Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 11:08 PM EDT

PDB ID	:	6UU1
Title	:	E. coli sigma-S transcription initiation complex with a 4-nt RNA and a CTP ("Fresh" crystal soaked with CTP, GTP, and ddTTP for 30 minutes)
Authors	:	Zuo, Y.; De, S.; Steitz, T.A.
Deposited on	:	2019-10-30
Resolution	:	4.10 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 (i) 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 (i)) were used in the production of this report:

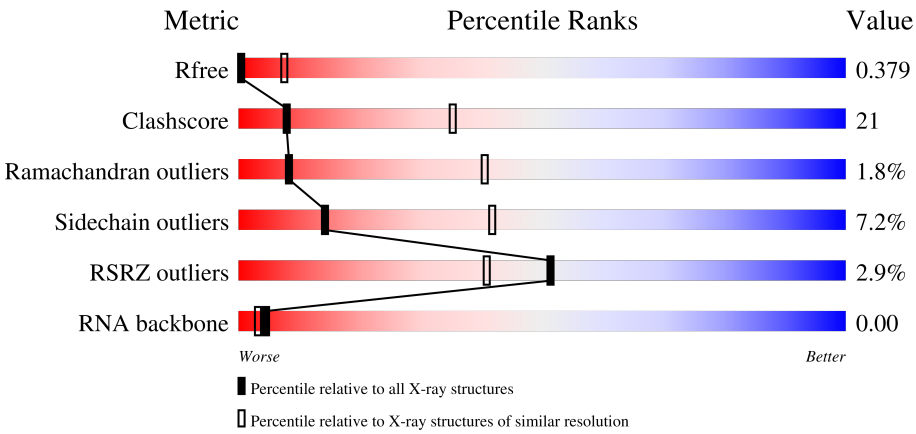
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)
RNA backbone	3102	1049 (5.04-3.00)

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 <=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	5% 62% 29% • 5%
1	BBB	242	5% 62% 29% • 6%
2	CCC	1342	2% 64% 33% •
3	DDD	1407	2% 58% 35% • •

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Mol	Chain	Length	Quality of chain
4	EEE	90	%, 60%, 26%, 12%
5	FFF	336	6%, 50%, 30%, 18%
6	111	50	6%, 30%, 30%, 40%
7	222	50	8%, 22%, 50%, 28%
8	333	4	50%, 50%

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
11	CTP	333	201	-	-	X	-
9	ZN	DDD	1502	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29064 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
			Total	C	N	O	S			
1	AAA	230	1787	1112	317	352	6	0	0	0
1	BBB	228	1767	1100	312	349	6	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP A0A377D9Q8
AAA	-5	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-4	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-3	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-2	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-1	HIS	-	expression tag	UNP A0A377D9Q8
AAA	0	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-6	ALA	-	expression tag	UNP A0A377D9Q8
BBB	-5	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-4	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-3	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-2	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-1	HIS	-	expression tag	UNP A0A377D9Q8
BBB	0	HIS	-	expression tag	UNP A0A377D9Q8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	CCC	1341	10576	6636	1842	2055	43	0	0	0

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

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

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

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

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

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

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
			Total	C	N	O	P			
6	111	30	619	294	114	181	30	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	222	36	738	352	137	214	35	0	0	0

- Molecule 8 is a RNA chain called RNA 4-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	333	4	96	40	17	33	6	0	0	0

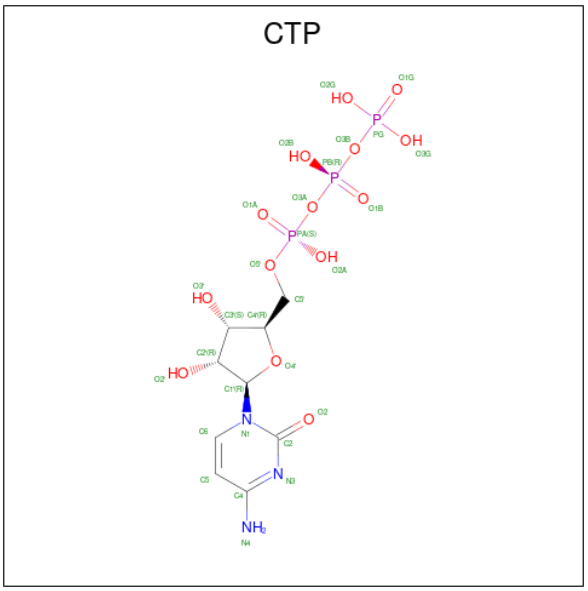
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



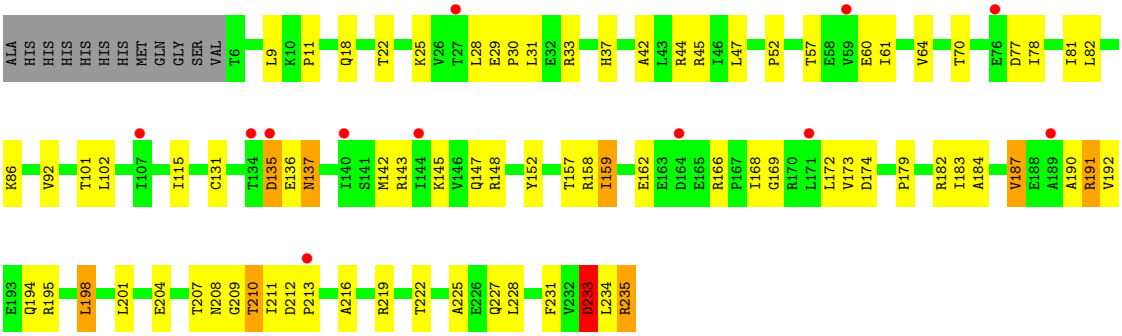
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	333	1	29	9	3	14	3	0	0

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.

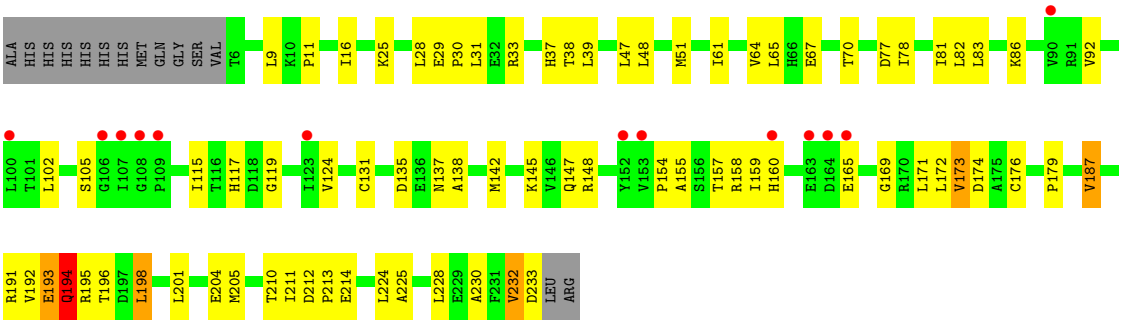
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain AAA:



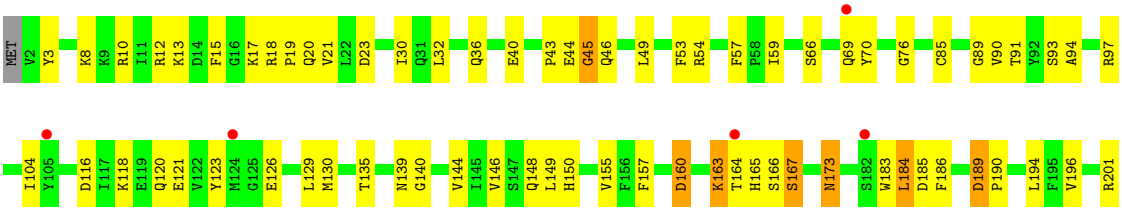
• Molecule 1: DNA-directed RNA polymerase subunit alpha

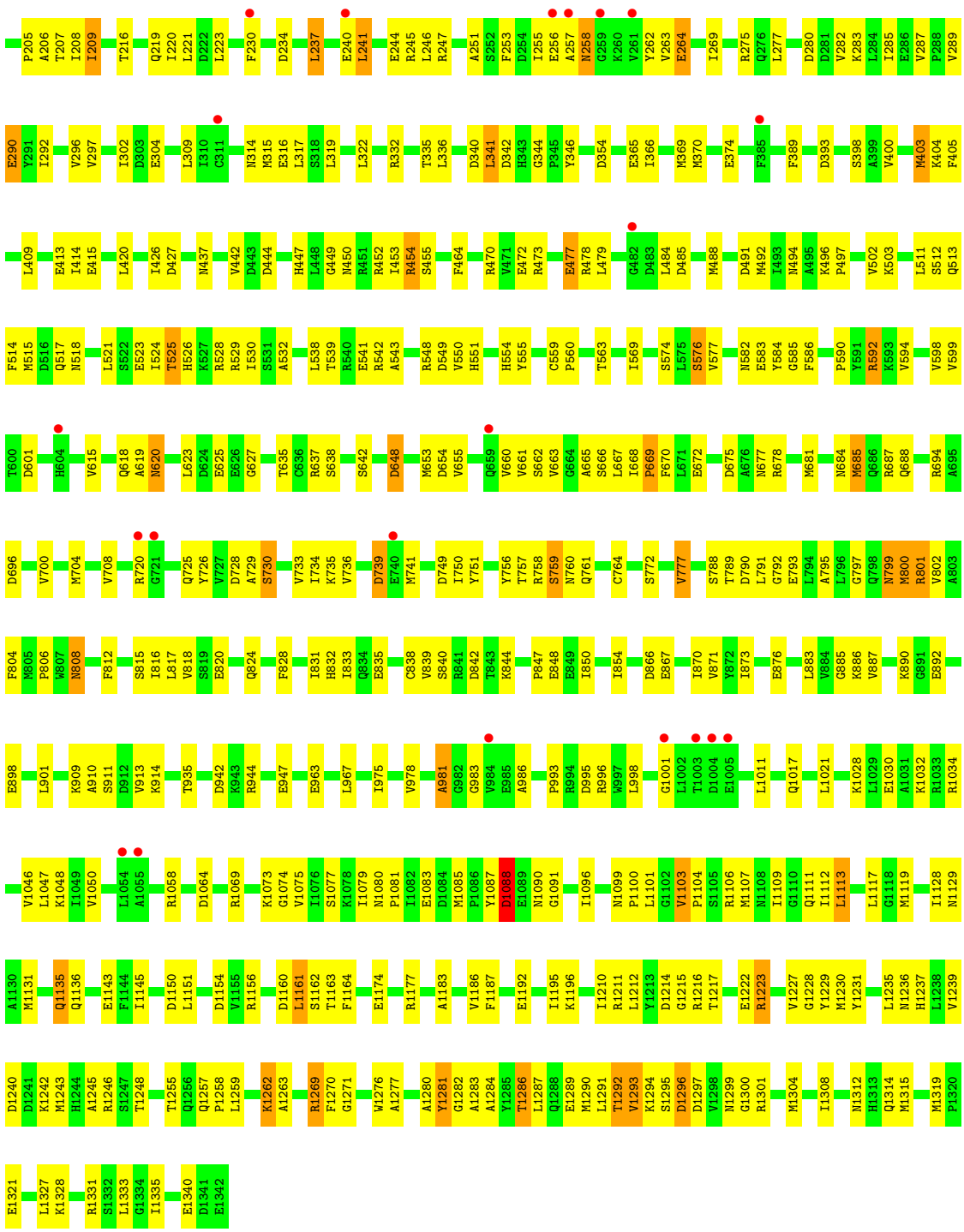
Chain BBB:



• Molecule 2: DNA-directed RNA polymerase subunit beta

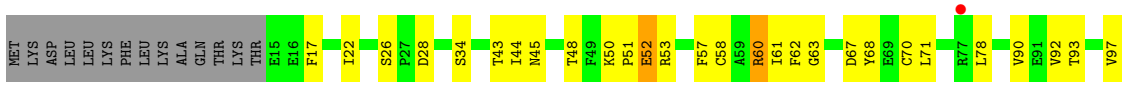
Chain CCC:

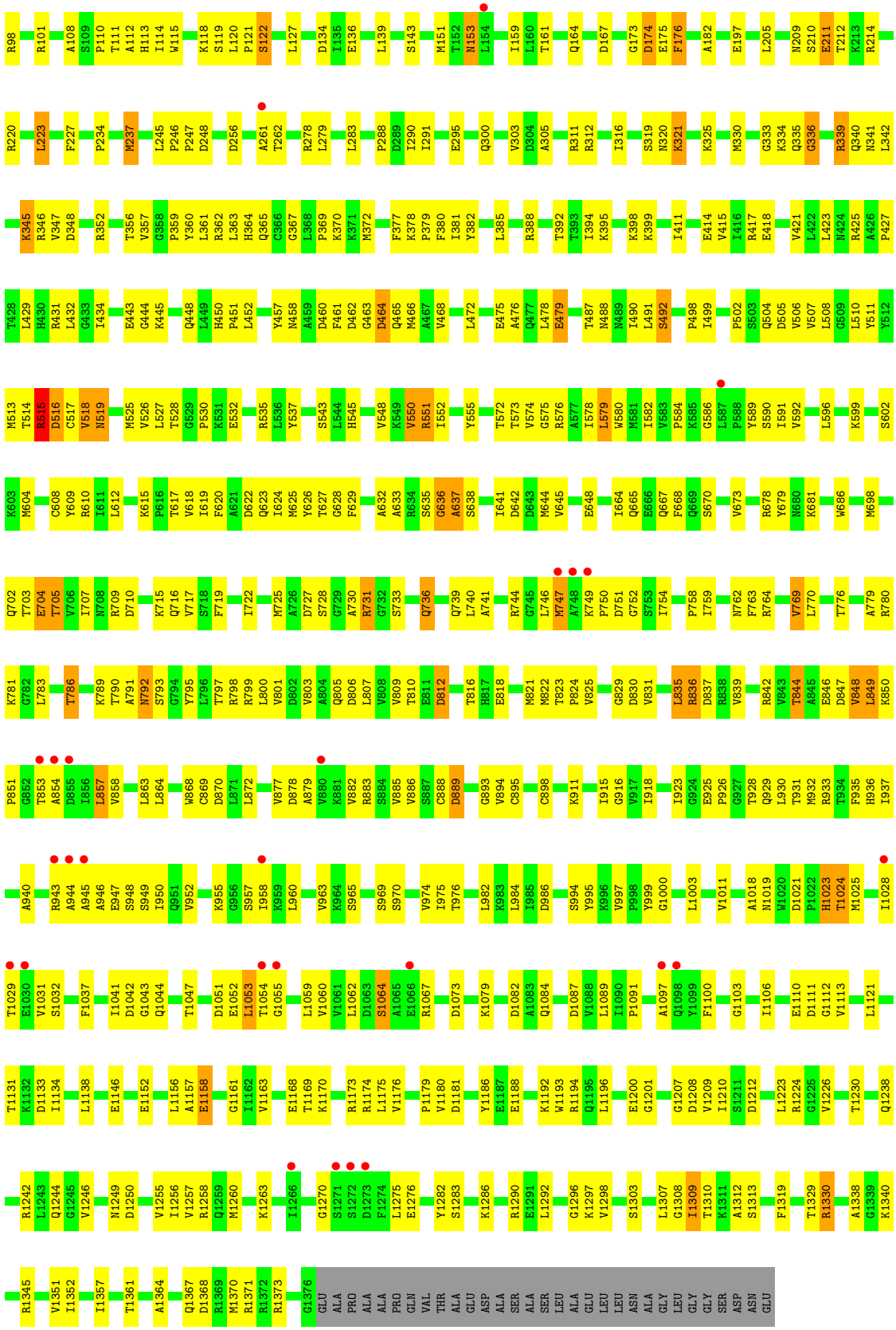




- Molecule 3: DNA-directed RNA polymerase subunit beta'

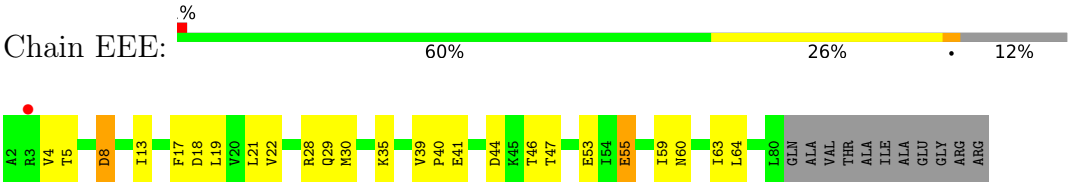
Chain DDD:





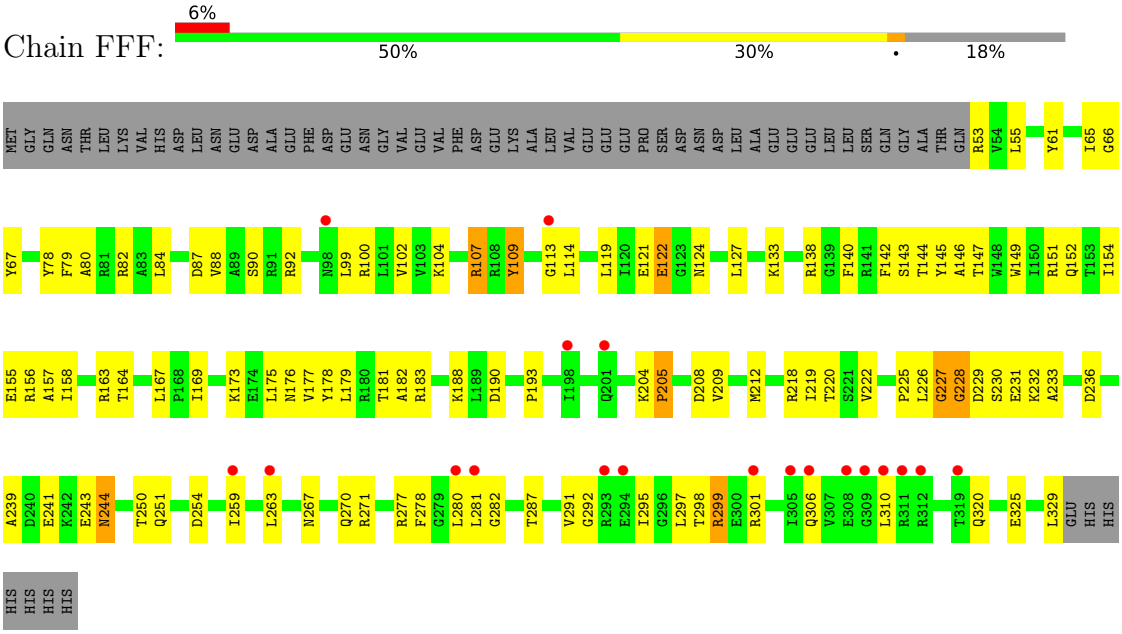
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain EEE:



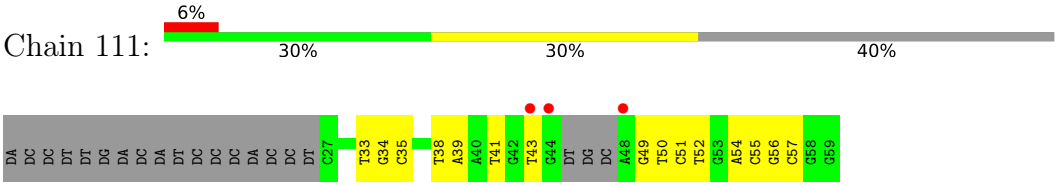
• Molecule 5: RNA polymerase sigma factor RpoS

Chain FFF:



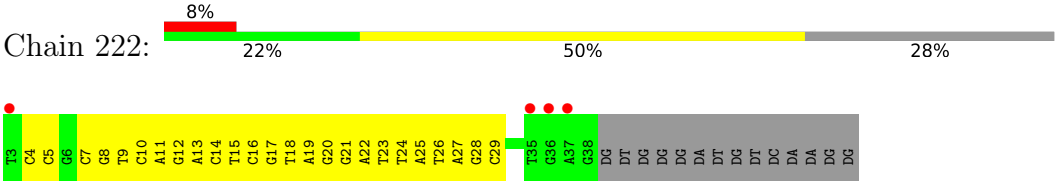
• Molecule 6: Synthetic DNA 50-MER (promoter non-template strand)

Chain 111:



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

Chain 222:



• Molecule 8: RNA 4-mer

Chain 333:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.85Å 154.25Å 230.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 4.10 49.18 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.18-4.10) 98.2 (49.18-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.332 , 0.396 0.319 , 0.379	Depositor DCC
R_{free} test set	1774 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	187.4	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 211.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29064	wwPDB-VP
Average B, all atoms (Å^2)	288.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2DT, MG, CTP, GTP, 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	AAA	0.63	0/1809	0.74	0/2450
1	BBB	0.64	0/1789	0.73	0/2425
2	CCC	0.62	0/10745	0.81	3/14499 (0.0%)
3	DDD	0.63	0/10729	0.80	5/14487 (0.0%)
4	EEE	0.62	0/629	0.80	0/847
5	FFF	0.65	0/2282	0.66	0/3076
6	111	0.29	0/693	0.61	0/1066
7	222	0.27	0/828	0.70	0/1277
8	333	0.19	0/50	0.56	0/76
All	All	0.62	0/29554	0.78	8/40203 (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	CCC	0	1
3	DDD	0	2
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DDD	636	GLY	C-N-CA	-7.74	102.34	121.70
3	DDD	636	GLY	N-CA-C	-7.16	95.20	113.10
3	DDD	636	GLY	CA-C-N	-6.29	103.37	117.20
2	CCC	1048	LYS	CB-CA-C	-5.97	98.46	110.40
3	DDD	637	ALA	CB-CA-C	5.75	118.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CCC	1088	ASP	CB-CA-C	-5.61	99.19	110.40
2	CCC	454	ARG	CB-CA-C	-5.44	99.53	110.40
3	DDD	460	ASP	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	CCC	1282	GLY	Peptide
3	DDD	636	GLY	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1787	0	1813	61	0
1	BBB	1767	0	1789	67	0
2	CCC	10576	0	10591	454	0
3	DDD	10568	0	10782	638	0
4	EEE	627	0	634	17	0
5	FFF	2253	0	2298	109	1
6	111	619	0	340	22	0
7	222	738	0	407	74	0
8	333	96	0	46	13	0
9	DDD	2	0	0	3	0
10	DDD	2	0	0	0	0
11	333	29	0	12	11	0
All	All	29064	0	28712	1238	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 21.

All (1238) 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)
3:DDD:504:GLN:NE2	3:DDD:731:ARG:HH21	1.12	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:750:PRO:HA	3:DDD:781:LYS:CG	1.57	1.35
7:222:21:DG:H4'	7:222:22:DA:C5'	1.54	1.34
3:DDD:750:PRO:CA	3:DDD:781:LYS:HG2	1.61	1.28
7:222:21:DG:C4'	7:222:22:DA:H5'	1.68	1.24
3:DDD:504:GLN:NE2	3:DDD:731:ARG:NH2	1.84	1.23
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	1.44	1.16
3:DDD:511:TYR:CE2	3:DDD:515:ARG:HD2	1.81	1.15
7:222:21:DG:H1'	7:222:22:DA:C8	1.82	1.13
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:HH12	1.03	1.11
5:FFF:109:TYR:OH	5:FFF:155:GLU:HG3	1.51	1.10
5:FFF:183:ARG:NH2	7:222:26:DT:OP2	1.83	1.09
8:333:101:2DT:H2'	11:333:201:CTP:C6	1.86	1.09
7:222:21:DG:H1'	7:222:22:DA:H8	1.04	1.08
3:DDD:451:PRO:HB2	3:DDD:625:MET:SD	1.94	1.06
2:CCC:514:PHE:HZ	7:222:19:DA:H4'	1.16	1.06
2:CCC:1269:ARG:N	7:222:15:DT:OP1	1.87	1.06
3:DDD:858:VAL:HG22	3:DDD:868:TRP:CE3	1.91	1.06
7:222:21:DG:N3	7:222:22:DA:N7	2.02	1.06
3:DDD:490:ILE:HD11	3:DDD:618:VAL:HG22	1.34	1.06
2:CCC:1223:ARG:CG	3:DDD:635:SER:O	2.04	1.05
3:DDD:395:LYS:HE2	5:FFF:329:LEU:HD22	1.39	1.04
2:CCC:549:ASP:CG	3:DDD:750:PRO:HG3	1.77	1.04
7:222:21:DG:C4'	7:222:22:DA:C5'	2.30	1.04
3:DDD:363:LEU:HD23	3:DDD:618:VAL:HG13	1.39	1.03
3:DDD:822:MET:HE2	3:DDD:882:VAL:HG21	1.41	1.01
3:DDD:519:ASN:ND2	3:DDD:709:ARG:HA	1.76	1.00
2:CCC:804:PHE:O	3:DDD:638:SER:HB2	1.61	1.00
3:DDD:388:ARG:NH2	3:DDD:414:GLU:OE1	1.94	1.00
3:DDD:392:THR:CG2	5:FFF:320:GLN:O	2.09	0.99
3:DDD:505:ASP:HB2	3:DDD:629:PHE:HD1	1.24	0.99
3:DDD:395:LYS:HG2	5:FFF:329:LEU:HD13	1.45	0.99
3:DDD:505:ASP:HB2	3:DDD:629:PHE:CD1	1.97	0.99
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.43	0.98
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.44	0.98
3:DDD:506:VAL:HG22	3:DDD:625:MET:O	1.64	0.98
2:CCC:1101:LEU:HD12	3:DDD:505:ASP:OD1	1.62	0.98
3:DDD:452:LEU:HD21	3:DDD:625:MET:HB2	1.46	0.97
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.44	0.96
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG11	1.48	0.96
3:DDD:504:GLN:HE22	3:DDD:731:ARG:HH21	0.97	0.95
3:DDD:511:TYR:CE2	3:DDD:515:ARG:CD	2.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:NH1	1.81	0.95
2:CCC:32:LEU:HA	2:CCC:130:MET:HE1	1.46	0.95
2:CCC:513:GLN:OE1	2:CCC:526:HIS:NE2	2.01	0.94
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HD13	1.47	0.94
3:DDD:504:GLN:HE22	3:DDD:731:ARG:NH2	1.55	0.94
3:DDD:932:MET:SD	11:333:201:CTP:H2'	2.07	0.94
5:FFF:109:TYR:OH	5:FFF:155:GLU:CG	2.15	0.94
1:BBB:83:LEU:HG	3:DDD:526:VAL:HG11	1.47	0.93
3:DDD:359:PRO:O	3:DDD:626:TYR:HE1	1.52	0.93
3:DDD:504:GLN:HE21	3:DDD:731:ARG:HH21	1.06	0.92
3:DDD:572:THR:OG1	3:DDD:576:ARG:HD2	1.70	0.91
3:DDD:895:CYS:HG	9:DDD:1502:ZN:ZN	0.60	0.91
7:222:21:DG:H4'	7:222:22:DA:H5"	1.51	0.91
2:CCC:514:PHE:CZ	7:222:19:DA:H4'	2.05	0.91
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	1.53	0.90
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.53	0.90
3:DDD:888:CYS:SG	9:DDD:1502:ZN:ZN	1.60	0.90
1:BBB:179:PRO:HG3	1:BBB:211:ILE:HD12	1.53	0.90
2:CCC:1101:LEU:CD1	3:DDD:505:ASP:OD1	2.20	0.90
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.07	0.90
3:DDD:1330:ARG:CZ	7:222:9:DT:H5"	2.02	0.89
2:CCC:251:ALA:CB	2:CCC:263:VAL:HG11	2.03	0.89
2:CCC:804:PHE:O	3:DDD:638:SER:CB	2.21	0.89
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.52	0.89
1:AAA:52:PRO:O	1:AAA:211:ILE:HD11	1.72	0.89
2:CCC:1223:ARG:HG3	3:DDD:635:SER:O	1.71	0.89
7:222:21:DG:N3	7:222:22:DA:C8	2.42	0.88
3:DDD:490:ILE:HD11	3:DDD:618:VAL:CG2	2.04	0.88
1:BBB:193:GLU:O	1:BBB:194:GLN:HB2	1.73	0.88
2:CCC:681:MET:O	2:CCC:685:MET:HG2	1.73	0.87
7:222:14:DC:O2	8:333:16:G:N2	2.07	0.87
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	1.57	0.87
3:DDD:1330:ARG:NH2	7:222:9:DT:OP1	2.06	0.87
3:DDD:519:ASN:HD22	3:DDD:709:ARG:HA	1.35	0.86
3:DDD:516:ASP:HB3	3:DDD:573:THR:HG21	1.57	0.86
2:CCC:1295:SER:OG	3:DDD:346:ARG:O	1.92	0.85
3:DDD:1133:ASP:OD2	3:DDD:1134:ILE:N	2.10	0.84
3:DDD:506:VAL:HA	3:DDD:628:GLY:HA3	1.60	0.84
2:CCC:1333:LEU:O	3:DDD:113:HIS:CE1	2.31	0.84
3:DDD:1156:LEU:HD22	3:DDD:1224:ARG:HH21	1.43	0.84
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:222:21:DG:O4'	7:222:22:DA:H5'	1.78	0.84
3:DDD:395:LYS:CG	5:FFF:329:LEU:HD13	2.07	0.83
3:DDD:793:SER:OG	3:DDD:928:THR:OG1	1.95	0.83
3:DDD:858:VAL:HG22	3:DDD:868:TRP:CZ3	2.12	0.83
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:HA	1.58	0.83
3:DDD:458:ASN:OD1	3:DDD:933:ARG:NH2	2.11	0.83
3:DDD:363:LEU:CD2	3:DDD:618:VAL:HG13	2.08	0.83
2:CCC:1222:GLU:OE1	3:DDD:537:TYR:OH	1.95	0.83
3:DDD:507:VAL:HG11	3:DDD:728:SER:O	1.77	0.82
5:FFF:152:GLN:OE1	7:222:27:DA:N6	2.12	0.82
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	1.60	0.82
3:DDD:516:ASP:CB	3:DDD:573:THR:CG2	2.57	0.82
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB2	1.80	0.82
1:BBB:83:LEU:HG	3:DDD:526:VAL:CG1	2.09	0.82
3:DDD:518:VAL:HG23	3:DDD:716:GLN:OE1	1.80	0.82
3:DDD:1158:GLU:OE2	3:DDD:1223:LEU:HD21	1.80	0.82
7:222:21:DG:C1'	7:222:22:DA:H8	1.91	0.81
3:DDD:22:ILE:HD11	3:DDD:1319:PHE:CE1	2.15	0.81
2:CCC:555:TYR:CD1	2:CCC:637:ARG:NH2	2.49	0.81
3:DDD:516:ASP:CB	3:DDD:573:THR:HG21	2.09	0.81
2:CCC:1107:MET:CE	3:DDD:739:GLN:HB2	2.11	0.81
1:AAA:9:LEU:HD21	1:AAA:198:LEU:HD11	1.63	0.81
3:DDD:516:ASP:HB3	3:DDD:573:THR:CG2	2.11	0.81
5:FFF:164:THR:HB	5:FFF:219:ILE:HD12	1.61	0.81
2:CCC:514:PHE:HZ	7:222:19:DA:C4'	1.92	0.80
3:DDD:506:VAL:HA	3:DDD:628:GLY:C	2.02	0.80
1:BBB:124:VAL:HG21	1:BBB:210:THR:HG22	1.63	0.80
3:DDD:506:VAL:HG13	3:DDD:624:ILE:O	1.80	0.80
3:DDD:525:MET:O	3:DDD:548:VAL:HG22	1.82	0.80
2:CCC:726:TYR:HB3	2:CCC:733:VAL:CG2	2.10	0.80
3:DDD:361:LEU:O	3:DDD:626:TYR:OH	2.00	0.80
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.63	0.80
3:DDD:506:VAL:HA	3:DDD:628:GLY:CA	2.12	0.79
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.16	0.79
3:DDD:516:ASP:HB2	3:DDD:573:THR:HG22	1.62	0.79
3:DDD:517:CYS:N	3:DDD:545:HIS:HB3	1.98	0.79
7:222:16:DC:H2'	7:222:17:DG:H5'	1.64	0.79
3:DDD:572:THR:HG21	3:DDD:589:TYR:OH	1.83	0.79
2:CCC:812:PHE:CE1	3:DDD:629:PHE:HZ	2.01	0.79
3:DDD:504:GLN:HE21	3:DDD:731:ARG:NH2	1.67	0.79
5:FFF:163:ARG:NH2	7:222:26:DT:O4	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:496:LYS:HB3	7:222:24:DT:OP1	1.83	0.78
3:DDD:673:VAL:CG1	3:DDD:678:ARG:HB2	2.13	0.78
3:DDD:895:CYS:SG	9:DDD:1502:ZN:ZN	1.72	0.78
2:CCC:790:ASP:O	2:CCC:792:GLY:N	2.16	0.78
5:FFF:163:ARG:NH2	7:222:25:DA:N1	2.31	0.78
2:CCC:237:LEU:HD12	2:CCC:289:VAL:HA	1.65	0.78
2:CCC:165:HIS:CE1	2:CCC:190:PRO:HG3	2.17	0.78
3:DDD:644:MET:O	3:DDD:764:ARG:NH1	2.15	0.78
3:DDD:572:THR:HG1	3:DDD:576:ARG:HD2	1.49	0.78
2:CCC:1333:LEU:O	3:DDD:113:HIS:HE1	1.67	0.78
2:CCC:186:PHE:CE1	2:CCC:196:VAL:HG22	2.18	0.77
2:CCC:1269:ARG:HB2	7:222:15:DT:P	2.23	0.77
3:DDD:312:ARG:HG2	3:DDD:312:ARG:O	1.85	0.77
3:DDD:816:THR:HG22	3:DDD:818:GLU:H	1.48	0.77
3:DDD:507:VAL:CG1	3:DDD:728:SER:O	2.32	0.76
3:DDD:750:PRO:HB3	3:DDD:781:LYS:HB2	1.67	0.76
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.66	0.76
3:DDD:1330:ARG:NH2	7:222:9:DT:P	2.59	0.76
2:CCC:514:PHE:CZ	7:222:19:DA:C4'	2.69	0.76
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.16	0.76
3:DDD:822:MET:CE	3:DDD:882:VAL:HG21	2.16	0.76
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HG3	1.68	0.76
2:CCC:3:TYR:O	2:CCC:8:LYS:HE3	1.85	0.75
3:DDD:121:PRO:O	3:DDD:122:SER:HB3	1.86	0.75
3:DDD:1029:THR:HG23	3:DDD:1121:LEU:HG	1.69	0.75
2:CCC:255:ILE:HD12	2:CCC:263:VAL:HG21	1.68	0.75
2:CCC:549:ASP:CG	3:DDD:750:PRO:CG	2.55	0.75
3:DDD:505:ASP:CB	3:DDD:629:PHE:HD1	2.00	0.75
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.68	0.75
3:DDD:359:PRO:O	3:DDD:626:TYR:CE1	2.40	0.75
5:FFF:226:LEU:O	5:FFF:228:GLY:N	2.20	0.75
2:CCC:549:ASP:OD2	3:DDD:750:PRO:CG	2.34	0.74
3:DDD:26:SER:OG	3:DDD:28:ASP:OD1	2.01	0.74
3:DDD:506:VAL:HG21	3:DDD:625:MET:HA	1.69	0.74
3:DDD:698:MET:O	3:DDD:702:GLN:HB3	1.86	0.74
3:DDD:703:THR:OG1	3:DDD:704:GLU:N	2.19	0.74
3:DDD:511:TYR:CZ	3:DDD:515:ARG:HD2	2.23	0.74
1:BBB:9:LEU:HD21	1:BBB:198:LEU:HD11	1.69	0.74
2:CCC:18:ARG:NH2	2:CCC:620:ASN:O	2.21	0.74
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD21	1.69	0.74
3:DDD:1152:GLU:CA	3:DDD:1194:ARG:HH22	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:555:TYR:CE1	2:CCC:637:ARG:NH2	2.56	0.74
2:CCC:898:GLU:HG3	5:FFF:259:ILE:CD1	2.17	0.73
3:DDD:395:LYS:HE2	5:FFF:329:LEU:CD2	2.18	0.73
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.69	0.73
2:CCC:1269:ARG:HB2	7:222:15:DT:OP1	1.88	0.73
3:DDD:452:LEU:HG	3:DDD:625:MET:SD	2.27	0.73
2:CCC:1107:MET:HE1	3:DDD:739:GLN:HB2	1.69	0.73
3:DDD:452:LEU:HD11	3:DDD:622:ASP:HA	1.70	0.73
1:BBB:65:LEU:O	1:BBB:169:GLY:HA2	1.89	0.73
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.70	0.73
2:CCC:93:SER:OG	2:CCC:126:GLU:OE1	2.06	0.73
3:DDD:822:MET:HE2	3:DDD:842:ARG:HD3	1.71	0.72
1:BBB:196:THR:HG21	3:DDD:370:LYS:NZ	2.04	0.72
3:DDD:528:THR:O	3:DDD:528:THR:OG1	2.03	0.72
2:CCC:201:ARG:HB2	2:CCC:369:MET:CE	2.20	0.72
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	1.70	0.72
2:CCC:663:VAL:O	2:CCC:666:SER:OG	2.07	0.72
2:CCC:806:PRO:HB2	3:DDD:633:ALA:HB2	1.71	0.72
3:DDD:517:CYS:CB	3:DDD:545:HIS:HB2	2.18	0.72
3:DDD:931:THR:O	3:DDD:935:PHE:CD2	2.43	0.72
7:222:21:DG:N2	7:222:22:DA:C6	2.57	0.72
3:DDD:511:TYR:O	3:DDD:515:ARG:HB2	1.90	0.72
2:CCC:1077:SER:HA	3:DDD:356:THR:CG2	2.20	0.71
2:CCC:1223:ARG:CD	3:DDD:635:SER:O	2.38	0.71
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:HE3	1.72	0.71
2:CCC:251:ALA:HB2	2:CCC:263:VAL:HG11	1.70	0.71
3:DDD:392:THR:HG21	5:FFF:320:GLN:C	2.11	0.71
7:222:19:DA:H2'	7:222:20:DG:C8	2.26	0.71
2:CCC:230:PHE:CD1	2:CCC:292:ILE:HD11	2.26	0.71
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.24	0.71
3:DDD:399:LYS:HE3	5:FFF:329:LEU:HD21	1.72	0.71
3:DDD:362:ARG:N	3:DDD:365:GLN:OE1	2.18	0.71
3:DDD:750:PRO:HA	3:DDD:781:LYS:CB	2.21	0.71
3:DDD:750:PRO:CA	3:DDD:781:LYS:CG	2.39	0.70
3:DDD:395:LYS:HG2	5:FFF:329:LEU:CD1	2.19	0.70
3:DDD:504:GLN:HA	3:DDD:730:ALA:O	1.92	0.70
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.19	0.70
3:DDD:525:MET:O	3:DDD:548:VAL:CG2	2.38	0.70
7:222:20:DG:H3'	7:222:21:DG:H5"	1.74	0.70
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:HD11	1.74	0.70
3:DDD:134:ASP:CG	3:DDD:159:ILE:HD11	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:475:GLU:O	3:DDD:479:GLU:HG2	1.90	0.70
5:FFF:228:GLY:HA3	8:333:14:GTP:O2G	1.92	0.69
3:DDD:363:LEU:HD23	3:DDD:618:VAL:CG1	2.21	0.69
3:DDD:792:ASN:N	3:DDD:792:ASN:OD1	2.25	0.69
2:CCC:163:LYS:HG2	2:CCC:164:THR:N	2.05	0.69
2:CCC:648:ASP:OD1	2:CCC:648:ASP:N	2.23	0.69
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:CE	2.22	0.69
2:CCC:1291:LEU:HA	3:DDD:345:LYS:HD2	1.74	0.69
2:CCC:1077:SER:HA	3:DDD:356:THR:HG21	1.73	0.69
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:H	1.56	0.69
7:222:21:DG:N2	7:222:22:DA:C5	2.60	0.69
3:DDD:958:ILE:HG23	3:DDD:982:LEU:CD1	2.23	0.69
2:CCC:257:ALA:HB3	2:CCC:262:TYR:CE2	2.28	0.69
3:DDD:516:ASP:HB2	3:DDD:573:THR:CG2	2.22	0.69
2:CCC:10:ARG:NH2	2:CCC:790:ASP:OD1	2.26	0.68
3:DDD:506:VAL:CA	3:DDD:628:GLY:HA3	2.22	0.68
3:DDD:572:THR:OG1	3:DDD:576:ARG:CD	2.41	0.68
5:FFF:182:ALA:HB1	5:FFF:193:PRO:HG3	1.73	0.68
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.76	0.68
3:DDD:886:VAL:HG21	3:DDD:1230:THR:HG21	1.74	0.68
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.75	0.68
5:FFF:163:ARG:HD3	5:FFF:167:LEU:HD12	1.76	0.68
3:DDD:504:GLN:HE21	3:DDD:731:ARG:CZ	2.07	0.68
7:222:16:DC:C2'	7:222:17:DG:H5'	2.24	0.68
2:CCC:1304:MET:HE1	3:DDD:472:LEU:HD13	1.75	0.68
3:DDD:339:ARG:NH2	7:222:11:DA:OP1	2.22	0.67
3:DDD:552:ILE:CG2	3:DDD:580:TRP:CD1	2.77	0.67
1:BBB:193:GLU:O	1:BBB:194:GLN:CB	2.42	0.67
3:DDD:511:TYR:HE2	3:DDD:515:ARG:HD2	1.53	0.67
1:AAA:60:GLU:HG3	1:AAA:169:GLY:O	1.94	0.67
2:CCC:223:LEU:HD13	2:CCC:426:ILE:HD13	1.76	0.67
2:CCC:1223:ARG:HD2	3:DDD:635:SER:O	1.93	0.67
6:111:54:DA:H2"	6:111:55:DC:H5'	1.76	0.67
2:CCC:1129:ASN:HA	2:CCC:1177:ARG:HG3	1.76	0.67
3:DDD:1156:LEU:HD22	3:DDD:1224:ARG:NH2	2.10	0.67
3:DDD:320:ASN:O	3:DDD:321:LYS:HB2	1.95	0.67
2:CCC:342:ASP:O	2:CCC:437:ASN:CG	2.33	0.67
2:CCC:1223:ARG:HG2	3:DDD:635:SER:O	1.93	0.67
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.10	0.66
3:DDD:823:THR:HB	3:DDD:824:PRO:HD2	1.77	0.66
3:DDD:839:VAL:HG12	3:DDD:864:LEU:CD1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:549:ASP:OD2	3:DDD:750:PRO:HG3	1.94	0.66
3:DDD:1156:LEU:CD2	3:DDD:1224:ARG:NH2	2.58	0.66
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG21	1.78	0.66
2:CCC:1276:TRP:CH2	3:DDD:798:ARG:HG3	2.31	0.66
3:DDD:555:TYR:O	3:DDD:586:GLY:HA2	1.95	0.66
2:CCC:1245:ALA:HB2	3:DDD:372:MET:HG3	1.76	0.66
8:333:101:2DT:H2"	11:333:201:CTP:O4'	1.96	0.66
2:CCC:184:LEU:HG	2:CCC:389:PHE:CE2	2.31	0.66
3:DDD:425:ARG:HH22	11:333:201:CTP:H4'	1.60	0.66
3:DDD:1330:ARG:CZ	7:222:9:DT:C5'	2.74	0.66
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	1.96	0.66
3:DDD:836:ARG:HG2	3:DDD:869:CYS:HB3	1.77	0.66
2:CCC:548:ARG:HD3	2:CCC:569:ILE:O	1.96	0.65
2:CCC:1107:MET:HE2	3:DDD:739:GLN:CB	2.26	0.65
3:DDD:516:ASP:CB	3:DDD:573:THR:HG22	2.26	0.65
3:DDD:750:PRO:CB	3:DDD:781:LYS:CD	2.74	0.65
1:AAA:227:GLN:OE1	1:BBB:11:PRO:HD3	1.97	0.65
3:DDD:1157:ALA:O	3:DDD:1207:GLY:N	2.27	0.65
3:DDD:97:VAL:HG12	3:DDD:101:ARG:HG3	1.79	0.65
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:H	1.99	0.65
2:CCC:541:GLU:HG3	2:CCC:542:ARG:N	2.12	0.65
3:DDD:750:PRO:HB3	3:DDD:781:LYS:HD3	1.78	0.65
3:DDD:895:CYS:SG	3:DDD:898:CYS:HB2	2.36	0.65
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:CG2	2.27	0.65
2:CCC:1269:ARG:HD3	7:222:14:DC:H5'	1.78	0.65
3:DDD:1023:HIS:O	3:DDD:1024:THR:HB	1.95	0.65
7:222:21:DG:H4'	7:222:22:DA:O5'	1.97	0.65
2:CCC:263:VAL:CG1	2:CCC:269:ILE:HD11	2.27	0.65
3:DDD:385:LEU:CD2	3:DDD:411:ILE:HD13	2.25	0.64
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.78	0.64
3:DDD:139:LEU:HD22	3:DDD:300:GLN:HE22	1.61	0.64
3:DDD:320:ASN:O	3:DDD:321:LYS:CB	2.45	0.64
1:AAA:211:ILE:CG2	1:AAA:216:ALA:HB2	2.26	0.64
2:CCC:19:PRO:HA	2:CCC:1156:ARG:HD2	1.79	0.64
3:DDD:504:GLN:NE2	3:DDD:731:ARG:CZ	2.59	0.64
6:111:49:DG:H2"	6:111:50:DT:C6	2.32	0.64
3:DDD:385:LEU:HD23	3:DDD:411:ILE:HD13	1.79	0.64
2:CCC:43:PRO:O	2:CCC:54:ARG:NH1	2.31	0.64
2:CCC:812:PHE:CE1	3:DDD:629:PHE:CZ	2.85	0.64
2:CCC:1106:ARG:CZ	11:333:201:CTP:O2G	2.46	0.64
3:DDD:395:LYS:CE	5:FFF:329:LEU:HD22	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:750:PRO:O	3:DDD:781:LYS:HE3	1.96	0.64
1:BBB:25:LYS:HG2	1:BBB:204:GLU:HG2	1.80	0.64
2:CCC:812:PHE:CD1	3:DDD:629:PHE:CZ	2.85	0.64
3:DDD:97:VAL:HG11	3:DDD:101:ARG:HE	1.63	0.64
3:DDD:750:PRO:HB2	3:DDD:781:LYS:HE3	1.79	0.64
3:DDD:502:PRO:HB2	3:DDD:506:VAL:HG11	1.79	0.63
3:DDD:750:PRO:CB	3:DDD:781:LYS:CG	2.76	0.63
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE2	1.79	0.63
2:CCC:1270:PHE:N	3:DDD:345:LYS:O	2.28	0.63
2:CCC:263:VAL:HG13	2:CCC:269:ILE:HD11	1.80	0.63
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.29	0.63
4:EEE:8:ASP:N	4:EEE:8:ASP:OD1	2.31	0.63
2:CCC:414:ILE:HG13	2:CCC:415:GLU:N	2.13	0.63
2:CCC:577:VAL:HG23	2:CCC:661:VAL:O	1.97	0.63
3:DDD:1338:ALA:HB3	3:DDD:1340:LYS:HG3	1.81	0.63
5:FFF:227:GLY:O	5:FFF:229:ASP:N	2.30	0.63
3:DDD:22:ILE:CD1	3:DDD:1319:PHE:CE1	2.82	0.63
3:DDD:363:LEU:HB2	3:DDD:622:ASP:OD2	1.98	0.63
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG21	1.79	0.63
2:CCC:3:TYR:O	2:CCC:8:LYS:CE	2.47	0.63
3:DDD:750:PRO:HA	3:DDD:781:LYS:HG2	0.73	0.63
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.27	0.63
1:AAA:37:HIS:NE2	1:AAA:187:VAL:HG21	2.14	0.63
2:CCC:146:VAL:O	2:CCC:511:LEU:HD13	1.98	0.63
3:DDD:1156:LEU:HD21	3:DDD:1209:VAL:HG22	1.81	0.63
3:DDD:58:CYS:SG	3:DDD:60:ARG:HB3	2.39	0.62
3:DDD:895:CYS:SG	3:DDD:898:CYS:CB	2.86	0.62
2:CCC:302:ILE:HG22	2:CCC:309:LEU:HD23	1.81	0.62
3:DDD:609:TYR:HA	3:DDD:617:THR:HG21	1.81	0.62
5:FFF:225:PRO:HB2	5:FFF:230:SER:HA	1.81	0.62
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD11	1.81	0.62
2:CCC:1276:TRP:HH2	3:DDD:798:ARG:HG3	1.63	0.62
3:DDD:288:PRO:HG3	5:FFF:92:ARG:HG2	1.82	0.62
2:CCC:139:ASN:ND2	7:222:20:DG:H5”	2.15	0.62
2:CCC:447:HIS:CD2	2:CCC:449:GLY:H	2.18	0.62
2:CCC:672:GLU:HG2	2:CCC:1187:PHE:HA	1.82	0.62
3:DDD:504:GLN:HE21	3:DDD:731:ARG:HE	1.47	0.62
3:DDD:515:ARG:O	3:DDD:545:HIS:ND1	2.30	0.62
3:DDD:504:GLN:HE21	3:DDD:731:ARG:NE	1.98	0.62
1:BBB:30:PRO:HB2	1:BBB:198:LEU:HD12	1.81	0.62
2:CCC:688:GLN:NE2	8:333:16:G:OP1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:993:PRO:HG2	2:CCC:996:ARG:NH1	2.15	0.62
3:DDD:750:PRO:HB3	3:DDD:781:LYS:CB	2.29	0.62
2:CCC:901:LEU:CD1	5:FFF:310:LEU:HD21	2.30	0.61
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:CD1	2.25	0.61
3:DDD:1282:TYR:CE1	3:DDD:1286:LYS:HD2	2.35	0.61
2:CCC:32:LEU:HD23	2:CCC:130:MET:CE	2.30	0.61
3:DDD:452:LEU:HD21	3:DDD:625:MET:CB	2.27	0.61
3:DDD:803:VAL:CG2	3:DDD:1313:SER:OG	2.48	0.61
3:DDD:807:LEU:CD2	3:DDD:1255:VAL:HG13	2.29	0.61
7:222:21:DG:C1'	7:222:22:DA:C8	2.70	0.61
3:DDD:752:GLY:O	3:DDD:1131:THR:OG1	2.18	0.61
3:DDD:858:VAL:HG22	3:DDD:868:TRP:HE3	1.62	0.61
2:CCC:1291:LEU:CD1	3:DDD:1351:VAL:HG13	2.30	0.61
3:DDD:1152:GLU:HB3	3:DDD:1194:ARG:NH2	2.16	0.61
2:CCC:12:ARG:NH2	2:CCC:793:GLU:OE1	2.33	0.61
2:CCC:1109:ILE:HG13	3:DDD:644:MET:HE3	1.83	0.61
3:DDD:492:SER:HB2	3:DDD:499:ILE:HD11	1.82	0.61
3:DDD:822:MET:HE2	3:DDD:882:VAL:CG2	2.23	0.61
1:BBB:86:LYS:CE	1:BBB:174:ASP:HB2	2.30	0.61
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.22	0.61
3:DDD:245:LEU:HD12	3:DDD:246:PRO:HD2	1.82	0.61
3:DDD:844:THR:HG23	3:DDD:864:LEU:HD11	1.82	0.61
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	1.82	0.61
2:CCC:340:ASP:HB3	2:CCC:341:LEU:HG	1.81	0.61
3:DDD:609:TYR:HA	3:DDD:617:THR:CG2	2.31	0.61
2:CCC:183:TRP:CZ2	6:111:50:DT:C4	2.89	0.60
2:CCC:262:TYR:OH	2:CCC:280:ASP:OD2	2.19	0.60
3:DDD:709:ARG:CG	3:DDD:709:ARG:O	2.49	0.60
2:CCC:118:LYS:HD3	2:CCC:488:MET:HG2	1.83	0.60
2:CCC:528:ARG:HD2	2:CCC:663:VAL:HG21	1.83	0.60
2:CCC:734:ILE:CG2	2:CCC:749:ASP:HB2	2.30	0.60
2:CCC:890:LYS:HD2	2:CCC:914:LYS:HE2	1.83	0.60
3:DDD:552:ILE:HG21	3:DDD:580:TRP:CD1	2.35	0.60
8:333:101:2DT:C2'	11:333:201:CTP:O4'	2.49	0.60
2:CCC:389:PHE:HB3	2:CCC:420:LEU:HD12	1.83	0.60
1:AAA:82:LEU:HD22	1:AAA:173:VAL:CG2	2.30	0.60
1:AAA:212:ASP:OD1	1:AAA:213:PRO:HD2	2.02	0.60
1:BBB:37:HIS:NE2	1:BBB:187:VAL:HG21	2.16	0.60
2:CCC:157:PHE:O	2:CCC:442:VAL:HG13	2.01	0.60
3:DDD:975:ILE:HD12	3:DDD:997:VAL:HG11	1.83	0.60
2:CCC:661:VAL:HG13	2:CCC:665:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:572:THR:HG21	3:DDD:589:TYR:HH	1.67	0.60
1:AAA:25:LYS:HG2	1:AAA:204:GLU:HG2	1.82	0.60
3:DDD:1003:LEU:HD23	3:DDD:1018:ALA:HB2	1.82	0.60
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	1.84	0.60
3:DDD:491:LEU:HA	3:DDD:498:PRO:HA	1.84	0.60
3:DDD:506:VAL:CG2	3:DDD:625:MET:O	2.46	0.60
3:DDD:1152:GLU:C	3:DDD:1194:ARG:HH22	2.03	0.60
2:CCC:700:VAL:HG13	2:CCC:1117:LEU:HD23	1.84	0.59
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:N	2.56	0.59
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.83	0.59
1:BBB:135:ASP:OD1	1:BBB:138:ALA:HB2	2.02	0.59
3:DDD:525:MET:N	3:DDD:548:VAL:HG23	2.16	0.59
3:DDD:552:ILE:CG2	3:DDD:580:TRP:NE1	2.65	0.59
3:DDD:1134:ILE:CD1	3:DDD:1244:GLN:HG3	2.31	0.59
2:CCC:1112:ILE:HG22	3:DDD:641:ILE:HG12	1.82	0.59
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:CD1	2.31	0.59
3:DDD:112:ALA:H	3:DDD:300:GLN:HE21	1.49	0.59
3:DDD:750:PRO:O	3:DDD:781:LYS:CE	2.49	0.59
5:FFF:263:LEU:HD13	5:FFF:281:LEU:HD11	1.84	0.59
7:222:4:DC:H1'	7:222:5:DC:H5'	1.84	0.59
3:DDD:510:LEU:O	3:DDD:514:THR:HG23	2.02	0.59
3:DDD:750:PRO:CB	3:DDD:781:LYS:HB2	2.32	0.59
3:DDD:1134:ILE:HD11	3:DDD:1244:GLN:HG3	1.84	0.59
1:AAA:145:LYS:HD3	1:AAA:147:GLN:HE21	1.68	0.59
2:CCC:524:ILE:O	2:CCC:528:ARG:HG2	2.02	0.59
2:CCC:550:VAL:HG21	3:DDD:776:THR:CG2	2.33	0.59
2:CCC:685:MET:HE2	2:CCC:1235:LEU:HD11	1.83	0.59
3:DDD:334:LYS:O	3:DDD:339:ARG:HB2	2.03	0.59
5:FFF:53:ARG:O	5:FFF:55:LEU:HG	2.01	0.59
1:AAA:30:PRO:HB2	1:AAA:198:LEU:HD12	1.84	0.59
2:CCC:292:ILE:CG2	2:CCC:322:LEU:HD11	2.32	0.59
4:EEE:29:GLN:HE22	4:EEE:64:LEU:HD22	1.67	0.59
2:CCC:1214:ASP:OD2	2:CCC:1217:THR:HG23	2.02	0.59
2:CCC:1242:LYS:HD3	3:DDD:465:GLN:NE2	2.17	0.59
3:DDD:513:MET:O	3:DDD:575:GLY:HA3	2.03	0.59
1:BBB:145:LYS:HD3	1:BBB:147:GLN:HE21	1.66	0.59
2:CCC:240:GLU:HA	2:CCC:283:LYS:O	2.03	0.59
2:CCC:297:VAL:HG13	2:CCC:317:LEU:HG	1.85	0.59
3:DDD:1163:VAL:HG13	3:DDD:1176:VAL:O	2.02	0.59
4:EEE:53:GLU:HB3	4:EEE:59:ILE:HG12	1.85	0.59
5:FFF:298:THR:HG21	5:FFF:301:ARG:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:222:21:DG:N3	7:222:22:DA:C5	2.69	0.59
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HD12	1.84	0.58
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE1	1.85	0.58
3:DDD:1156:LEU:CD2	3:DDD:1224:ARG:HH21	2.11	0.58
3:DDD:750:PRO:O	3:DDD:781:LYS:NZ	2.36	0.58
3:DDD:857:LEU:O	3:DDD:868:TRP:HZ3	1.86	0.58
3:DDD:506:VAL:HG11	3:DDD:625:MET:HA	1.85	0.58
3:DDD:822:MET:CE	3:DDD:842:ARG:HD3	2.33	0.58
5:FFF:82:ARG:HG2	5:FFF:87:ASP:HB2	1.84	0.58
2:CCC:292:ILE:HB	2:CCC:322:LEU:HD11	1.85	0.58
2:CCC:734:ILE:HD11	2:CCC:777:VAL:HG23	1.86	0.58
3:DDD:452:LEU:HD12	3:DDD:622:ASP:OD1	2.03	0.58
3:DDD:510:LEU:CD2	3:DDD:579:LEU:HD21	2.32	0.58
3:DDD:886:VAL:HG21	3:DDD:1230:THR:CG2	2.34	0.58
2:CCC:736:VAL:HB	2:CCC:741:MET:HE2	1.86	0.58
3:DDD:395:LYS:CD	5:FFF:329:LEU:HD13	2.32	0.58
3:DDD:511:TYR:OH	3:DDD:727:ASP:OD2	2.12	0.58
1:BBB:67:GLU:CB	1:BBB:171:LEU:HD22	2.31	0.58
2:CCC:36:GLN:O	2:CCC:40:GLU:HB2	2.03	0.58
2:CCC:559:CYS:HB2	2:CCC:662:SER:HB3	1.86	0.58
5:FFF:244:ASN:N	5:FFF:244:ASN:OD1	2.36	0.58
5:FFF:61:TYR:CE2	5:FFF:65:ILE:HD11	2.39	0.58
5:FFF:122:GLU:HG2	5:FFF:157:ALA:HB2	1.85	0.58
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG13	1.84	0.58
3:DDD:43:THR:OG1	3:DDD:44:ILE:N	2.37	0.58
3:DDD:750:PRO:CB	3:DDD:781:LYS:HD3	2.34	0.58
5:FFF:107:ARG:HD3	6:111:43:DT:H4'	1.85	0.58
2:CCC:720:ARG:HD2	2:CCC:736:VAL:HG21	1.85	0.58
3:DDD:1110:GLU:O	3:DDD:1113:VAL:HG23	2.02	0.58
5:FFF:259:ILE:CG2	5:FFF:280:LEU:HD21	2.34	0.58
2:CCC:582:ASN:OD1	2:CCC:586:PHE:N	2.36	0.57
2:CCC:1304:MET:CE	3:DDD:472:LEU:HD13	2.33	0.57
3:DDD:883:ARG:HG2	3:DDD:898:CYS:HA	1.86	0.57
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.34	0.57
3:DDD:510:LEU:HD22	3:DDD:579:LEU:HD21	1.86	0.57
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:CD1	2.35	0.57
1:AAA:211:ILE:HG21	1:AAA:216:ALA:HB2	1.85	0.57
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HG	2.34	0.57
3:DDD:1161:GLY:HA3	3:DDD:1179:PRO:HA	1.85	0.57
3:DDD:1275:LEU:HG	3:DDD:1276:GLU:H	1.70	0.57
1:AAA:179:PRO:HG3	1:AAA:211:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:518:VAL:CG2	3:DDD:716:GLN:OE1	2.52	0.57
3:DDD:1000:GLY:HA2	3:DDD:1028:ILE:HD12	1.86	0.57
3:DDD:1158:GLU:HA	3:DDD:1223:LEU:HD22	1.85	0.57
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	1.85	0.57
2:CCC:1281:TYR:OH	3:DDD:431:ARG:O	2.22	0.57
3:DDD:176:PHE:O	3:DDD:176:PHE:CD2	2.58	0.57
2:CCC:150:HIS:CE1	2:CCC:454:ARG:HG3	2.39	0.57
2:CCC:1286:THR:HG23	3:DDD:476:ALA:HB1	1.85	0.57
3:DDD:936:HIS:CE1	3:DDD:937:ILE:HG13	2.39	0.57
3:DDD:950:ILE:HD13	3:DDD:995:TYR:HB3	1.87	0.57
3:DDD:1158:GLU:OE2	3:DDD:1223:LEU:CD2	2.51	0.57
3:DDD:1309:ILE:HG22	3:DDD:1310:THR:N	2.20	0.57
5:FFF:61:TYR:CZ	5:FFF:65:ILE:HD11	2.40	0.57
2:CCC:241:LEU:HD13	2:CCC:285:ILE:HD12	1.85	0.57
3:DDD:68:TYR:C	3:DDD:92:VAL:HG13	2.26	0.57
3:DDD:506:VAL:CG2	3:DDD:625:MET:HA	2.34	0.57
3:DDD:803:VAL:HG23	3:DDD:1313:SER:OG	2.05	0.57
2:CCC:582:ASN:ND2	2:CCC:586:PHE:HB2	2.18	0.57
7:222:21:DG:C2	7:222:22:DA:C5	2.93	0.57
1:BBB:212:ASP:OD1	1:BBB:213:PRO:HD2	2.04	0.56
2:CCC:302:ILE:CG2	2:CCC:309:LEU:HD23	2.34	0.56
2:CCC:993:PRO:HG2	2:CCC:996:ARG:CZ	2.36	0.56
3:DDD:68:TYR:CD2	3:DDD:78:LEU:HD23	2.39	0.56
5:FFF:263:LEU:HD13	5:FFF:281:LEU:CD1	2.35	0.56
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.35	0.56
3:DDD:609:TYR:CA	3:DDD:617:THR:HG21	2.35	0.56
1:AAA:209:GLY:O	1:AAA:210:THR:C	2.43	0.56
2:CCC:263:VAL:HG22	2:CCC:269:ILE:HD12	1.87	0.56
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CD2	2.41	0.56
2:CCC:1192:GLU:OE2	3:DDD:764:ARG:NH2	2.24	0.56
2:CCC:1312:ASN:OD1	2:CCC:1312:ASN:O	2.22	0.56
3:DDD:367:GLY:HA3	3:DDD:448:GLN:HB2	1.85	0.56
3:DDD:929:GLN:O	3:DDD:933:ARG:HB2	2.05	0.56
5:FFF:144:THR:HG22	6:111:39:DA:H8	1.69	0.56
5:FFF:226:LEU:CB	7:222:19:DA:H61	2.18	0.56
5:FFF:226:LEU:HB3	7:222:19:DA:H61	1.70	0.56
3:DDD:279:LEU:HD13	3:DDD:295:GLU:HB3	1.87	0.56
1:AAA:135:ASP:OD1	1:AAA:136:GLU:N	2.38	0.56
2:CCC:563:THR:HG21	3:DDD:780:ARG:NH2	2.21	0.56
2:CCC:1099:ASN:OD1	2:CCC:1100:PRO:HD2	2.06	0.56
3:DDD:451:PRO:CB	3:DDD:625:MET:SD	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:502:PRO:CB	3:DDD:506:VAL:HG11	2.35	0.56
2:CCC:289:VAL:HG12	2:CCC:319:LEU:HD23	1.87	0.56
2:CCC:342:ASP:O	2:CCC:437:ASN:ND2	2.38	0.56
3:DDD:572:THR:HG1	3:DDD:576:ARG:CD	2.16	0.56
3:DDD:1169:THR:OG1	3:DDD:1174:ARG:NH2	2.37	0.56
2:CCC:369:MET:HG3	2:CCC:370:MET:N	2.21	0.56
2:CCC:1223:ARG:NH2	3:DDD:719:PHE:O	2.38	0.56
3:DDD:97:VAL:HG11	3:DDD:101:ARG:NE	2.20	0.56
3:DDD:800:LEU:CD2	3:DDD:1309:ILE:HD11	2.35	0.56
2:CCC:804:PHE:O	3:DDD:638:SER:HB3	2.04	0.56
4:EEE:30:MET:HG2	4:EEE:35:LYS:O	2.05	0.56
3:DDD:974:VAL:CG1	3:DDD:1028:ILE:HD13	2.36	0.56
5:FFF:78:TYR:OH	5:FFF:82:ARG:NH1	2.38	0.56
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:CE	2.36	0.55
3:DDD:620:PHE:O	3:DDD:624:ILE:HG13	2.07	0.55
1:BBB:47:LEU:HA	1:BBB:51:MET:HG2	1.87	0.55
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.22	0.55
5:FFF:109:TYR:CD2	5:FFF:154:ILE:HG21	2.41	0.55
2:CCC:661:VAL:CG1	2:CCC:665:ALA:HB3	2.36	0.55
5:FFF:119:LEU:CD2	5:FFF:158:ILE:HD11	2.37	0.55
2:CCC:444:ASP:O	2:CCC:450:ASN:ND2	2.39	0.55
3:DDD:858:VAL:CG2	3:DDD:868:TRP:CE3	2.81	0.55
3:DDD:974:VAL:HG11	3:DDD:1028:ILE:HD13	1.88	0.55
2:CCC:1107:MET:CE	3:DDD:739:GLN:CB	2.81	0.55
3:DDD:673:VAL:HG11	3:DDD:678:ARG:HB2	1.86	0.55
3:DDD:709:ARG:O	3:DDD:710:ASP:C	2.44	0.55
3:DDD:812:ASP:OD1	3:DDD:812:ASP:N	2.38	0.55
3:DDD:1157:ALA:HB3	3:DDD:1208:ASP:H	1.72	0.55
2:CCC:123:TYR:CE1	5:FFF:190:ASP:O	2.60	0.55
2:CCC:257:ALA:O	2:CCC:258:ASN:HB3	2.07	0.55
3:DDD:394:ILE:HD13	5:FFF:250:THR:HG22	1.89	0.55
3:DDD:686:TRP:CD2	3:DDD:758:PRO:HG3	2.42	0.55
5:FFF:143:SER:CB	6:111:41:DT:H72	2.37	0.55
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CZ	2.42	0.55
2:CCC:1270:PHE:CE1	2:CCC:1290:MET:CE	2.90	0.55
3:DDD:797:THR:O	3:DDD:801:VAL:HG23	2.07	0.55
2:CCC:253:PHE:CE1	2:CCC:287:VAL:HG12	2.42	0.55
3:DDD:427:PRO:HG2	3:DDD:429:LEU:HD21	1.88	0.55
8:333:101:2DT:H2'	11:333:201:CTP:N1	2.19	0.55
2:CCC:1104:PRO:HA	3:DDD:740:LEU:HD11	1.89	0.54
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:488:ASN:OD1	4:EEE:5:THR:HG23	2.06	0.54
3:DDD:502:PRO:HB2	3:DDD:506:VAL:CG1	2.37	0.54
1:BBB:196:THR:HG21	3:DDD:370:LYS:HZ1	1.72	0.54
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HG3	2.38	0.54
1:AAA:45:ARG:NH1	2:CCC:1216:ARG:HA	2.21	0.54
1:BBB:83:LEU:CG	3:DDD:526:VAL:CG1	2.84	0.54
2:CCC:369:MET:CG	2:CCC:370:MET:N	2.69	0.54
2:CCC:369:MET:HG2	2:CCC:370:MET:HG2	1.90	0.54
2:CCC:764:CYS:SG	2:CCC:833:ILE:HD11	2.48	0.54
2:CCC:1112:ILE:CG2	3:DDD:641:ILE:HG12	2.37	0.54
3:DDD:791:ALA:HA	7:222:12:DG:C8	2.41	0.54
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HD11	2.37	0.54
3:DDD:1042:ASP:OD1	3:DDD:1043:GLY:N	2.40	0.54
2:CCC:494:ASN:ND2	7:222:25:DA:OP1	2.40	0.54
2:CCC:599:VAL:HG21	2:CCC:623:LEU:HD21	1.89	0.54
2:CCC:666:SER:HA	2:CCC:1186:VAL:HG21	1.90	0.54
1:AAA:22:THR:OG1	1:AAA:207:THR:O	2.19	0.54
2:CCC:139:ASN:HD22	7:222:20:DG:H5"	1.72	0.54
2:CCC:1107:MET:HE2	3:DDD:739:GLN:HB3	1.89	0.54
3:DDD:506:VAL:CG1	3:DDD:624:ILE:O	2.52	0.54
3:DDD:517:CYS:N	3:DDD:545:HIS:CB	2.69	0.54
3:DDD:530:PRO:HD3	3:DDD:552:ILE:CD1	2.38	0.54
4:EEE:18:ASP:O	4:EEE:22:VAL:HG23	2.08	0.54
2:CCC:890:LYS:HB2	2:CCC:914:LYS:HG3	1.89	0.54
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CD2	2.40	0.54
3:DDD:747:MET:HA	3:DDD:940:ALA:HA	1.89	0.54
2:CCC:277:LEU:HD12	2:CCC:282:VAL:HG21	1.90	0.54
2:CCC:808:ASN:HD22	2:CCC:808:ASN:N	2.04	0.54
2:CCC:1269:ARG:CB	7:222:15:DT:OP1	2.55	0.54
3:DDD:552:ILE:HG23	3:DDD:580:TRP:CD1	2.42	0.54
6:111:51:DC:H2"	6:111:52:DT:H5'	1.90	0.54
2:CCC:560:PRO:CB	3:DDD:776:THR:HG21	2.32	0.54
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG22	1.87	0.54
3:DDD:114:ILE:HG12	3:DDD:311:ARG:HD2	1.89	0.54
3:DDD:555:TYR:O	3:DDD:586:GLY:CA	2.56	0.54
5:FFF:102:VAL:HG11	5:FFF:124:ASN:OD1	2.08	0.54
2:CCC:1186:VAL:HG12	2:CCC:1187:PHE:CD2	2.42	0.53
2:CCC:1196:LYS:NZ	3:DDD:642:ASP:OD2	2.41	0.53
3:DDD:635:SER:OG	3:DDD:637:ALA:HB2	2.08	0.53
1:BBB:86:LYS:HE2	1:BBB:174:ASP:HB2	1.90	0.53
2:CCC:155:VAL:CG2	2:CCC:405:PHE:CD2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG23	1.89	0.53
3:DDD:517:CYS:CB	3:DDD:545:HIS:CB	2.84	0.53
3:DDD:1064:SER:HA	3:DDD:1067:ARG:HB3	1.90	0.53
5:FFF:144:THR:HG22	6:111:39:DA:C8	2.43	0.53
2:CCC:49:LEU:CD2	2:CCC:464:PHE:CE2	2.91	0.53
2:CCC:244:GLU:HG2	2:CCC:245:ARG:N	2.23	0.53
5:FFF:80:ALA:O	5:FFF:84:LEU:HG	2.08	0.53
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.91	0.53
1:AAA:44:ARG:NH2	2:CCC:1215:GLY:HA2	2.23	0.53
2:CCC:290:GLU:O	2:CCC:290:GLU:HG2	2.08	0.53
2:CCC:521:LEU:HD13	2:CCC:667:LEU:HD11	1.91	0.53
2:CCC:734:ILE:HD11	2:CCC:777:VAL:CG2	2.38	0.53
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:CD	2.38	0.53
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HE	2.22	0.53
3:DDD:574:VAL:O	3:DDD:578:ILE:HG13	2.09	0.53
3:DDD:807:LEU:HD23	3:DDD:1255:VAL:HG13	1.91	0.53
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD21	1.90	0.53
2:CCC:13:LYS:NZ	2:CCC:1151:LEU:HB3	2.24	0.53
3:DDD:1052:GLU:HG2	3:DDD:1053:LEU:H	1.73	0.53
8:333:101:2DT:H2"	11:333:201:CTP:C1'	2.39	0.53
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD13	1.89	0.53
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.38	0.53
3:DDD:476:ALA:HA	3:DDD:479:GLU:HG3	1.91	0.53
3:DDD:747:MET:SD	3:DDD:759:ILE:HD12	2.50	0.53
3:DDD:1292:LEU:O	3:DDD:1296:GLY:N	2.37	0.53
7:222:27:DA:H2"	7:222:28:DG:C8	2.44	0.53
2:CCC:800:MET:SD	2:CCC:828:PHE:HE2	2.31	0.52
2:CCC:901:LEU:CD1	5:FFF:278:PHE:CE2	2.89	0.52
1:AAA:31:LEU:CD1	1:AAA:201:LEU:HB2	2.39	0.52
1:BBB:64:VAL:HG13	1:BBB:78:ILE:HD13	1.91	0.52
1:BBB:192:VAL:O	1:BBB:194:GLN:N	2.42	0.52
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.90	0.52
3:DDD:97:VAL:CG1	3:DDD:101:ARG:NE	2.72	0.52
3:DDD:278:ARG:HB3	3:DDD:295:GLU:OE2	2.09	0.52
3:DDD:839:VAL:CG1	3:DDD:882:VAL:HG11	2.32	0.52
2:CCC:477:GLU:HG3	2:CCC:478:ARG:N	2.22	0.52
3:DDD:492:SER:HB2	3:DDD:499:ILE:CD1	2.40	0.52
3:DDD:839:VAL:O	3:DDD:864:LEU:HD12	2.09	0.52
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.92	0.52
1:BBB:179:PRO:HG3	1:BBB:211:ILE:CD1	2.34	0.52
3:DDD:506:VAL:HG13	3:DDD:628:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:86:LYS:CE	1:BBB:173:VAL:HG12	2.39	0.52
3:DDD:709:ARG:O	3:DDD:709:ARG:HG3	2.09	0.52
3:DDD:1152:GLU:CD	3:DDD:1193:TRP:HH2	2.12	0.52
2:CCC:503:LYS:HD2	7:222:23:DT:OP1	2.09	0.52
2:CCC:1160:ASP:O	2:CCC:1161:LEU:C	2.48	0.52
3:DDD:835:LEU:HD13	3:DDD:878:ASP:O	2.10	0.52
2:CCC:812:PHE:HD2	3:DDD:461:PHE:HE2	1.56	0.52
5:FFF:226:LEU:HB3	7:222:19:DA:N6	2.25	0.52
2:CCC:555:TYR:CE1	2:CCC:637:ARG:CZ	2.93	0.51
3:DDD:421:VAL:CG1	3:DDD:468:VAL:HG13	2.40	0.51
3:DDD:1270:GLY:HA2	3:DDD:1298:VAL:O	2.11	0.51
5:FFF:104:LYS:HG3	6:111:41:DT:H4'	1.91	0.51
2:CCC:820:GLU:O	2:CCC:824:GLN:HG3	2.10	0.51
2:CCC:847:PRO:HB3	2:CCC:1047:LEU:HD11	1.91	0.51
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CE2	2.45	0.51
2:CCC:1283:ALA:HB1	2:CCC:1286:THR:OG1	2.10	0.51
3:DDD:111:THR:HG21	3:DDD:303:VAL:HG11	1.92	0.51
3:DDD:511:TYR:CZ	3:DDD:727:ASP:OD2	2.63	0.51
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	1.92	0.51
2:CCC:1312:ASN:OD1	2:CCC:1312:ASN:C	2.49	0.51
3:DDD:750:PRO:HB3	3:DDD:781:LYS:CD	2.37	0.51
2:CCC:89:GLY:HA2	2:CCC:140:GLY:HA3	1.93	0.51
3:DDD:519:ASN:HD21	3:DDD:709:ARG:HA	1.72	0.51
5:FFF:208:ASP:O	5:FFF:212:MET:HG2	2.10	0.51
5:FFF:228:GLY:CA	8:333:14:GTP:O2G	2.59	0.51
2:CCC:297:VAL:HG22	2:CCC:315:MET:O	2.10	0.51
2:CCC:739:ASP:OD1	2:CCC:739:ASP:N	2.43	0.51
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	1.92	0.51
3:DDD:464:ASP:OD1	3:DDD:464:ASP:N	2.43	0.51
3:DDD:885:VAL:O	3:DDD:1258:ARG:HD2	2.10	0.51
5:FFF:178:TYR:CE1	5:FFF:209:VAL:HG22	2.46	0.51
2:CCC:1161:LEU:O	2:CCC:1163:THR:N	2.44	0.51
2:CCC:532:ALA:HB1	2:CCC:538:LEU:HD12	1.93	0.51
3:DDD:114:ILE:HG23	3:DDD:115:TRP:N	2.24	0.51
3:DDD:115:TRP:CZ2	3:DDD:1329:THR:HG22	2.46	0.51
3:DDD:525:MET:H	3:DDD:548:VAL:HG23	1.76	0.51
3:DDD:836:ARG:CG	3:DDD:869:CYS:HB3	2.41	0.51
2:CCC:1001:GLY:HA2	2:CCC:1011:LEU:CD2	2.41	0.51
3:DDD:888:CYS:CB	3:DDD:898:CYS:SG	2.99	0.51
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.91	0.51
2:CCC:521:LEU:HD13	2:CCC:667:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG21	1.92	0.51
2:CCC:1263:ALA:HB2	7:222:17:DG:OP1	2.11	0.51
3:DDD:462:ASP:OD2	11:333:201:CTP:O1G	2.28	0.51
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.93	0.51
2:CCC:400:VAL:HG13	2:CCC:584:TYR:HB3	1.92	0.50
3:DDD:295:GLU:OE1	5:FFF:121:GLU:HG2	2.11	0.50
3:DDD:508:LEU:HD13	3:DDD:725:MET:HA	1.93	0.50
5:FFF:66:GLY:HA2	5:FFF:100:ARG:NH2	2.26	0.50
1:AAA:86:LYS:HE2	1:AAA:174:ASP:HB2	1.92	0.50
3:DDD:63:GLY:O	3:DDD:98:ARG:HD2	2.11	0.50
3:DDD:750:PRO:C	3:DDD:781:LYS:HE3	2.32	0.50
5:FFF:231:GLU:HG2	5:FFF:232:LYS:N	2.26	0.50
2:CCC:1077:SER:HA	3:DDD:356:THR:HG23	1.92	0.50
3:DDD:335:GLN:O	3:DDD:336:GLY:O	2.29	0.50
3:DDD:965:SER:CB	3:DDD:975:ILE:HA	2.40	0.50
2:CCC:1101:LEU:HD22	3:DDD:731:ARG:HB2	1.92	0.50
3:DDD:1079:LYS:HE3	3:DDD:1087:ASP:OD1	2.10	0.50
2:CCC:551:HIS:H	2:CCC:554:HIS:CE1	2.29	0.50
2:CCC:1214:ASP:OD1	2:CCC:1214:ASP:C	2.50	0.50
3:DDD:279:LEU:O	3:DDD:283:LEU:HG	2.11	0.50
3:DDD:889:ASP:OD1	3:DDD:1290:ARG:NH2	2.43	0.50
7:222:20:DG:C3'	7:222:21:DG:H5"	2.40	0.50
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.94	0.50
1:AAA:227:GLN:OE1	1:BBB:11:PRO:CD	2.59	0.50
2:CCC:135:THR:HG21	2:CCC:515:MET:HE1	1.93	0.50
3:DDD:707:ILE:HD12	3:DDD:716:GLN:HE21	1.77	0.50
3:DDD:1368:ASP:O	3:DDD:1371:ARG:HG2	2.11	0.50
3:DDD:622:ASP:HB3	3:DDD:626:TYR:HE2	1.77	0.50
1:BBB:47:LEU:HD13	1:BBB:205:MET:HE2	1.93	0.50
3:DDD:101:ARG:O	3:DDD:246:PRO:HG3	2.11	0.50
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.32	0.50
3:DDD:360:TYR:OH	3:DDD:448:GLN:OE1	2.24	0.50
3:DDD:432:LEU:HD12	3:DDD:499:ILE:HD12	1.93	0.50
2:CCC:201:ARG:CB	2:CCC:369:MET:HE2	2.42	0.50
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	1.93	0.50
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.26	0.50
3:DDD:423:LEU:HB3	3:DDD:466:MET:HE1	1.93	0.50
3:DDD:1238:GLN:O	3:DDD:1242:ARG:HB2	2.11	0.50
1:AAA:135:ASP:OD1	1:AAA:137:ASN:N	2.36	0.49
2:CCC:165:HIS:HB3	2:CCC:167:SER:HB3	1.94	0.49
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1308:GLY:O	3:DDD:1310:THR:N	2.45	0.49
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.42	0.49
2:CCC:642:SER:CB	3:DDD:770:LEU:HD21	2.42	0.49
2:CCC:812:PHE:CD2	3:DDD:461:PHE:HE2	2.29	0.49
2:CCC:1280:ALA:O	2:CCC:1281:TYR:O	2.30	0.49
3:DDD:795:TYR:CZ	3:DDD:799:ARG:HD3	2.48	0.49
3:DDD:1082:ASP:OD1	3:DDD:1084:GLN:N	2.45	0.49
5:FFF:225:PRO:CB	5:FFF:230:SER:HA	2.41	0.49
1:AAA:102:LEU:HB2	1:AAA:115:ILE:HG12	1.94	0.49
1:BBB:16:ILE:HD13	1:BBB:214:GLU:OE2	2.12	0.49
2:CCC:66:SER:HB2	2:CCC:479:LEU:HD22	1.94	0.49
2:CCC:598:VAL:HG13	2:CCC:627:GLY:HA2	1.94	0.49
2:CCC:720:ARG:HD3	2:CCC:736:VAL:HG11	1.94	0.49
3:DDD:377:PHE:O	3:DDD:381:ILE:HG13	2.13	0.49
2:CCC:155:VAL:HG23	2:CCC:405:PHE:CD2	2.47	0.49
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.94	0.49
3:DDD:506:VAL:O	3:DDD:628:GLY:HA3	2.12	0.49
3:DDD:645:VAL:HG23	3:DDD:645:VAL:O	2.13	0.49
2:CCC:555:TYR:CD1	2:CCC:637:ARG:CZ	2.96	0.49
5:FFF:133:LYS:NZ	6:111:35:DC:OP2	2.36	0.49
7:222:25:DA:O5'	7:222:25:DA:H8	1.96	0.49
2:CCC:374:GLU:OE2	6:111:43:DT:H72	2.13	0.49
2:CCC:453:ILE:HD11	2:CCC:530:ILE:HD13	1.94	0.49
2:CCC:799:ASN:C	2:CCC:800:MET:HG2	2.32	0.49
3:DDD:505:ASP:HB2	3:DDD:629:PHE:CE1	2.45	0.49
7:222:23:DT:H2'	7:222:24:DT:C6	2.47	0.49
1:BBB:158:ARG:HD2	1:BBB:172:LEU:HD21	1.95	0.49
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CE2	2.48	0.49
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.76	0.49
3:DDD:750:PRO:HB3	3:DDD:781:LYS:CG	2.42	0.49
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CG	2.90	0.49
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	1.94	0.49
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.94	0.49
2:CCC:97:ARG:NH2	5:FFF:188:LYS:O	2.45	0.49
2:CCC:478:ARG:NH1	2:CCC:491:ASP:O	2.46	0.49
2:CCC:797:GLY:O	2:CCC:1231:TYR:OH	2.31	0.49
2:CCC:675:ASP:HA	3:DDD:763:PHE:CZ	2.48	0.49
3:DDD:161:THR:H	3:DDD:164:GLN:HB2	1.78	0.49
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:HA	1.94	0.49
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.43	0.49
3:DDD:1163:VAL:HG11	3:DDD:1175:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:156:ARG:HE	6:111:33:DT:H72	1.78	0.49
2:CCC:244:GLU:HG2	2:CCC:245:ARG:H	1.78	0.48
2:CCC:870:ILE:HD12	2:CCC:1050:VAL:HG11	1.94	0.48
2:CCC:1017:GLN:NE2	2:CCC:1021:LEU:HG	2.28	0.48
2:CCC:1083:GLU:H	2:CCC:1083:GLU:CD	2.15	0.48
3:DDD:115:TRP:O	3:DDD:119:SER:HB3	2.13	0.48
3:DDD:1249:ASN:OD1	3:DDD:1250:ASP:N	2.45	0.48
8:333:15:A:H2'	8:333:16:G:H5'	1.95	0.48
2:CCC:263:VAL:HG12	2:CCC:264:GLU:O	2.13	0.48
3:DDD:399:LYS:NZ	5:FFF:329:LEU:HG	2.28	0.48
3:DDD:506:VAL:CG1	3:DDD:625:MET:HA	2.43	0.48
3:DDD:1134:ILE:HG23	3:DDD:1138:LEU:HG	1.94	0.48
3:DDD:1152:GLU:HA	3:DDD:1194:ARG:HH22	1.78	0.48
2:CCC:685:MET:HE2	2:CCC:1235:LEU:CD1	2.43	0.48
3:DDD:608:CYS:SG	3:DDD:612:LEU:HD12	2.52	0.48
3:DDD:746:LEU:O	3:DDD:940:ALA:HB1	2.13	0.48
3:DDD:1037:PHE:CZ	3:DDD:1059:LEU:CD1	2.96	0.48
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.78	0.48
7:222:16:DC:C3'	7:222:17:DG:H5'	2.43	0.48
2:CCC:277:LEU:CD1	2:CCC:282:VAL:HG21	2.43	0.48
2:CCC:517:GLN:N	2:CCC:761:GLN:OE1	2.47	0.48
2:CCC:898:GLU:OE2	5:FFF:259:ILE:HD13	2.13	0.48
3:DDD:333:GLY:O	3:DDD:336:GLY:N	2.39	0.48
3:DDD:458:ASN:HD22	3:DDD:929:GLN:HE22	1.62	0.48
4:EEE:13:ILE:HD12	4:EEE:19:LEU:HA	1.95	0.48
5:FFF:122:GLU:HG2	5:FFF:157:ALA:CB	2.43	0.48
1:AAA:86:LYS:CE	1:AAA:174:ASP:HB2	2.43	0.48
3:DDD:750:PRO:CB	3:DDD:781:LYS:HE3	2.44	0.48
3:DDD:334:LYS:NZ	7:222:13:DA:OP2	2.37	0.48
2:CCC:93:SER:HG	2:CCC:126:GLU:HB3	1.78	0.48
2:CCC:734:ILE:HG22	2:CCC:749:ASP:HB2	1.96	0.48
3:DDD:395:LYS:HE2	5:FFF:329:LEU:HD13	1.96	0.48
3:DDD:615:LYS:HE3	4:EEE:5:THR:HB	1.96	0.48
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.95	0.48
3:DDD:1364:ALA:O	3:DDD:1367:GLN:HG2	2.13	0.48
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.31	0.48
6:111:54:DA:C2	6:111:55:DC:C2	3.02	0.48
1:AAA:44:ARG:HH21	2:CCC:1215:GLY:HA2	1.79	0.48
3:DDD:506:VAL:HG21	3:DDD:625:MET:CA	2.41	0.48
3:DDD:1330:ARG:NH1	7:222:9:DT:H5"	2.29	0.48
5:FFF:177:VAL:O	5:FFF:181:THR:OG1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:20:GLN:O	2:CCC:20:GLN:HG3	2.14	0.48
2:CCC:549:ASP:CB	3:DDD:750:PRO:HG3	2.44	0.48
2:CCC:677:ASN:OD1	3:DDD:779:ALA:HB1	2.14	0.48
3:DDD:795:TYR:CE2	3:DDD:799:ARG:NE	2.82	0.48
8:333:14:GTP:O5'	8:333:14:GTP:H8	1.97	0.48
2:CCC:194:LEU:HA	2:CCC:194:LEU:HD12	1.77	0.47
2:CCC:660:VAL:HG21	3:DDD:769:VAL:CG1	2.44	0.47
2:CCC:871:VAL:CG2	2:CCC:883:LEU:HA	2.44	0.47
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:OE2	2.14	0.47
2:CCC:1292:THR:CG2	2:CCC:1293:VAL:N	2.77	0.47
2:CCC:44:GLU:HG3	2:CCC:45:GLY:H	1.79	0.47
2:CCC:216:THR:HG23	2:CCC:219:GLN:OE1	2.14	0.47
2:CCC:297:VAL:HG13	2:CCC:317:LEU:CG	2.45	0.47
2:CCC:549:ASP:OD2	3:DDD:750:PRO:HG2	2.14	0.47
2:CCC:661:VAL:HG12	2:CCC:662:SER:O	2.14	0.47
3:DDD:151:MET:SD	3:DDD:151:MET:N	2.87	0.47
5:FFF:138:ARG:HG2	5:FFF:140:PHE:HD2	1.80	0.47
2:CCC:244:GLU:O	2:CCC:245:ARG:C	2.51	0.47
1:AAA:29:GLU:CB	1:AAA:30:PRO:HA	2.43	0.47
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	2.13	0.47
2:CCC:839:VAL:HG13	2:CCC:1046:VAL:HG13	1.96	0.47
3:DDD:108:ALA:HB3	3:DDD:279:LEU:HD23	1.96	0.47
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.97	0.47
3:DDD:824:PRO:HG3	3:DDD:878:ASP:OD1	2.15	0.47
3:DDD:1111:ASP:OD1	3:DDD:1112:GLY:N	2.47	0.47
1:AAA:211:ILE:HG22	1:AAA:216:ALA:HB2	1.95	0.47
2:CCC:206:ALA:O	2:CCC:209:ILE:HG22	2.15	0.47
2:CCC:660:VAL:HG21	3:DDD:769:VAL:HG12	1.97	0.47
2:CCC:720:ARG:HB2	2:CCC:749:ASP:OD2	2.15	0.47
2:CCC:1117:LEU:HD13	2:CCC:1195:ILE:HG12	1.96	0.47
3:DDD:931:THR:O	3:DDD:935:PHE:HD2	1.95	0.47
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.44	0.47
2:CCC:447:HIS:HD2	2:CCC:449:GLY:H	1.59	0.47
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.77	0.47
2:CCC:812:PHE:HE1	3:DDD:629:PHE:HZ	1.56	0.47
2:CCC:838:CYS:SG	2:CCC:886:LYS:HE2	2.55	0.47
2:CCC:842:ASP:HB3	2:CCC:1047:LEU:HD21	1.97	0.47
3:DDD:68:TYR:CE1	3:DDD:93:THR:HA	2.50	0.47
3:DDD:161:THR:N	3:DDD:164:GLN:HB2	2.30	0.47
3:DDD:707:ILE:HD12	3:DDD:716:GLN:NE2	2.29	0.47
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1307:LEU:HB2	3:DDD:1312:ALA:HB2	1.97	0.47
5:FFF:143:SER:HB3	6:111:41:DT:H72	1.96	0.47
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.15	0.47
1:BBB:64:VAL:CG1	1:BBB:78:ILE:HD13	2.44	0.47
1:BBB:86:LYS:HG2	1:BBB:174:ASP:O	2.15	0.47
3:DDD:516:ASP:C	3:DDD:545:HIS:HB3	2.34	0.47
2:CCC:277:LEU:HD12	2:CCC:277:LEU:HA	1.82	0.47
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CE1	2.50	0.47
3:DDD:45:ASN:HB2	3:DDD:52:GLU:OE1	2.15	0.47
2:CCC:473:ARG:O	2:CCC:477:GLU:HB3	2.15	0.47
3:DDD:399:LYS:HZ2	5:FFF:329:LEU:HG	1.80	0.47
3:DDD:750:PRO:CA	3:DDD:781:LYS:CB	2.85	0.47
4:EEE:60:ASN:HB3	4:EEE:63:ILE:HD12	1.96	0.47
2:CCC:1243:MET:SD	3:DDD:445:LYS:HG2	2.55	0.46
3:DDD:382:TYR:OH	3:DDD:398:LYS:HG2	2.15	0.46
3:DDD:803:VAL:HG22	3:DDD:1313:SER:OG	2.15	0.46
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CD1	2.94	0.46
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	1.97	0.46
5:FFF:182:ALA:CB	5:FFF:193:PRO:HG3	2.43	0.46
5:FFF:227:GLY:HA2	7:222:18:DT:H3	1.80	0.46
6:111:56:DG:H2"	6:111:57:DC:OP2	2.14	0.46
7:222:27:DA:C2'	7:222:28:DG:C8	2.98	0.46
1:AAA:190:ALA:O	1:AAA:192:VAL:N	2.48	0.46
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	2.16	0.46
2:CCC:292:ILE:CB	2:CCC:322:LEU:HD11	2.45	0.46
2:CCC:720:ARG:HB3	2:CCC:736:VAL:HG13	1.96	0.46
2:CCC:806:PRO:HB2	3:DDD:633:ALA:CB	2.44	0.46
2:CCC:1214:ASP:OD1	2:CCC:1215:GLY:N	2.48	0.46
3:DDD:395:LYS:HE3	5:FFF:251:GLN:OE1	2.14	0.46
3:DDD:450:HIS:NE2	3:DDD:622:ASP:OD1	2.48	0.46
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.48	0.46
2:CCC:594:VAL:HG22	2:CCC:599:VAL:HG22	1.96	0.46
2:CCC:812:PHE:HD2	3:DDD:461:PHE:CE2	2.33	0.46
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.96	0.46
3:DDD:174:ASP:N	3:DDD:174:ASP:OD1	2.48	0.46
3:DDD:290:ILE:H	3:DDD:290:ILE:HD12	1.80	0.46
3:DDD:511:TYR:CE1	3:DDD:727:ASP:OD2	2.68	0.46
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	1.97	0.46
3:DDD:836:ARG:NH2	3:DDD:870:ASP:OD1	2.47	0.46
3:DDD:960:LEU:HB3	3:DDD:963:VAL:HG11	1.98	0.46
2:CCC:524:ILE:HD12	2:CCC:708:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:848:GLU:OE1	2:CCC:886:LYS:HD3	2.15	0.46
2:CCC:873:ILE:HD11	2:CCC:944:ARG:HH22	1.79	0.46
2:CCC:1111:GLN:HB2	2:CCC:1230:MET:HE1	1.97	0.46
3:DDD:511:TYR:CE2	3:DDD:515:ARG:HD3	2.43	0.46
3:DDD:584:PRO:HD3	3:DDD:620:PHE:CD1	2.51	0.46
5:FFF:277:ARG:CD	5:FFF:306:GLN:HE21	2.29	0.46
1:BBB:31:LEU:CD1	1:BBB:201:LEU:HB2	2.46	0.46
1:BBB:86:LYS:HE2	1:BBB:173:VAL:HG12	1.98	0.46
2:CCC:514:PHE:CZ	7:222:19:DA:C5'	2.98	0.46
2:CCC:1269:ARG:HA	3:DDD:346:ARG:HA	1.97	0.46
3:DDD:209:ASN:HB2	3:DDD:214:ARG:HG3	1.97	0.46
3:DDD:805:GLN:HG2	3:DDD:806:ASP:N	2.29	0.46
4:EEE:41:GLU:O	4:EEE:44:ASP:HB2	2.15	0.46
1:AAA:225:ALA:HB2	1:BBB:228:LEU:HD13	1.97	0.46
1:AAA:233:ASP:O	1:AAA:235:ARG:N	2.48	0.46
2:CCC:53:PHE:HB3	2:CCC:70:TYR:CD2	2.50	0.46
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:N	2.26	0.46
3:DDD:118:LYS:NZ	3:DDD:136:GLU:OE2	2.48	0.46
4:EEE:17:PHE:O	4:EEE:21:LEU:HG	2.15	0.46
5:FFF:169:ILE:O	5:FFF:173:LYS:HG2	2.15	0.46
7:222:7:DC:C4	7:222:8:DG:C6	3.03	0.46
2:CCC:1028:LYS:O	2:CCC:1032:LYS:HG2	2.15	0.46
3:DDD:44:ILE:HG22	3:DDD:51:PRO:HA	1.97	0.46
5:FFF:204:LYS:HB3	5:FFF:205:PRO:HD2	1.98	0.46
1:AAA:135:ASP:OD1	1:AAA:135:ASP:C	2.54	0.46
2:CCC:1327:LEU:O	2:CCC:1331:ARG:HG3	2.16	0.46
3:DDD:334:LYS:HB2	3:DDD:339:ARG:NH1	2.31	0.46
7:222:20:DG:O3'	7:222:22:DA:H5"	2.15	0.46
1:AAA:195:ARG:HD2	1:AAA:198:LEU:HD23	1.97	0.46
2:CCC:538:LEU:HD23	2:CCC:542:ARG:NH2	2.31	0.46
3:DDD:667:GLN:O	3:DDD:670:SER:OG	2.21	0.46
1:AAA:222:THR:OG1	1:BBB:233:ASP:CB	2.60	0.46
2:CCC:409:LEU:HD13	2:CCC:427:ASP:HB3	1.98	0.46
2:CCC:479:LEU:HD21	2:CCC:492:MET:HE1	1.98	0.46
2:CCC:871:VAL:HG23	2:CCC:883:LEU:O	2.16	0.46
2:CCC:1131:MET:HG2	2:CCC:1136:GLN:OE1	2.16	0.46
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:CD1	2.45	0.46
2:CCC:840:SER:HB3	2:CCC:850:ILE:HD11	1.97	0.45
2:CCC:1081:PRO:CB	2:CCC:1083:GLU:OE2	2.65	0.45
2:CCC:1129:ASN:CA	2:CCC:1177:ARG:HG3	2.46	0.45
3:DDD:516:ASP:HA	3:DDD:545:HIS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:886:VAL:CG1	3:DDD:1226:VAL:CG1	2.95	0.45
3:DDD:925:GLU:HB3	3:DDD:926:PRO:CD	2.47	0.45
1:BBB:157:THR:HG22	1:BBB:157:THR:O	2.15	0.45
2:CCC:104:ILE:HD13	2:CCC:484:LEU:HB3	1.98	0.45
2:CCC:515:MET:HG2	2:CCC:517:GLN:HG3	1.98	0.45
2:CCC:736:VAL:O	2:CCC:741:MET:HE3	2.16	0.45
2:CCC:1290:MET:SD	3:DDD:347:VAL:HG11	2.56	0.45
3:DDD:291:ILE:HD11	5:FFF:99:LEU:HD21	1.99	0.45
3:DDD:872:LEU:CD2	3:DDD:877:VAL:HG21	2.45	0.45
3:DDD:945:ALA:O	3:DDD:947:GLU:N	2.46	0.45
5:FFF:156:ARG:HE	6:111:33:DT:C7	2.30	0.45
7:222:17:DG:H2'	7:222:18:DT:O4'	2.16	0.45
2:CCC:1269:ARG:HH21	2:CCC:1271:GLY:HA2	1.82	0.45
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.47	0.45
1:BBB:225:ALA:HA	1:BBB:228:LEU:HD12	1.98	0.45
2:CCC:812:PHE:HB3	3:DDD:357:VAL:HG21	1.98	0.45
3:DDD:248:ASP:N	3:DDD:248:ASP:OD1	2.49	0.45
3:DDD:703:THR:O	3:DDD:704:GLU:C	2.55	0.45
3:DDD:733:SER:H	3:DDD:736:GLN:HG3	1.82	0.45
3:DDD:943:ARG:HG2	3:DDD:944:ALA:N	2.32	0.45
2:CCC:967:LEU:HD12	2:CCC:967:LEU:HA	1.86	0.45
3:DDD:347:VAL:HG12	3:DDD:348:ASP:O	2.17	0.45
3:DDD:923:ILE:HD12	3:DDD:1256:ILE:HD12	1.98	0.45
3:DDD:925:GLU:OE1	3:DDD:926:PRO:N	2.49	0.45
2:CCC:183:TRP:CH2	6:111:50:DT:C5	3.05	0.45
2:CCC:850:ILE:HG22	2:CCC:850:ILE:O	2.17	0.45
2:CCC:909:LYS:C	2:CCC:911:SER:H	2.19	0.45
2:CCC:1314:GLN:HA	4:EEE:28:ARG:NH2	2.31	0.45
3:DDD:197:GLU:OE1	3:DDD:220:ARG:NH2	2.49	0.45
3:DDD:205:LEU:HD22	3:DDD:214:ARG:HG2	1.97	0.45
3:DDD:487:THR:O	3:DDD:490:ILE:HG13	2.17	0.45
1:AAA:228:LEU:HD11	1:BBB:224:LEU:HG	1.99	0.45
2:CCC:207:THR:CG2	2:CCC:354:ASP:HB2	2.46	0.45
2:CCC:669:PRO:HB2	2:CCC:670:PHE:H	1.55	0.45
2:CCC:871:VAL:HG23	2:CCC:883:LEU:HA	1.99	0.45
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:NZ	2.31	0.45
3:DDD:665:GLN:O	3:DDD:668:PHE:HB3	2.17	0.45
3:DDD:1330:ARG:NH2	7:222:9:DT:C5'	2.80	0.45
1:AAA:231:PHE:O	1:AAA:235:ARG:OXT	2.35	0.45
2:CCC:173:ASN:C	2:CCC:173:ASN:OD1	2.54	0.45
3:DDD:121:PRO:O	3:DDD:122:SER:CB	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:491:LEU:HD23	3:DDD:498:PRO:HB3	1.98	0.45
3:DDD:507:VAL:HG12	3:DDD:728:SER:HB2	1.99	0.45
3:DDD:664:ILE:HG21	3:DDD:681:LYS:HD3	1.99	0.45
2:CCC:21:VAL:HG21	2:CCC:592:ARG:CZ	2.47	0.45
2:CCC:32:LEU:CD2	2:CCC:130:MET:CE	2.94	0.45
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CD2	2.52	0.45
2:CCC:150:HIS:CE1	2:CCC:452:ARG:HD3	2.52	0.45
2:CCC:582:ASN:HD21	2:CCC:586:PHE:HB2	1.82	0.45
2:CCC:806:PRO:HG2	3:DDD:633:ALA:HA	1.99	0.45
2:CCC:854:ILE:HD11	2:CCC:885:GLY:HA3	1.98	0.45
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	2.17	0.45
3:DDD:342:LEU:HD22	3:DDD:1352:ILE:O	2.17	0.45
3:DDD:750:PRO:HB2	3:DDD:781:LYS:CE	2.44	0.45
3:DDD:1100:PHE:CE1	3:DDD:1192:LYS:HE2	2.52	0.45
3:DDD:1174:ARG:O	3:DDD:1176:VAL:HG23	2.16	0.45
1:AAA:64:VAL:CG1	1:AAA:78:ILE:HD13	2.47	0.45
2:CCC:150:HIS:HE1	2:CCC:452:ARG:HH11	1.64	0.45
2:CCC:257:ALA:HB3	2:CCC:262:TYR:HE2	1.81	0.45
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD21	1.99	0.45
2:CCC:515:MET:SD	2:CCC:523:GLU:HG3	2.56	0.45
2:CCC:751:TYR:CD2	2:CCC:751:TYR:N	2.85	0.45
2:CCC:944:ARG:O	2:CCC:947:GLU:HG2	2.17	0.45
2:CCC:1280:ALA:HB1	3:DDD:918:ILE:HG12	1.98	0.45
3:DDD:58:CYS:SG	3:DDD:61:ILE:HG13	2.57	0.45
3:DDD:789:LYS:O	3:DDD:792:ASN:N	2.50	0.45
2:CCC:296:VAL:HB	2:CCC:336:LEU:HD12	1.99	0.44
2:CCC:978:VAL:O	2:CCC:981:ALA:HB3	2.17	0.44
3:DDD:1152:GLU:CB	3:DDD:1194:ARG:HH22	2.29	0.44
6:111:34:DG:N2	7:222:29:DC:O2	2.35	0.44
2:CCC:57:PHE:CE1	2:CCC:59:ILE:HD12	2.52	0.44
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.53	0.44
3:DDD:423:LEU:HB3	3:DDD:466:MET:CE	2.46	0.44
3:DDD:425:ARG:HD3	3:DDD:457:TYR:O	2.16	0.44
1:AAA:11:PRO:O	1:BBB:230:ALA:HB2	2.16	0.44
1:AAA:52:PRO:HG2	1:AAA:219:ARG:NH1	2.33	0.44
2:CCC:569:ILE:O	2:CCC:569:ILE:HG23	2.16	0.44
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.98	0.44
5:FFF:119:LEU:HD22	5:FFF:158:ILE:HD11	1.99	0.44
1:BBB:83:LEU:CD1	3:DDD:526:VAL:HG12	2.48	0.44
2:CCC:263:VAL:HG22	2:CCC:269:ILE:CD1	2.45	0.44
2:CCC:816:ILE:HD11	2:CCC:1074:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:364:HIS:CD2	4:EEE:4:VAL:HG13	2.52	0.44
3:DDD:622:ASP:HB3	3:DDD:626:TYR:CE2	2.52	0.44
3:DDD:795:TYR:CE2	3:DDD:799:ARG:CZ	3.00	0.44
3:DDD:858:VAL:HA	3:DDD:868:TRP:CZ3	2.53	0.44
3:DDD:1082:ASP:OD1	3:DDD:1082:ASP:C	2.56	0.44
1:AAA:152:TYR:CE2	2:CCC:824:GLN:HA	2.52	0.44
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	2.00	0.44
2:CCC:684:ASN:CG	2:CCC:687:ARG:HH21	2.21	0.44
5:FFF:241:GLU:C	5:FFF:243:GLU:N	2.71	0.44
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.50	0.44
2:CCC:196:VAL:CG2	2:CCC:206:ALA:HA	2.32	0.44
2:CCC:366:ILE:O	2:CCC:369:MET:HG2	2.16	0.44
2:CCC:832:HIS:CD2	2:CCC:1058:ARG:HD2	2.53	0.44
2:CCC:1075:VAL:HG21	3:DDD:463:GLY:HA2	2.00	0.44
3:DDD:622:ASP:O	3:DDD:626:TYR:CD2	2.70	0.44
3:DDD:750:PRO:CA	3:DDD:781:LYS:HB2	2.48	0.44
2:CCC:1280:ALA:C	2:CCC:1281:TYR:O	2.56	0.44
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.83	0.44
2:CCC:32:LEU:HD23	2:CCC:130:MET:HE1	1.99	0.44
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB3	2.00	0.44
2:CCC:512:SER:O	2:CCC:512:SER:OG	2.32	0.44
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG22	2.00	0.44
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.83	0.44
3:DDD:502:PRO:HG3	3:DDD:624:ILE:CG2	2.48	0.44
5:FFF:87:ASP:OD2	5:FFF:90:SER:HB2	2.17	0.44
6:111:54:DA:C2'	6:111:55:DC:H5'	2.47	0.44
1:AAA:195:ARG:HD2	1:AAA:198:LEU:CD2	2.48	0.44
1:BBB:86:LYS:HE3	1:BBB:173:VAL:HG12	1.99	0.44
2:CCC:1109:ILE:HD13	2:CCC:1109:ILE:HA	1.87	0.44
2:CCC:1269:ARG:NH1	3:DDD:340:GLN:O	2.48	0.44
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CD1	2.53	0.44
3:DDD:517:CYS:SG	3:DDD:518:VAL:N	2.91	0.44
3:DDD:551:ARG:O	3:DDD:551:ARG:HG2	2.17	0.44
3:DDD:505:ASP:O	3:DDD:632:ALA:HB2	2.18	0.43
3:DDD:572:THR:CG2	3:DDD:589:TYR:OH	2.59	0.43
3:DDD:965:SER:HB2	3:DDD:975:ILE:HA	2.00	0.43
3:DDD:1156:LEU:HD21	3:DDD:1224:ARG:NH2	2.31	0.43
1:BBB:83:LEU:HD11	3:DDD:526:VAL:HB	2.01	0.43
3:DDD:325:LYS:HE2	3:DDD:330:MET:HG2	2.00	0.43
3:DDD:530:PRO:HD3	3:DDD:552:ILE:HD12	1.98	0.43
2:CCC:15:PHE:O	2:CCC:17:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:32:LEU:CD2	2:CCC:130:MET:HE3	2.48	0.43
2:CCC:599:VAL:HG21	2:CCC:623:LEU:CD2	2.48	0.43
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CE1	2.54	0.43
2:CCC:812:PHE:HD1	3:DDD:629:PHE:CZ	2.36	0.43
2:CCC:1335:ILE:CG2	3:DDD:22:ILE:HG23	2.48	0.43
3:DDD:305:ALA:CB	3:DDD:316:ILE:HD12	2.48	0.43
3:DDD:936:HIS:CE1	11:333:201:CTP:O1B	2.71	0.43
2:CCC:453:ILE:CD1	2:CCC:530:ILE:HD13	2.49	0.43
2:CCC:576:SER:OG	2:CCC:577:VAL:N	2.51	0.43
2:CCC:582:ASN:OD1	2:CCC:585:GLY:N	2.50	0.43
2:CCC:1212:LEU:HD23	2:CCC:1212:LEU:HA	1.85	0.43
2:CCC:1293:VAL:HG12	2:CCC:1300:GLY:C	2.39	0.43
3:DDD:1152:GLU:OE1	3:DDD:1193:TRP:HH2	2.01	0.43
3:DDD:1370:MET:O	3:DDD:1373:ARG:HB2	2.18	0.43
4:EEE:8:ASP:HB2	4:EEE:55:GLU:CG	2.48	0.43
2:CCC:668:ILE:HG12	2:CCC:1069:ARG:O	2.19	0.43
2:CCC:818:VAL:HG23	2:CCC:1079:ILE:HG12	1.99	0.43
2:CCC:1075:VAL:CG2	3:DDD:463:GLY:HA2	2.48	0.43
2:CCC:1257:GLN:NE2	3:DDD:341:ASN:O	2.52	0.43
3:DDD:58:CYS:SG	3:DDD:61:ILE:N	2.92	0.43
3:DDD:1168:GLU:OE2	3:DDD:1173:ARG:NH1	2.52	0.43
5:FFF:145:TYR:CZ	5:FFF:149:TRP:NE1	2.85	0.43
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CZ	2.53	0.43
2:CCC:909:LYS:C	2:CCC:911:SER:N	2.72	0.43
3:DDD:127:LEU:HD23	3:DDD:127:LEU:HA	1.87	0.43
3:DDD:380:PHE:HB3	3:DDD:415:VAL:HG11	2.00	0.43
7:222:12:DG:H2'	7:222:13:DA:O5'	2.19	0.43
2:CCC:118:LYS:NZ	2:CCC:485:ASP:O	2.29	0.43
5:FFF:176:ASN:ND2	7:222:26:DT:H2'	2.33	0.43
5:FFF:225:PRO:HA	5:FFF:233:ALA:HA	2.01	0.43
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD11	2.01	0.43
2:CCC:90:VAL:HG12	2:CCC:91:THR:N	2.33	0.43
2:CCC:189:ASP:OD1	2:CCC:190:PRO:N	2.52	0.43
2:CCC:1109:ILE:HG22	2:CCC:1113:LEU:HD12	2.01	0.43
3:DDD:119:SER:O	3:DDD:122:SER:N	2.52	0.43
3:DDD:528:THR:HG23	3:DDD:532:GLU:OE1	2.19	0.43
3:DDD:572:THR:OG1	3:DDD:573:THR:N	2.50	0.43
3:DDD:579:LEU:HB3	3:DDD:592:VAL:HG21	2.01	0.43
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	2.18	0.43
3:DDD:1186:TYR:CZ	3:DDD:1188:GLU:OE2	2.72	0.43
3:DDD:1212:ASP:OD1	3:DDD:1212:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:30:PRO:HB2	1:BBB:198:LEU:CD1	2.49	0.43
2:CCC:963:GLU:O	2:CCC:967:LEU:HB2	2.19	0.43
2:CCC:1128:ILE:HD11	2:CCC:1145:ILE:HG12	2.00	0.43
2:CCC:1269:ARG:CA	7:222:15:DT:OP1	2.65	0.43
3:DDD:664:ILE:HD13	3:DDD:681:LYS:HG2	2.00	0.43
3:DDD:703:THR:O	3:DDD:705:THR:N	2.52	0.43
3:DDD:1196:LEU:HD22	3:DDD:1210:ILE:HG22	2.01	0.43
2:CCC:555:TYR:OH	2:CCC:654:ASP:OD2	2.20	0.43
2:CCC:1064:ASP:OD1	2:CCC:1239:VAL:HG12	2.18	0.43
2:CCC:1269:ARG:CB	7:222:15:DT:P	3.02	0.43
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.18	0.43
3:DDD:579:LEU:HD23	3:DDD:579:LEU:HA	1.87	0.43
3:DDD:848:VAL:HG12	3:DDD:848:VAL:O	2.19	0.43
6:111:38:DT:H2"	6:111:39:DA:C8	2.53	0.43
1:BBB:160:HIS:CD2	1:BBB:160:HIS:C	2.93	0.42
2:CCC:160:ASP:HB3	2:CCC:163:LYS:HD3	2.01	0.42
2:CCC:1296:ASP:CB	2:CCC:1321:GLU:H	2.31	0.42
3:DDD:398:LYS:HZ2	5:FFF:251:GLN:HB2	1.84	0.42
7:222:12:DG:C2'	7:222:13:DA:O5'	2.66	0.42
1:BBB:124:VAL:HG21	1:BBB:210:THR:CG2	2.42	0.42
2:CCC:1087:TYR:HD2	2:CCC:1091:GLY:HA2	1.84	0.42
2:CCC:1262:LYS:H	7:222:16:DC:H5'	1.84	0.42
3:DDD:703:THR:C	3:DDD:705:THR:N	2.71	0.42
3:DDD:994:SER:O	3:DDD:995:TYR:CG	2.72	0.42
3:DDD:1031:VAL:HG21	3:DDD:1097:ALA:CB	2.49	0.42
5:FFF:259:ILE:HG23	5:FFF:280:LEU:HD21	2.01	0.42
1:AAA:61:ILE:HG12	1:AAA:142:MET:HB3	2.01	0.42
1:BBB:102:LEU:HB2	1:BBB:115:ILE:HG12	2.01	0.42
1:BBB:154:PRO:HD2	1:BBB:157:THR:HB	2.00	0.42
1:BBB:195:ARG:HD2	1:BBB:198:LEU:CD2	2.50	0.42
2:CCC:148:GLN:OE1	2:CCC:454:ARG:HD2	2.18	0.42
2:CCC:1255:THR:HG21	3:DDD:341:ASN:CG	2.40	0.42
3:DDD:234:PRO:O	3:DDD:237:MET:HG3	2.20	0.42
3:DDD:525:MET:O	3:DDD:548:VAL:HG23	2.18	0.42
3:DDD:1106:ILE:HG22	3:DDD:1106:ILE:O	2.18	0.42
3:DDD:1357:ILE:H	3:DDD:1357:ILE:HG13	1.52	0.42
7:222:21:DG:C2	7:222:22:DA:N7	2.79	0.42
1:AAA:222:THR:HG23	1:BBB:233:ASP:HB3	2.01	0.42
2:CCC:160:ASP:OD1	2:CCC:160:ASP:N	2.52	0.42
2:CCC:543:ALA:HB3	2:CCC:548:ARG:HH21	1.83	0.42
2:CCC:619:ALA:HB2	2:CCC:654:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:525:MET:C	3:DDD:548:VAL:CG2	2.87	0.42
3:DDD:679:TYR:HE1	3:DDD:754:ILE:O	2.03	0.42
3:DDD:810:THR:OG1	3:DDD:893:GLY:HA3	2.19	0.42
1:AAA:159:ILE:O	1:AAA:159:ILE:HG23	2.19	0.42
2:CCC:1304:MET:HE1	3:DDD:472:LEU:CD1	2.46	0.42
3:DDD:71:LEU:HB2	3:DDD:90:VAL:HG21	2.00	0.42
6:111:49:DG:H2"	6:111:50:DT:C5	2.54	0.42
2:CCC:670:PHE:CD2	2:CCC:1113:LEU:HB3	2.55	0.42
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.49	0.42
3:DDD:450:HIS:HE1	3:DDD:626:TYR:OH	2.02	0.42
3:DDD:749:LYS:CB	3:DDD:750:PRO:HD2	2.50	0.42
3:DDD:952:VAL:HG11	3:DDD:984:LEU:HD13	2.02	0.42
2:CCC:237:LEU:HD11	2:CCC:292:ILE:HD12	2.02	0.42
3:DDD:452:LEU:CD2	3:DDD:625:MET:SD	3.08	0.42
3:DDD:452:LEU:CG	3:DDD:625:MET:SD	3.04	0.42
3:DDD:809:VAL:HG22	3:DDD:915:ILE:CD1	2.50	0.42
6:111:51:DC:H2"	6:111:52:DT:C5'	2.48	0.42
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HG13	2.02	0.42
2:CCC:93:SER:OG	2:CCC:126:GLU:HB3	2.18	0.42
2:CCC:1030:GLU:HG3	2:CCC:1034:ARG:CZ	2.49	0.42
3:DDD:385:LEU:CD2	3:DDD:411:ILE:CD1	2.97	0.42
5:FFF:228:GLY:N	8:333:14:GTP:O2G	2.52	0.42
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.35	0.42
1:AAA:30:PRO:HB2	1:AAA:198:LEU:CD1	2.49	0.42
2:CCC:76:GLY:O	2:CCC:94:ALA:HB1	2.19	0.42
2:CCC:403:MET:HB3	2:CCC:403:MET:HE2	1.81	0.42
2:CCC:666:SER:HB2	2:CCC:704:MET:HG3	2.01	0.42
2:CCC:799:ASN:ND2	2:CCC:799:ASN:H	2.18	0.42
3:DDD:510:LEU:HD22	3:DDD:579:LEU:CG	2.49	0.42
3:DDD:750:PRO:CB	3:DDD:781:LYS:CB	2.95	0.42
3:DDD:786:THR:HB	3:DDD:932:MET:HA	2.01	0.42
8:333:101:2DT:C2'	11:333:201:CTP:C1'	2.98	0.42
1:BBB:78:ILE:HA	1:BBB:81:ILE:HD12	2.01	0.42
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.20	0.42
3:DDD:262:THR:O	5:FFF:222:VAL:HG12	2.20	0.42
3:DDD:511:TYR:HD1	3:DDD:596:LEU:O	2.03	0.42
2:CCC:49:LEU:HD22	2:CCC:464:PHE:CE2	2.55	0.41
2:CCC:1017:GLN:HE21	2:CCC:1021:LEU:HG	1.84	0.41
3:DDD:421:VAL:HG11	3:DDD:468:VAL:HG13	2.02	0.41
3:DDD:510:LEU:HD22	3:DDD:579:LEU:CD2	2.49	0.41
3:DDD:1047:THR:HB	3:DDD:1062:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:222:9:DT:H2"	7:222:10:DC:O5'	2.20	0.41
2:CCC:149:LEU:HB2	2:CCC:530:ILE:CG2	2.50	0.41
2:CCC:216:THR:O	2:CCC:220:ILE:HG13	2.20	0.41
2:CCC:1080:ASN:HB3	2:CCC:1085:MET:SD	2.59	0.41
2:CCC:1284:ALA:HB3	3:DDD:1361:THR:HB	2.02	0.41
3:DDD:783:LEU:HD12	3:DDD:783:LEU:HA	1.84	0.41
3:DDD:816:THR:HG22	3:DDD:818:GLU:N	2.25	0.41
3:DDD:1041:ILE:CG2	3:DDD:1044:GLN:HG3	2.50	0.41
3:DDD:1152:GLU:HA	3:DDD:1194:ARG:NH2	2.35	0.41
1:AAA:78:ILE:HA	1:AAA:81:ILE:HD12	2.02	0.41
2:CCC:12:ARG:HD3	2:CCC:1183:ALA:HB2	2.01	0.41
2:CCC:667:LEU:HD23	2:CCC:704:MET:HB2	2.01	0.41
2:CCC:1242:LYS:HD3	3:DDD:465:GLN:HE21	1.84	0.41
2:CCC:1328:LYS:HA	2:CCC:1328:LYS:HD3	1.91	0.41
3:DDD:514:THR:HA	3:DDD:576:ARG:HG3	2.02	0.41
3:DDD:705:THR:HG23	3:DDD:707:ILE:HG13	2.02	0.41
3:DDD:1152:GLU:HB3	3:DDD:1194:ARG:HH22	1.84	0.41
1:BBB:48:LEU:HD22	3:DDD:535:ARG:HG3	2.02	0.41
2:CCC:898:GLU:OE1	2:CCC:898:GLU:N	2.52	0.41
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:CD	2.40	0.41
3:DDD:1146:GLU:OE2	3:DDD:1309:ILE:CG2	2.68	0.41
1:BBB:86:LYS:HE2	1:BBB:174:ASP:H	1.85	0.41
1:BBB:232:VAL:HB	1:BBB:233:ASP:H	1.60	0.41
2:CCC:750:ILE:HG23	2:CCC:750:ILE:O	2.20	0.41
2:CCC:890:LYS:HB2	2:CCC:914:LYS:HE3	2.03	0.41
3:DDD:506:VAL:O	3:DDD:628:GLY:CA	2.68	0.41
1:AAA:179:PRO:HG3	1:AAA:211:ILE:CG1	2.51	0.41
2:CCC:592:ARG:NH1	2:CCC:653:MET:HE1	2.35	0.41
2:CCC:818:VAL:HG12	2:CCC:1096:ILE:HG12	2.02	0.41
2:CCC:818:VAL:CG2	2:CCC:1079:ILE:HG12	2.50	0.41
3:DDD:161:THR:N	3:DDD:164:GLN:OE1	2.47	0.41
3:DDD:821:MET:HE3	3:DDD:879:ALA:HB1	2.03	0.41
1:AAA:231:PHE:CZ	1:BBB:39:LEU:HD13	2.56	0.41
2:CCC:563:THR:HG21	3:DDD:780:ARG:CZ	2.51	0.41
2:CCC:1340:GLU:O	3:DDD:17:PHE:HB2	2.20	0.41
3:DDD:644:MET:HG3	3:DDD:722:ILE:CD1	2.51	0.41
3:DDD:1041:ILE:HG21	3:DDD:1044:GLN:HG3	2.03	0.41
5:FFF:175:LEU:O	5:FFF:179:LEU:HG	2.21	0.41
2:CCC:726:TYR:CZ	2:CCC:728:ASP:HB2	2.55	0.41
3:DDD:1031:VAL:HG11	3:DDD:1089:LEU:O	2.21	0.41
3:DDD:1263:LYS:CG	3:DDD:1307:LEU:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:61:ILE:HG12	1:BBB:142:MET:HB3	2.03	0.41
2:CCC:479:LEU:HD23	2:CCC:479:LEU:HA	1.92	0.41
2:CCC:975:ILE:HG23	2:CCC:1011:LEU:CD1	2.50	0.41
2:CCC:1109:ILE:HG13	3:DDD:644:MET:CE	2.50	0.41
3:DDD:151:MET:HB3	3:DDD:153:ASN:ND2	2.35	0.41
3:DDD:325:LYS:HE2	3:DDD:330:MET:CG	2.51	0.41
3:DDD:369:PRO:HB3	3:DDD:444:GLY:O	2.21	0.41
3:DDD:608:CYS:SG	3:DDD:617:THR:HG22	2.61	0.41
3:DDD:844:THR:HG21	3:DDD:858:VAL:HG11	2.02	0.41
3:DDD:955:LYS:HG2	3:DDD:1011:VAL:O	2.21	0.41
3:DDD:976:THR:HA	3:DDD:999:TYR:CE1	2.56	0.41
5:FFF:142:PHE:CE2	5:FFF:146:ALA:HB2	2.56	0.41
2:CCC:515:MET:HG2	2:CCC:517:GLN:CG	2.51	0.41
2:CCC:725:GLN:HB2	2:CCC:735:LYS:HG3	2.03	0.41
3:DDD:110:PRO:O	3:DDD:182:ALA:HB3	2.20	0.41
3:DDD:385:LEU:HD21	3:DDD:411:ILE:HD13	2.00	0.41
3:DDD:395:LYS:HD2	5:FFF:251:GLN:CD	2.42	0.41
3:DDD:750:PRO:C	3:DDD:781:LYS:HG2	2.33	0.41
3:DDD:1180:VAL:HG23	3:DDD:1181:ASP:H	1.85	0.41
5:FFF:87:ASP:OD1	5:FFF:88:VAL:N	2.53	0.41
1:BBB:155:ALA:HB1	1:BBB:172:LEU:HD23	2.02	0.40
2:CCC:518:ASN:OD1	2:CCC:1236:ASN:ND2	2.54	0.40
2:CCC:1246:ARG:NH2	2:CCC:1258:PRO:HB3	2.36	0.40
3:DDD:211:GLU:HG2	3:DDD:212:THR:HG23	2.04	0.40
3:DDD:352:ARG:HA	3:DDD:466:MET:O	2.21	0.40
3:DDD:741:ALA:O	3:DDD:762:ASN:ND2	2.54	0.40
3:DDD:746:LEU:HD23	3:DDD:758:PRO:HB3	2.03	0.40
3:DDD:1163:VAL:O	3:DDD:1201:GLY:HA2	2.21	0.40
2:CCC:583:GLU:HG3	2:CCC:584:TYR:CD2	2.56	0.40
2:CCC:1293:VAL:O	2:CCC:1301:ARG:HB3	2.21	0.40
3:DDD:417:ARG:HG2	3:DDD:418:GLU:HG2	2.03	0.40
3:DDD:948:SER:OG	3:DDD:1019:ASN:ND2	2.55	0.40
3:DDD:1054:THR:OG1	3:DDD:1055:GLY:N	2.54	0.40
5:FFF:267:ASN:HB2	5:FFF:270:GLN:HB2	2.03	0.40
1:AAA:101:THR:HG22	1:AAA:143:ARG:HG2	2.03	0.40
2:CCC:144:VAL:HB	2:CCC:526:HIS:CE1	2.56	0.40
2:CCC:758:ARG:HD2	2:CCC:835:GLU:HB2	2.04	0.40
2:CCC:1160:ASP:O	2:CCC:1161:LEU:O	2.39	0.40
2:CCC:1289:GLU:HG3	2:CCC:1315:MET:HE1	2.02	0.40
3:DDD:872:LEU:HD23	3:DDD:877:VAL:HG21	2.03	0.40
3:DDD:1152:GLU:CA	3:DDD:1194:ARG:NH2	2.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:114:ILE:CG2	3:DDD:115:TRP:N	2.84	0.40
3:DDD:261:ALA:HA	5:FFF:220:THR:O	2.22	0.40
2:CCC:759:SER:OG	2:CCC:760:ASN:N	2.53	0.40
2:CCC:1277:ALA:HB3	3:DDD:434:ILE:HD12	2.04	0.40
3:DDD:916:GLY:HA2	3:DDD:1255:VAL:HG11	2.04	0.40
3:DDD:1152:GLU:CD	3:DDD:1193:TRP:CH2	2.94	0.40
7:222:21:DG:C4	7:222:22:DA:N7	2.85	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)
5:FFF:67:TYR:O	5:FFF:299:ARG:NH2[3_644]	1.95	0.25

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	210 (92%)	12 (5%)	6 (3%)	5	34
1	BBB	226/242 (93%)	207 (92%)	14 (6%)	5 (2%)	6	37
2	CCC	1339/1342 (100%)	1241 (93%)	72 (5%)	26 (2%)	8	39
3	DDD	1360/1407 (97%)	1246 (92%)	92 (7%)	22 (2%)	9	43
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	275/336 (82%)	254 (92%)	16 (6%)	5 (2%)	8	40
All	All	3505/3659 (96%)	3231 (92%)	210 (6%)	64 (2%)	8	40

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS

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Mol	Chain	Res	Type
1	BBB	119	GLY
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN
2	CCC	247	ARG
2	CCC	791	LEU
2	CCC	1162	SER
2	CCC	1281	TYR
3	DDD	53	ARG
3	DDD	519	ASN
5	FFF	227	GLY
5	FFF	228	GLY
1	AAA	168	ILE
1	AAA	234	LEU
2	CCC	258	ASN
2	CCC	625	GLU
2	CCC	730	SER
2	CCC	756	TYR
2	CCC	1161	LEU
3	DDD	122	SER
3	DDD	174	ASP
3	DDD	321	LYS
3	DDD	336	GLY
3	DDD	515	ARG
3	DDD	1309	ILE
1	AAA	191	ARG
1	AAA	233	ASP
1	BBB	232	VAL
2	CCC	669	PRO
2	CCC	981	ALA
2	CCC	1103	VAL
2	CCC	1135	GLN
3	DDD	1053	LEU
3	DDD	1200	GLU
2	CCC	45	GLY
2	CCC	163	LYS
2	CCC	234	ASP
2	CCC	246	LEU
2	CCC	341	LEU
2	CCC	455	SER
2	CCC	729	ALA
2	CCC	867	GLU

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Mol	Chain	Res	Type
2	CCC	910	ALA
2	CCC	986	ALA
2	CCC	1297	ASP
3	DDD	854	ALA
3	DDD	946	ALA
3	DDD	1024	THR
3	DDD	1091	PRO
1	AAA	162	GLU
1	AAA	210	THR
3	DDD	153	ASN
3	DDD	846	GLU
3	DDD	847	ASP
3	DDD	986	ASP
3	DDD	1170	LYS
3	DDD	1297	LYS
5	FFF	113	GLY
5	FFF	282	GLY
3	DDD	1103	GLY
2	CCC	983	GLY
5	FFF	295	ILE
3	DDD	829	GLY

5.3.2 Protein sidechains (i)

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%)	180 (91%)	18 (9%)	9 33
1	BBB	196/208 (94%)	182 (93%)	14 (7%)	14 42
2	CCC	1156/1157 (100%)	1065 (92%)	91 (8%)	12 39
3	DDD	1135/1168 (97%)	1059 (93%)	76 (7%)	16 44
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	27 54
5	FFF	240/292 (82%)	226 (94%)	14 (6%)	20 48
All	All	2992/3107 (96%)	2776 (93%)	216 (7%)	14 42

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	18	GLN
1	AAA	28	LEU
1	AAA	33	ARG
1	AAA	70	THR
1	AAA	77	ASP
1	AAA	131	CYS
1	AAA	135	ASP
1	AAA	137	ASN
1	AAA	157	THR
1	AAA	159	ILE
1	AAA	166	ARG
1	AAA	187	VAL
1	AAA	191	ARG
1	AAA	194	GLN
1	AAA	198	LEU
1	AAA	208	ASN
1	AAA	233	ASP
1	AAA	235	ARG
1	BBB	28	LEU
1	BBB	33	ARG
1	BBB	70	THR
1	BBB	77	ASP
1	BBB	105	SER
1	BBB	131	CYS
1	BBB	137	ASN
1	BBB	159	ILE
1	BBB	173	VAL
1	BBB	176	CYS
1	BBB	187	VAL
1	BBB	191	ARG
1	BBB	194	GLN
1	BBB	198	LEU
2	CCC	23	ASP
2	CCC	30	ILE
2	CCC	69	GLN
2	CCC	85	CYS
2	CCC	116	ASP
2	CCC	120	GLN
2	CCC	121	GLU
2	CCC	160	ASP
2	CCC	166	SER
2	CCC	167	SER

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Mol	Chain	Res	Type
2	CCC	173	ASN
2	CCC	184	LEU
2	CCC	185	ASP
2	CCC	189	ASP
2	CCC	209	ILE
2	CCC	237	LEU
2	CCC	241	LEU
2	CCC	256	GLU
2	CCC	264	GLU
2	CCC	275	ARG
2	CCC	290	GLU
2	CCC	304	GLU
2	CCC	316	GLU
2	CCC	332	ARG
2	CCC	335	THR
2	CCC	393	ASP
2	CCC	398	SER
2	CCC	403	MET
2	CCC	404	LYS
2	CCC	413	GLU
2	CCC	470	ARG
2	CCC	472	GLU
2	CCC	477	GLU
2	CCC	502	VAL
2	CCC	525	THR
2	CCC	529	ARG
2	CCC	539	THR
2	CCC	574	SER
2	CCC	576	SER
2	CCC	592	ARG
2	CCC	601	ASP
2	CCC	618	GLN
2	CCC	620	ASN
2	CCC	635	THR
2	CCC	648	ASP
2	CCC	678	ARG
2	CCC	685	MET
2	CCC	694	ARG
2	CCC	730	SER
2	CCC	739	ASP
2	CCC	757	THR
2	CCC	759	SER

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Mol	Chain	Res	Type
2	CCC	772	SER
2	CCC	777	VAL
2	CCC	788	SER
2	CCC	789	THR
2	CCC	799	ASN
2	CCC	800	MET
2	CCC	801	ARG
2	CCC	802	VAL
2	CCC	808	ASN
2	CCC	815	SER
2	CCC	817	LEU
2	CCC	831	ILE
2	CCC	844	LYS
2	CCC	866	ASP
2	CCC	876	GLU
2	CCC	892	GLU
2	CCC	935	THR
2	CCC	942	ASP
2	CCC	995	ASP
2	CCC	998	LEU
2	CCC	1073	LYS
2	CCC	1088	ASP
2	CCC	1113	LEU
2	CCC	1135	GLN
2	CCC	1143	GLU
2	CCC	1150	ASP
2	CCC	1154	ASP
2	CCC	1174	GLU
2	CCC	1223	ARG
2	CCC	1240	ASP
2	CCC	1248	THR
2	CCC	1262	LYS
2	CCC	1269	ARG
2	CCC	1286	THR
2	CCC	1292	THR
2	CCC	1293	VAL
2	CCC	1296	ASP
2	CCC	1299	ASN
2	CCC	1319	MET
3	DDD	34	SER
3	DDD	52	GLU
3	DDD	60	ARG

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Mol	Chain	Res	Type
3	DDD	67	ASP
3	DDD	70	CYS
3	DDD	143	SER
3	DDD	167	ASP
3	DDD	176	PHE
3	DDD	210	SER
3	DDD	211	GLU
3	DDD	223	LEU
3	DDD	237	MET
3	DDD	256	ASP
3	DDD	319	SER
3	DDD	339	ARG
3	DDD	345	LYS
3	DDD	443	GLU
3	DDD	464	ASP
3	DDD	479	GLU
3	DDD	492	SER
3	DDD	515	ARG
3	DDD	516	ASP
3	DDD	518	VAL
3	DDD	543	SER
3	DDD	550	VAL
3	DDD	551	ARG
3	DDD	579	LEU
3	DDD	590	SER
3	DDD	591	ILE
3	DDD	599	LYS
3	DDD	602	SER
3	DDD	604	MET
3	DDD	610	ARG
3	DDD	619	ILE
3	DDD	627	THR
3	DDD	648	GLU
3	DDD	704	GLU
3	DDD	705	THR
3	DDD	715	LYS
3	DDD	717	VAL
3	DDD	731	ARG
3	DDD	736	GLN
3	DDD	747	MET
3	DDD	751	ASP
3	DDD	769	VAL

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Mol	Chain	Res	Type
3	DDD	786	THR
3	DDD	790	THR
3	DDD	792	ASN
3	DDD	812	ASP
3	DDD	830	ASP
3	DDD	831	VAL
3	DDD	835	LEU
3	DDD	836	ARG
3	DDD	837	ASP
3	DDD	844	THR
3	DDD	848	VAL
3	DDD	849	LEU
3	DDD	857	LEU
3	DDD	863	LEU
3	DDD	889	ASP
3	DDD	911	LYS
3	DDD	957	SER
3	DDD	969	SER
3	DDD	970	SER
3	DDD	1021	ASP
3	DDD	1023	HIS
3	DDD	1025	MET
3	DDD	1032	SER
3	DDD	1051	ASP
3	DDD	1064	SER
3	DDD	1073	ASP
3	DDD	1158	GLU
3	DDD	1283	SER
3	DDD	1303	SER
3	DDD	1330	ARG
3	DDD	1345	ARG
4	EEE	8	ASP
4	EEE	46	THR
4	EEE	55	GLU
5	FFF	107	ARG
5	FFF	109	TYR
5	FFF	114	LEU
5	FFF	122	GLU
5	FFF	127	LEU
5	FFF	151	ARG
5	FFF	205	PRO
5	FFF	218	ARG

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Mol	Chain	Res	Type
5	FFF	236	ASP
5	FFF	244	ASN
5	FFF	254	ASP
5	FFF	271	ARG
5	FFF	299	ARG
5	FFF	325	GLU

Sometimes 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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	2DT	333	101	7	17,20,21	1.51	4 (23%)	22,28,31	2.70	8 (36%)

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	2DT	333	101	7	-	1/7/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	333	101	2DT	C2-N1	2.76	1.42	1.38
8	333	101	2DT	C6-C5	2.70	1.39	1.34
8	333	101	2DT	C4-C5	2.28	1.48	1.44
8	333	101	2DT	C4-N3	-2.14	1.34	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	333	101	2DT	C4-N3-C2	-5.22	120.59	127.35
8	333	101	2DT	C5-C4-N3	4.80	119.41	115.31
8	333	101	2DT	O4-C4-C5	-4.80	119.34	124.90
8	333	101	2DT	C3'-C2'-C1'	4.73	108.24	102.78
8	333	101	2DT	N3-C2-N1	4.50	120.86	114.89
8	333	101	2DT	C5-C6-N1	-3.74	119.50	123.34
8	333	101	2DT	C5M-C5-C4	2.39	121.40	118.77
8	333	101	2DT	C5M-C5-C6	-2.16	119.96	122.85

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	333	101	2DT	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	333	101	2DT	6	0

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	CTP	333	201	10	26,30,30	0.54	0	39,47,47	0.52	0

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	CTP	333	201	10	-	5/22/38/38	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	333	201	CTP	PB-O3A-PA-O1A
11	333	201	CTP	PB-O3B-PG-O1G
11	333	201	CTP	PB-O3B-PG-O2G
11	333	201	CTP	PB-O3B-PG-O3G
11	333	201	CTP	PB-O3A-PA-O2A

There are no ring outliers.

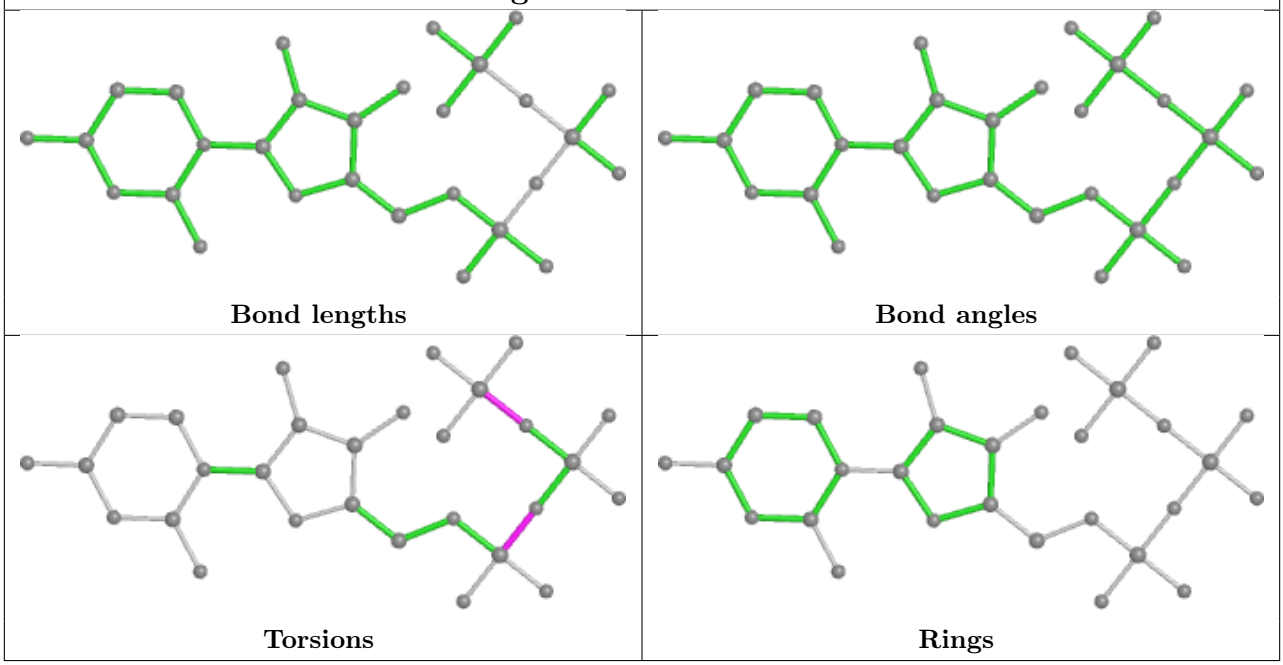
1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	333	201	CTP	11	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 then 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.

Ligand CTP 333 201



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'	101:2DT	P	1.78

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	AAA	230/242 (95%)	0.12	12 (5%)	27	23	232, 309, 389, 488	0
1	BBB	228/242 (94%)	0.02	13 (5%)	23	20	215, 331, 426, 456	0
2	CCC	1341/1342 (99%)	-0.11	26 (1%)	66	58	149, 259, 404, 485	0
3	DDD	1362/1407 (96%)	-0.17	27 (1%)	65	56	142, 269, 383, 504	0
4	EEE	79/90 (87%)	-0.29	1 (1%)	77	68	249, 322, 473, 567	0
5	FFF	277/336 (82%)	0.15	19 (6%)	16	13	215, 334, 439, 467	0
6	111	30/50 (60%)	-0.16	3 (10%)	7	7	272, 329, 405, 531	0
7	222	36/50 (72%)	0.40	4 (11%)	5	6	230, 334, 489, 507	0
8	333	2/4 (50%)	0.92	0	100	100	231, 231, 231, 302	0
All	All	3585/3763 (95%)	-0.09	105 (2%)	51	41	142, 281, 411, 567	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	853	THR	5.5
7	222	36	DG	5.3
3	DDD	1272	SER	4.9
1	AAA	144	ILE	4.7
1	BBB	108	GLY	4.5
2	CCC	740	GLU	4.5
5	FFF	263	LEU	4.3
2	CCC	259	GLY	4.3
3	DDD	854	ALA	4.2
6	111	48	DA	4.0
3	DDD	1266	ILE	4.0
2	CCC	1004	ASP	3.9
2	CCC	1003	THR	3.8
3	DDD	1028	ILE	3.8
3	DDD	1271	SER	3.8

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Mol	Chain	Res	Type	RSRZ
5	FFF	306	GLN	3.8
1	AAA	171	LEU	3.7
6	111	44	DG	3.7
1	BBB	164	ASP	3.6
1	AAA	59	VAL	3.5
2	CCC	257	ALA	3.5
1	BBB	160	HIS	3.5
3	DDD	1030	GLU	3.5
2	CCC	261	VAL	3.4
2	CCC	1001	GLY	3.4
5	FFF	293	ARG	3.4
2	CCC	659	GLN	3.3
2	CCC	124	MET	3.3
7	222	37	DA	3.3
7	222	35	DT	3.2
5	FFF	201	GLN	3.2
3	DDD	944	ALA	3.2
2	CCC	240	GLU	3.2
5	FFF	310	LEU	3.1
3	DDD	1097	ALA	3.1
5	FFF	305	ILE	3.1
1	BBB	165	GLU	3.1
2	CCC	482	GLY	3.1
3	DDD	1273	ASP	3.1
3	DDD	747	MET	3.0
1	AAA	134	THR	3.0
1	AAA	164	ASP	2.9
5	FFF	259	ILE	2.9
2	CCC	1055	ALA	2.9
3	DDD	1098	GLN	2.8
2	CCC	182	SER	2.8
2	CCC	256	GLU	2.8
7	222	3	DT	2.8
1	AAA	27	THR	2.8
5	FFF	98	ASN	2.7
2	CCC	1005	GLU	2.7
5	FFF	301	ARG	2.7
5	FFF	312	ARG	2.6
3	DDD	1055	GLY	2.6
1	BBB	123	ILE	2.6
3	DDD	261	ALA	2.6
5	FFF	198	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	189	ALA	2.6
1	AAA	213	PRO	2.6
5	FFF	294	GLU	2.5
2	CCC	230	PHE	2.5
3	DDD	1066	GLU	2.5
2	CCC	385	PHE	2.5
3	DDD	1054	THR	2.5
2	CCC	721	GLY	2.5
1	AAA	76	GLU	2.5
1	BBB	109	PRO	2.4
2	CCC	105	TYR	2.4
5	FFF	308	GLU	2.4
2	CCC	984	VAL	2.4
5	FFF	319	THR	2.4
2	CCC	311	CYS	2.4
1	BBB	152	TYR	2.3
5	FFF	309	GLY	2.3
3	DDD	749	LYS	2.3
1	AAA	135	ASP	2.3
1	AAA	140	ILE	2.3
1	BBB	100	LEU	2.3
2	CCC	164	THR	2.3
3	DDD	855	ASP	2.3
3	DDD	1029	THR	2.3
1	BBB	163	GLU	2.2
3	DDD	748	ALA	2.2
5	FFF	280	LEU	2.2
2	CCC	604	HIS	2.2
5	FFF	281	LEU	2.2
2	CCC	1054	LEU	2.2
3	DDD	154	LEU	2.2
2	CCC	69	GLN	2.2
3	DDD	880	VAL	2.2
3	DDD	958	ILE	2.2
3	DDD	945	ALA	2.1
5	FFF	113	GLY	2.1
5	FFF	311	ARG	2.1
3	DDD	587	LEU	2.1
1	BBB	107	ILE	2.1
6	111	43	DT	2.1
1	BBB	153	VAL	2.1
1	AAA	107	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	90	VAL	2.0
3	DDD	77	ARG	2.0
4	EEE	3	ARG	2.0
2	CCC	720	ARG	2.0
1	BBB	106	GLY	2.0
3	DDD	943	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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(Å^2)	Q<0.9
8	2DT	333	101	19/20	0.89	0.27	223,258,283,290	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

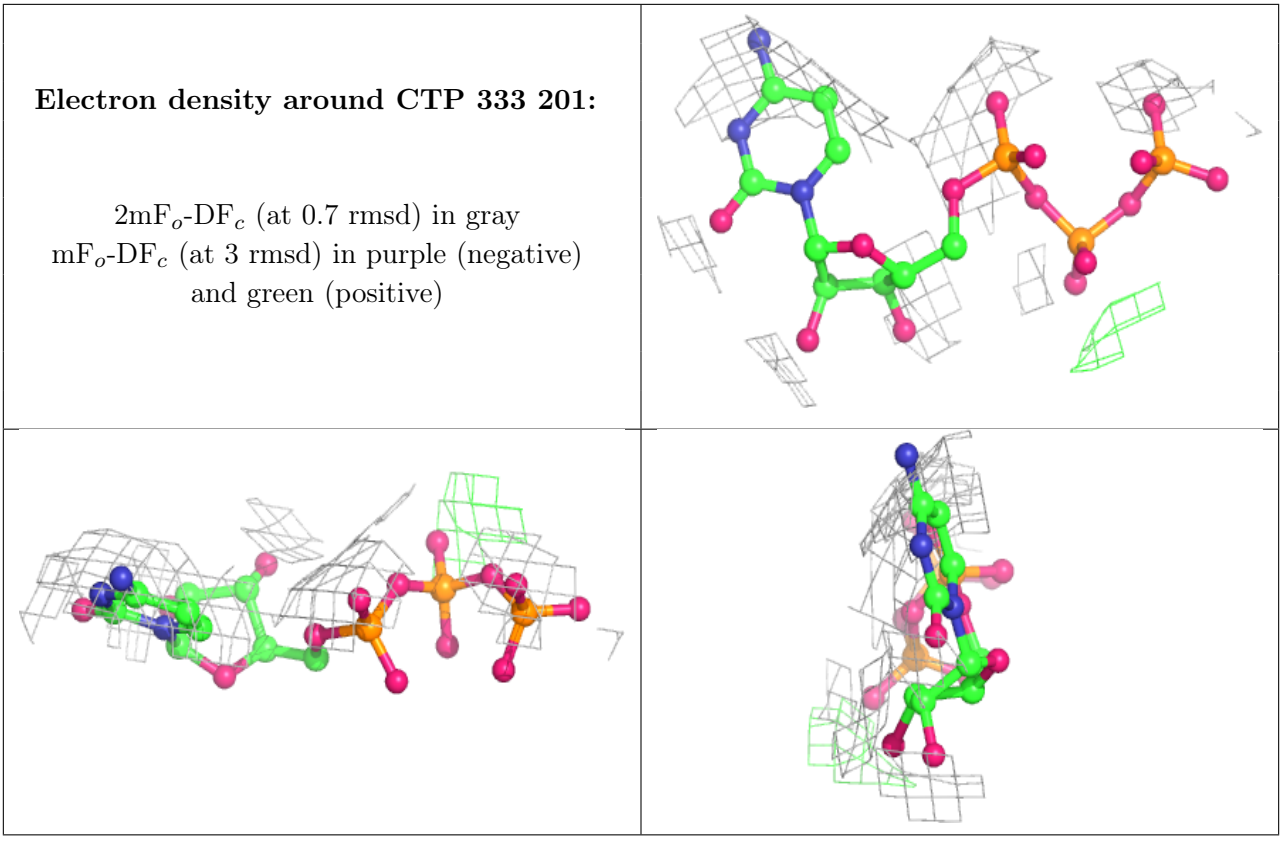
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	ZN	DDD	1502	1/1	0.94	0.17	293,293,293,293	0
11	CTP	333	201	29/29	0.94	0.29	172,203,288,301	0
9	ZN	DDD	1501	1/1	0.96	0.19	421,421,421,421	0
10	MG	DDD	1504	1/1	0.97	0.20	205,205,205,205	0
10	MG	DDD	1503	1/1	0.99	0.30	133,133,133,133	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.

Electron density around CTP 333 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.