0.42
3:DDD:1078:LEU:HD12	3:DDD:1121:LEU:HB3	2.02	0.42
3:DDD:364:HIS:HB3	3:DDD:487:THR:CG2	2.49	0.42
3:DDD:490:ILE:HD11	3:DDD:614:LEU:HD13	2.00	0.42
3:DDD:739:GLN:HG3	3:DDD:744:ARG:HD2	2.01	0.42
5:FFF:152:GLN:HE22	5:FFF:156:ARG:HD3	1.83	0.42
2:CCC:1159:VAL:HG22	2:CCC:1159:VAL:O	2.18	0.42
2:CCC:144:VAL:HG23	2:CCC:515:MET:HB2	2.02	0.42
2:CCC:525:THR:CG2	2:CCC:687:ARG:HD2	2.48	0.42
3:DDD:430:HIS:CD2	3:DDD:432:LEU:HB2	2.54	0.42
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	2.02	0.42
5:FFF:217:GLU:HA	5:FFF:217:GLU:OE1	2.20	0.42
6:111:49:DG:H4'	6:111:50:DT:OP1	2.19	0.42
2:CCC:1291:LEU:CD1	3:DDD:1351:VAL:HG13	2.49	0.42
2:CCC:194:LEU:HA	2:CCC:194:LEU:HD12	1.85	0.42
2:CCC:68:LEU:HD23	2:CCC:102:LEU:HA	2.01	0.42
6:111:51:DC:H2"	6:111:52:DT:O5'	2.19	0.42
2:CCC:518:ASN:O	2:CCC:519:ASN:HB2	2.18	0.42
2:CCC:942:ASP:O	2:CCC:946:LEU:HG	2.20	0.42
3:DDD:1053:LEU:HD23	3:DDD:1053:LEU:HA	1.91	0.42
3:DDD:295:GLU:OE1	5:FFF:121:GLU:HG3	2.20	0.42
3:DDD:452:LEU:HB3	3:DDD:500:ILE:HG23	2.02	0.42
2:CCC:1119:MET:HG2	2:CCC:1204:LEU:HD13	2.00	0.42
3:DDD:1050:THR:HG22	3:DDD:1051:ASP:N	2.35	0.42
3:DDD:147:ILE:HD11	3:DDD:179:LYS:HB2	2.01	0.42
3:DDD:582:ILE:HD12	3:DDD:623:GLN:HB3	2.01	0.42
3:DDD:846:GLU:HA	3:DDD:860:ARG:NH2	2.35	0.42
1:AAA:195:ARG:HG2	1:AAA:198:LEU:CG	2.48	0.42
1:AAA:86:LYS:HE2	1:AAA:174:ASP:H	1.85	0.42
2:CCC:241:LEU:CD2	2:CCC:277:LEU:CD2	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:839:VAL:HG13	2:CCC:839:VAL:O	2.20	0.42
3:DDD:133:ARG:O	3:DDD:137:ARG:HG3	2.20	0.42
3:DDD:67:ASP:OD1	3:DDD:95:THR:HG22	2.20	0.42
3:DDD:644:MET:CE	3:DDD:740:LEU:HB3	2.50	0.42
5:FFF:65:ILE:HG22	5:FFF:99:LEU:CD1	2.49	0.42
6:111:34:DG:C2	7:222:30:DA:C2	3.08	0.42
2:CCC:1075:VAL:HG21	3:DDD:463:GLY:HA2	2.02	0.42
2:CCC:277:LEU:HD12	2:CCC:282:VAL:HG21	2.01	0.42
3:DDD:975:ILE:HD11	3:DDD:1003:LEU:HG	2.02	0.42
5:FFF:148:TRP:O	5:FFF:152:GLN:HB3	2.19	0.42
5:FFF:190:ASP:CG	5:FFF:191:HIS:N	2.72	0.42
6:111:45:DT:O3'	6:111:46:DG:C4'	2.67	0.41
3:DDD:1268:ASN:OD1	3:DDD:1269:ALA:N	2.53	0.41
3:DDD:591:ILE:HD11	3:DDD:604:MET:HA	2.02	0.41
5:FFF:170:HIS:O	5:FFF:174:GLU:HG2	2.19	0.41
5:FFF:54:VAL:HG13	5:FFF:59:GLN:OE1	2.19	0.41
2:CCC:819:SER:HB2	2:CCC:1085:MET:HG3	2.01	0.41
2:CCC:848:GLU:CG	2:CCC:888:THR:HG22	2.48	0.41
4:EEE:30:MET:HE1	4:EEE:37:PRO:HB3	2.02	0.41
5:FFF:155:GLU:O	5:FFF:159:MET:HG3	2.19	0.41
7:222:13:DA:C2'	7:222:14:DC:H5'	2.46	0.41
2:CCC:123:TYR:CG	5:FFF:190:ASP:HA	2.55	0.41
2:CCC:61:SER:CB	2:CCC:479:LEU:HB3	2.51	0.41
2:CCC:615:VAL:O	2:CCC:615:VAL:HG13	2.19	0.41
3:DDD:1366:HIS:O	3:DDD:1370:MET:HG2	2.20	0.41
2:CCC:812:PHE:HB3	3:DDD:357:VAL:HG11	2.02	0.41
3:DDD:612:LEU:HB3	3:DDD:616:PRO:HG2	2.02	0.41
5:FFF:98:ASN:ND2	5:FFF:142:PHE:CE2	2.89	0.41
2:CCC:253:PHE:CE2	2:CCC:287:VAL:HG12	2.54	0.41
2:CCC:634:VAL:HG12	2:CCC:636:CYS:SG	2.60	0.41
3:DDD:1155:ILE:HG13	3:DDD:1194:ARG:NH2	2.36	0.41
3:DDD:865:HIS:H	3:DDD:868:TRP:HD1	1.69	0.41
3:DDD:868:TRP:HE3	3:DDD:871:LEU:HD12	1.84	0.41
6:111:56:DG:H2''	6:111:57:DC:C6	2.56	0.41
1:BBB:22:THR:O	1:BBB:206:GLU:HA	2.21	0.41
2:CCC:1146:GLN:HB2	2:CCC:1161:LEU:HD12	2.02	0.41
2:CCC:619:ALA:HB2	2:CCC:654:ASP:HB2	2.01	0.41
3:DDD:1075:ARG:CD	3:DDD:1193:TRP:HB3	2.50	0.41
2:CCC:57:PHE:CE2	2:CCC:100:LEU:HD11	2.56	0.41
2:CCC:737:ASN:O	2:CCC:741:MET:HB2	2.21	0.41
3:DDD:1069:ALA:HA	3:DDD:1072:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:327:LEU:HD23	5:FFF:327:LEU:C	2.41	0.41
2:CCC:1151:LEU:HD22	2:CCC:1198:LEU:HD12	2.03	0.41
2:CCC:582:ASN:HB3	2:CCC:586:PHE:H	1.85	0.41
2:CCC:59:ILE:CG2	2:CCC:476:LYS:HE3	2.50	0.41
3:DDD:552:ILE:HG13	3:DDD:589:TYR:CE1	2.55	0.41
3:DDD:843:VAL:HG21	3:DDD:897:HIS:HA	2.02	0.41
5:FFF:170:HIS:CE1	6:111:32:DA:N7	2.89	0.41
6:111:57:DC:C2'	6:111:58:DG:OP2	2.63	0.41
1:AAA:150:ARG:NH1	1:BBB:7:GLU:H	2.18	0.41
2:CCC:242:VAL:HA	2:CCC:243:PRO:HD2	1.88	0.41
3:DDD:1364:ALA:O	3:DDD:1367:GLN:HG2	2.21	0.41
3:DDD:505:ASP:OD1	3:DDD:505:ASP:N	2.53	0.41
2:CCC:1046:VAL:HG11	2:CCC:1049:ILE:HD11	2.03	0.41
3:DDD:609:TYR:HA	3:DDD:617:THR:CG2	2.48	0.41
2:CCC:1107:MET:HG2	3:DDD:740:LEU:HD21	2.02	0.41
3:DDD:803:VAL:CG1	3:DDD:803:VAL:O	2.66	0.41
3:DDD:790:THR:CG2	3:DDD:932:MET:HG3	2.51	0.41
7:222:22:DA:H1'	7:222:23:DT:H5'	2.03	0.41
1:BBB:49:SER:O	1:BBB:151:GLY:CA	2.69	0.41
3:DDD:1025:MET:CB	3:DDD:1126:GLN:HE21	2.33	0.41
3:DDD:519:ASN:OD1	3:DDD:520:ALA:N	2.46	0.41
3:DDD:858:VAL:HG12	3:DDD:859:PRO:CD	2.51	0.41
5:FFF:166:ARG:NH1	5:FFF:168:PRO:HA	2.29	0.41
5:FFF:169:ILE:CG2	5:FFF:173:LYS:HD2	2.51	0.41
1:BBB:205:MET:HE1	1:BBB:217:ILE:HG13	2.01	0.41
1:AAA:228:LEU:HD11	1:BBB:224:LEU:HG	2.03	0.41
2:CCC:967:LEU:CD2	2:CCC:1021:LEU:HD22	2.50	0.41
2:CCC:868:SER:OG	2:CCC:944:ARG:N	2.51	0.41
3:DDD:975:ILE:HD12	3:DDD:1001:ALA:HB3	2.02	0.41
3:DDD:429:LEU:HD23	3:DDD:429:LEU:HA	1.93	0.41
3:DDD:478:LEU:HG	4:EEE:47:THR:CG2	2.50	0.41
3:DDD:816:THR:HG22	3:DDD:818:GLU:H	1.86	0.41
3:DDD:923:ILE:HD12	3:DDD:1256:ILE:HD13	2.03	0.41
6:111:48:DA:H2'	6:111:49:DG:O4'	2.21	0.40
1:AAA:58:GLU:OE1	1:AAA:170:ARG:NE	2.49	0.40
2:CCC:1149:TYR:HB3	2:CCC:1159:VAL:HG13	2.01	0.40
2:CCC:858:GLY:HA2	5:FFF:328:PHE:HE1	1.86	0.40
3:DDD:395:LYS:HD3	5:FFF:329:LEU:HD13	2.02	0.40
3:DDD:646:ILE:HD11	3:DDD:764:ARG:HD3	2.03	0.40
4:EEE:30:MET:HB3	4:EEE:30:MET:HE2	1.84	0.40
1:AAA:190:ALA:HB2	1:AAA:199:ASP:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.21	0.40
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.83	0.40
3:DDD:478:LEU:CD2	4:EEE:47:THR:HG23	2.51	0.40
3:DDD:570:LYS:HG3	3:DDD:589:TYR:CD2	2.56	0.40
6:111:27:DC:N4	7:222:36:DG:H1	2.08	0.40
1:AAA:112:ALA:HB1	1:AAA:123:ILE:HG21	2.02	0.40
1:AAA:158:ARG:HB3	1:AAA:172:LEU:CD2	2.48	0.40
1:AAA:162:GLU:HB2	1:AAA:163:GLU:H	1.63	0.40
2:CCC:1149:TYR:CD1	2:CCC:1159:VAL:HG11	2.57	0.40
3:DDD:398:LYS:HE2	3:DDD:402:GLU:HG3	2.02	0.40
3:DDD:552:ILE:HG21	3:DDD:589:TYR:CD1	2.56	0.40
3:DDD:650:LYS:HE3	3:DDD:654:ILE:HD12	2.03	0.40
3:DDD:963:VAL:HG23	3:DDD:975:ILE:HG23	2.03	0.40
1:AAA:22:THR:HG23	1:AAA:23:HIS:N	2.36	0.40
2:CCC:228:VAL:O	2:CCC:335:THR:OG1	2.35	0.40
2:CCC:519:ASN:ND2	2:CCC:796:LEU:HD22	2.37	0.40
3:DDD:305:ALA:CB	3:DDD:316:ILE:HD12	2.52	0.40
3:DDD:660:GLU:HG3	3:DDD:685:ILE:HD13	2.02	0.40
2:CCC:1107:MET:HE2	3:DDD:739:GLN:CB	2.46	0.40
5:FFF:63:GLY:O	5:FFF:67:TYR:CD2	2.74	0.40

All (1) 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)
1:BBB:166:ARG:NH2	3:DDD:1055:GLY:O[4_445]	1.99	0.21

## 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	AAA	228/242 (94%)	204 (90%)	20 (9%)	4 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	226/242 (93%)	211 (93%)	13 (6%)	2 (1%)	17	53
2	CCC	1338/1342 (100%)	1243 (93%)	84 (6%)	11 (1%)	19	56
3	DDD	1360/1407 (97%)	1261 (93%)	81 (6%)	18 (1%)	12	46
4	EEE	77/90 (86%)	74 (96%)	3 (4%)	0	100	100
5	FFF	275/336 (82%)	256 (93%)	16 (6%)	3 (1%)	14	50
All	All	3504/3659 (96%)	3249 (93%)	217 (6%)	38 (1%)	14	50

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	192	VAL
3	DDD	174	ASP
3	DDD	519	ASN
3	DDD	710	ASP
3	DDD	861	ASN
3	DDD	1053	LEU
3	DDD	1132	LYS
3	DDD	1135	THR
3	DDD	1268	ASN
5	FFF	190	ASP
2	CCC	756	TYR
2	CCC	894	GLN
3	DDD	829	GLY
3	DDD	947	GLU
1	BBB	8	PHE
1	BBB	232	VAL
2	CCC	1137	GLU
2	CCC	1297	ASP
3	DDD	321	LYS
1	AAA	208	ASN
1	AAA	210	THR
1	AAA	211	ILE
2	CCC	986	ALA
2	CCC	1103	VAL
3	DDD	49	PHE
3	DDD	805	GLN
3	DDD	860	ARG
5	FFF	228	GLY
2	CCC	45	GLY
3	DDD	846	GLU

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Mol	Chain	Res	Type
3	DDD	854	ALA
2	CCC	507	GLY
2	CCC	43	PRO
2	CCC	112	GLY
2	CCC	519	ASN
3	DDD	1091	PRO
3	DDD	828	GLY
5	FFF	295	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	AAA	198/208 (95%)	189 (96%)	9 (4%)	27	55
1	BBB	196/208 (94%)	188 (96%)	8 (4%)	30	57
2	CCC	1155/1157 (100%)	1124 (97%)	31 (3%)	44	67
3	DDD	1135/1168 (97%)	1094 (96%)	41 (4%)	35	61
4	EEE	67/74 (90%)	65 (97%)	2 (3%)	41	64
5	FFF	240/292 (82%)	232 (97%)	8 (3%)	38	63
All	All	2991/3107 (96%)	2892 (97%)	99 (3%)	38	63

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	12	ARG
1	AAA	28	LEU
1	AAA	32	GLU
1	AAA	70	THR
1	AAA	131	CYS
1	AAA	157	THR
1	AAA	166	ARG
1	AAA	173	VAL
1	AAA	176	CYS
1	BBB	12	ARG

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Mol	Chain	Res	Type
1	BBB	28	LEU
1	BBB	32	GLU
1	BBB	70	THR
1	BBB	131	CYS
1	BBB	159	ILE
1	BBB	197	ASP
1	BBB	198	LEU
2	CCC	12	ARG
2	CCC	23	ASP
2	CCC	30	ILE
2	CCC	70	TYR
2	CCC	290	GLU
2	CCC	338	THR
2	CCC	368	ARG
2	CCC	412	GLU
2	CCC	443	ASP
2	CCC	538	LEU
2	CCC	553	THR
2	CCC	554	HIS
2	CCC	561	ILE
2	CCC	571	LEU
2	CCC	653	MET
2	CCC	657	THR
2	CCC	697	LYS
2	CCC	700	VAL
2	CCC	851	THR
2	CCC	886	LYS
2	CCC	887	VAL
2	CCC	913	VAL
2	CCC	914	LYS
2	CCC	1078	LYS
2	CCC	1089	GLU
2	CCC	1159	VAL
2	CCC	1207	SER
2	CCC	1223	ARG
2	CCC	1250	SER
2	CCC	1273	MET
2	CCC	1299	ASN
3	DDD	93	THR
3	DDD	99	ARG
3	DDD	153	ASN
3	DDD	216	LYS

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Mol	Chain	Res	Type
3	DDD	223	LEU
3	DDD	227	PHE
3	DDD	240	THR
3	DDD	256	ASP
3	DDD	298	MET
3	DDD	321	LYS
3	DDD	384	LYS
3	DDD	398	LYS
3	DDD	399	LYS
3	DDD	417	ARG
3	DDD	453	VAL
3	DDD	505	ASP
3	DDD	536	LEU
3	DDD	538	ARG
3	DDD	547	ARG
3	DDD	548	VAL
3	DDD	579	LEU
3	DDD	599	LYS
3	DDD	619	ILE
3	DDD	641	ILE
3	DDD	695	LYS
3	DDD	736	GLN
3	DDD	738	ARG
3	DDD	746	LEU
3	DDD	798	ARG
3	DDD	830	ASP
3	DDD	849	LEU
3	DDD	860	ARG
3	DDD	867	GLN
3	DDD	943	ARG
3	DDD	1108	GLN
3	DDD	1165	PHE
3	DDD	1175	LEU
3	DDD	1180	VAL
3	DDD	1189	MET
3	DDD	1199	PHE
3	DDD	1227	HIS
4	EEE	43	ASN
4	EEE	45	LYS
5	FFF	107	ARG
5	FFF	152	GLN
5	FFF	156	ARG

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Mol	Chain	Res	Type
5	FFF	241	GLU
5	FFF	244	ASN
5	FFF	259	ILE
5	FFF	265	GLU
5	FFF	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	1/4 (25%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	16	G

There are no RNA pucker outliers to report.

## 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 monosaccharides 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	$\# Z  > 2$
11	DPO	DDD	1504	-	6,8,8	0.75	0	13,13,13	1.53	1 (7%)

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
11	DPO	DDD	1504	-	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	DDD	1504	DPO	P2-O4-P1	-4.60	117.04	132.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	DDD	1504	DPO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	333	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	333	16:G	O3'	17:U	P	3.64

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	230/242 (95%)	0.08	7 (3%) 50 39	179, 261, 332, 374	0
1	BBB	228/242 (94%)	0.09	17 (7%) 14 11	181, 267, 336, 412	0
2	CCC	1340/1342 (99%)	-0.01	32 (2%) 59 49	135, 229, 361, 488	0
3	DDD	1362/1407 (96%)	0.18	94 (6%) 16 12	124, 243, 361, 437	0
4	EEE	79/90 (87%)	-0.07	6 (7%) 13 10	196, 282, 469, 527	0
5	FFF	277/336 (82%)	0.26	25 (9%) 9 7	155, 272, 410, 502	0
6	111	33/50 (66%)	-0.22	2 (6%) 21 16	226, 286, 414, 428	0
7	222	35/50 (70%)	-0.37	0 100 100	175, 280, 384, 460	0
8	333	3/4 (75%)	0.92	0 100 100	176, 176, 176, 210	0
All	All	3587/3763 (95%)	0.09	183 (5%) 28 24	124, 246, 370, 527	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	1130	GLY	17.7
5	FFF	291	VAL	9.3
5	FFF	310	LEU	7.9
5	FFF	290	ASP	6.2
3	DDD	879	ALA	5.9
5	FFF	263	LEU	5.8
3	DDD	1121	LEU	5.7
3	DDD	1068	THR	5.7
3	DDD	958	ILE	5.3
3	DDD	944	ALA	5.3
3	DDD	1065	ALA	5.2
5	FFF	302	VAL	5.2
3	DDD	941	ALA	5.0
2	CCC	939	VAL	4.9
3	DDD	960	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	CCC	169	LYS	4.6
3	DDD	1030	GLU	4.6
3	DDD	982	LEU	4.5
3	DDD	1078	LEU	4.5
2	CCC	998	LEU	4.4
3	DDD	1066	GLU	4.3
2	CCC	1004	ASP	4.3
3	DDD	997	VAL	4.3
4	EEE	79	GLU	4.2
3	DDD	1129	GLY	4.2
3	DDD	1099	TYR	4.2
2	CCC	940	GLU	4.2
3	DDD	382	TYR	4.2
2	CCC	1180	MET	4.1
5	FFF	280	LEU	4.0
3	DDD	1098	GLN	4.0
1	AAA	144	ILE	4.0
5	FFF	309	GLY	3.9
3	DDD	856	ILE	3.9
5	FFF	303	ARG	3.9
3	DDD	1069	ALA	3.8
5	FFF	285	ALA	3.8
2	CCC	986	ALA	3.8
3	DDD	1109	LEU	3.8
3	DDD	976	THR	3.7
3	DDD	1131	THR	3.7
3	DDD	216	LYS	3.7
3	DDD	91	GLU	3.7
3	DDD	1076	PRO	3.7
3	DDD	940	ALA	3.6
3	DDD	1028	ILE	3.6
3	DDD	1376	GLY	3.6
3	DDD	1185	PRO	3.6
1	BBB	133	LEU	3.6
1	BBB	201	LEU	3.6
3	DDD	1166	GLY	3.6
5	FFF	259	ILE	3.5
3	DDD	1122	ALA	3.5
3	DDD	1054	THR	3.5
1	BBB	90	VAL	3.4
5	FFF	53	ARG	3.4
3	DDD	945	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
3	DDD	992	LYS	3.3
5	FFF	283	TYR	3.3
5	FFF	287	THR	3.3
5	FFF	295	ILE	3.3
2	CCC	493	ILE	3.3
2	CCC	975	ILE	3.3
2	CCC	124	MET	3.3
3	DDD	76	LYS	3.2
1	BBB	160	HIS	3.1
3	DDD	942	SER	3.1
4	EEE	78	ALA	3.1
2	CCC	1054	LEU	3.1
3	DDD	983	LYS	3.1
1	AAA	51	MET	3.0
3	DDD	1029	THR	3.0
3	DDD	1123	ARG	3.0
5	FFF	288	LEU	3.0
3	DDD	212	THR	3.0
2	CCC	261	VAL	3.0
2	CCC	883	LEU	3.0
3	DDD	880	VAL	2.9
2	CCC	1159	VAL	2.9
1	BBB	168	ILE	2.9
5	FFF	294	GLU	2.9
5	FFF	110	GLY	2.9
3	DDD	75	TYR	2.9
6	111	45	DT	2.9
2	CCC	938	GLY	2.9
3	DDD	1017	VAL	2.9
3	DDD	1051	ASP	2.9
3	DDD	1266	ILE	2.9
3	DDD	1075	ARG	2.8
3	DDD	995	TYR	2.8
3	DDD	1035	VAL	2.8
5	FFF	289	GLU	2.8
2	CCC	94	ALA	2.8
2	CCC	127	ILE	2.7
1	BBB	98	VAL	2.7
3	DDD	1053	LEU	2.7
3	DDD	952	VAL	2.7
2	CCC	1055	ALA	2.7
3	DDD	993	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
4	EEE	76	GLU	2.6
4	EEE	2	ALA	2.6
3	DDD	1187	GLU	2.6
3	DDD	957	SER	2.6
3	DDD	80	HIS	2.6
3	DDD	977	SER	2.6
2	CCC	230	PHE	2.6
3	DDD	1115	ILE	2.6
5	FFF	74	GLU	2.5
3	DDD	1101	LEU	2.5
2	CCC	492	MET	2.5
3	DDD	1038	THR	2.5
3	DDD	1190	ILE	2.5
3	DDD	969	SER	2.5
1	BBB	144	ILE	2.5
3	DDD	1124	ILE	2.5
1	BBB	74	VAL	2.5
1	BBB	131	CYS	2.5
1	BBB	107	ILE	2.5
3	DDD	1040	MET	2.4
3	DDD	1120	THR	2.4
1	AAA	135	ASP	2.4
3	DDD	92	VAL	2.4
3	DDD	986	ASP	2.4
3	DDD	1203	ARG	2.4
3	DDD	854	ALA	2.4
3	DDD	959	LYS	2.4
3	DDD	1004	ALA	2.4
5	FFF	293	ARG	2.4
2	CCC	870	ILE	2.4
3	DDD	855	ASP	2.4
1	BBB	164	ASP	2.4
3	DDD	996	LYS	2.4
1	BBB	142	MET	2.4
2	CCC	239	MET	2.3
5	FFF	111	ASN	2.3
1	BBB	203	ILE	2.3
3	DDD	939	GLY	2.3
2	CCC	696	ASP	2.3
3	DDD	853	THR	2.3
2	CCC	385	PHE	2.3
2	CCC	333	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	130	ILE	2.3
6	111	46	DG	2.3
3	DDD	1077	ALA	2.3
5	FFF	305	ILE	2.3
3	DDD	1128	SER	2.2
3	DDD	951	GLN	2.2
3	DDD	1167	LYS	2.2
5	FFF	273	VAL	2.2
3	DDD	954	ASN	2.2
1	BBB	28	LEU	2.2
3	DDD	984	LEU	2.2
3	DDD	732	GLY	2.2
3	DDD	1052	GLU	2.2
1	AAA	133	LEU	2.2
3	DDD	830	ASP	2.2
3	DDD	1097	ALA	2.1
4	EEE	75	GLN	2.1
2	CCC	241	LEU	2.1
1	AAA	134	THR	2.1
3	DDD	1049	GLN	2.1
2	CCC	721	GLY	2.1
3	DDD	964	LYS	2.1
3	DDD	991	THR	2.1
1	BBB	123	ILE	2.1
3	DDD	1186	TYR	2.1
3	DDD	1189	MET	2.1
4	EEE	80	LEU	2.1
5	FFF	313	LEU	2.1
2	CCC	1010	GLN	2.1
5	FFF	306	GLN	2.1
2	CCC	113	THR	2.1
3	DDD	381	ILE	2.1
2	CCC	795	ALA	2.1
3	DDD	68	TYR	2.1
3	DDD	1039	ASP	2.0
1	AAA	52	PRO	2.0
3	DDD	1011	VAL	2.0
1	BBB	200	LYS	2.0
2	CCC	941	LYS	2.0
3	DDD	980	THR	2.0
1	AAA	96	ASP	2.0
2	CCC	240	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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
9	MG	CCC	1401	1/1	0.27	0.43	138,138,138,138	0
11	DPO	DDD	1504	9/9	0.89	0.44	153,178,187,193	0
9	MG	DDD	1503	1/1	0.90	0.23	105,105,105,105	0
10	ZN	DDD	1501	1/1	0.96	0.04	298,298,298,298	0
10	ZN	DDD	1502	1/1	0.99	0.15	228,228,228,228	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.