



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:06 PM BST

PDB ID : 6UUB
Title : E. coli sigma-S transcription initiation complex with a mismatching UTP
("Fresh" crystal soaked with UTP for 2 hours)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 3.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

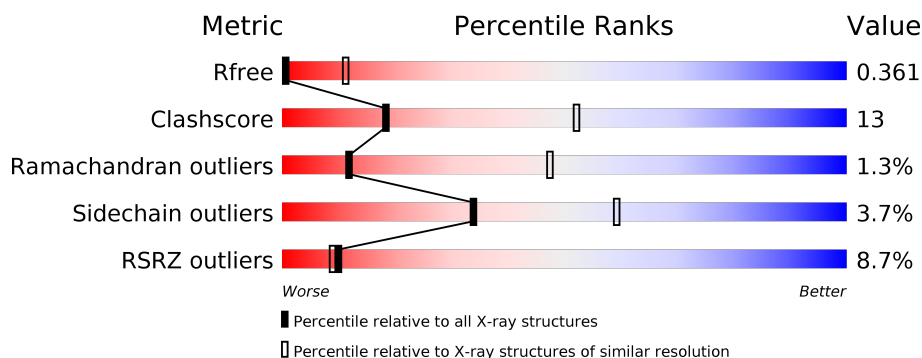
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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.



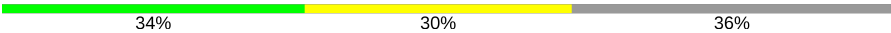

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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

Mol	Chain	Length	Quality of chain
1	AAA	242	<div> <div>7%</div> <div>68%</div> <div>24%</div> <div>5%</div> </div>
1	BBB	242	<div> <div>11%</div> <div>71%</div> <div>21%</div> <div>6%</div> </div>
2	CCC	1342	<div> <div>6%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
3	DDD	1407	<div> <div>11%</div> <div>72%</div> <div>23%</div> <div>.</div> </div>
4	EEE	90	<div> <div>7%</div> <div>71%</div> <div>16%</div> <div>12%</div> </div>
5	FFF	336	<div> <div>10%</div> <div>65%</div> <div>16%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
6	111	50	 34% 30% 36%
7	222	50	 6% 48% 20% 32%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	UTP	DDD	1504	-	-	-	X
9	ZN	DDD	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28871 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1350	Total	C	N	O	S	0	0	0
			10478	6578	1867	1984	49			

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	32	Total	C	N	O	P	0	0	0
			661	314	121	194	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	34	Total	C	N	O	P	0	0	0
			695	332	127	203	33			

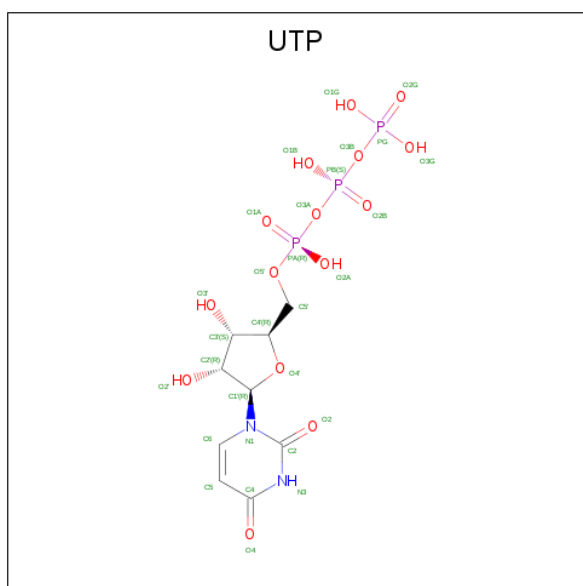
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

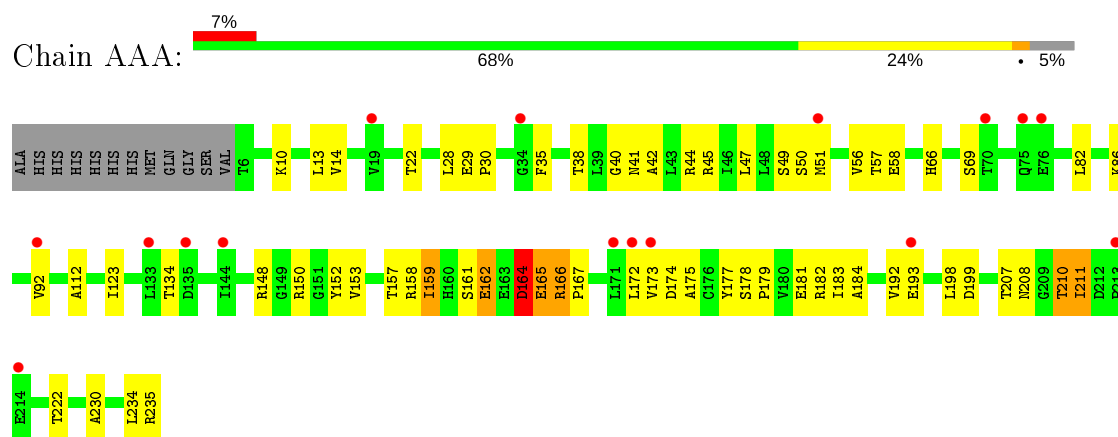
- Molecule 10 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



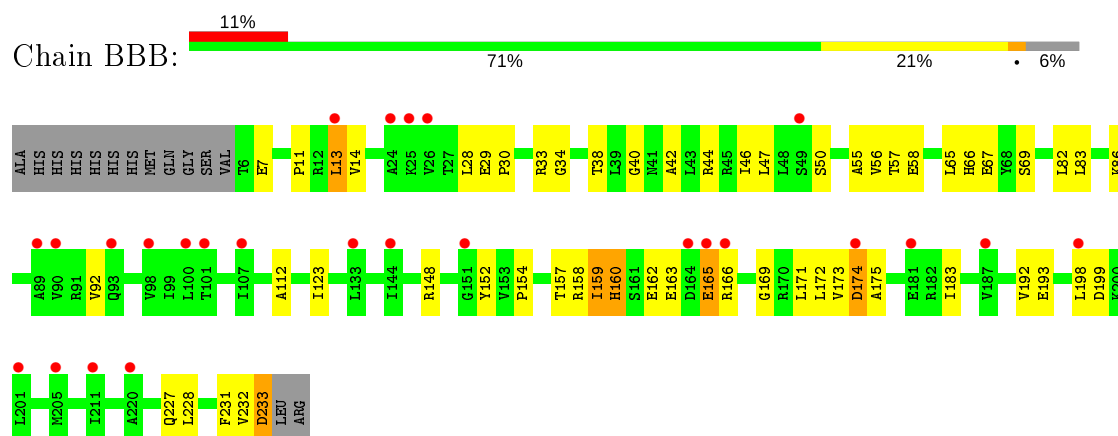
3 Residue-property plots [i](#)

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

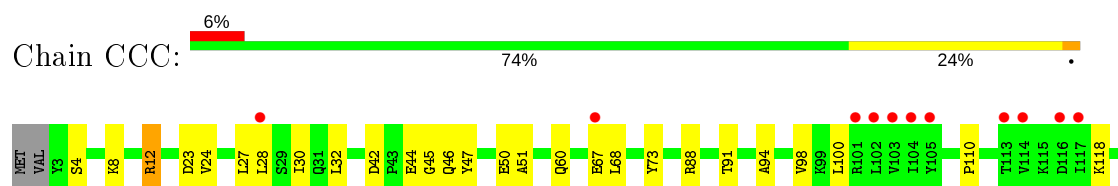
- Molecule 1: DNA-directed RNA polymerase subunit alpha

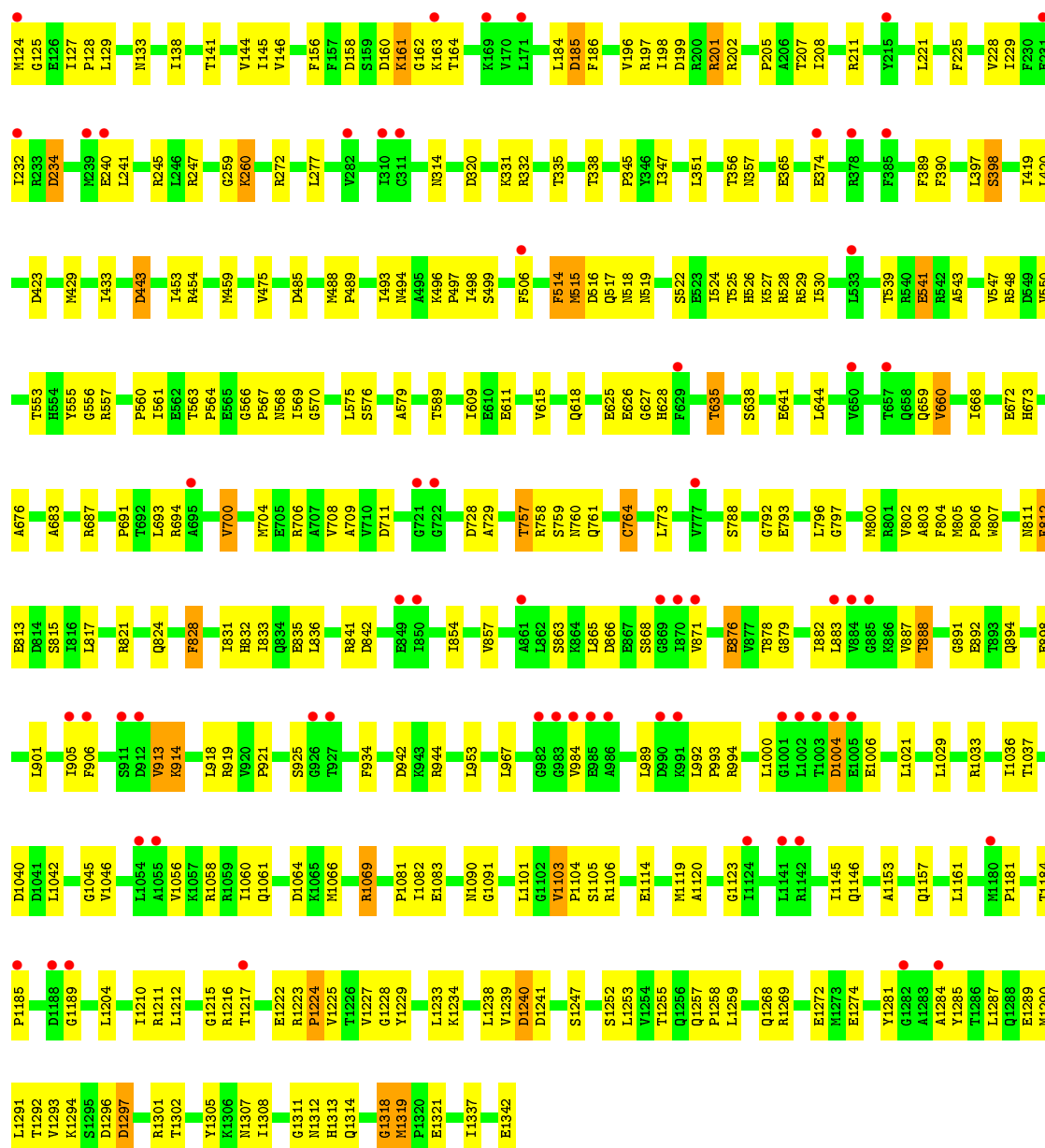


- Molecule 1: DNA-directed RNA polymerase subunit alpha

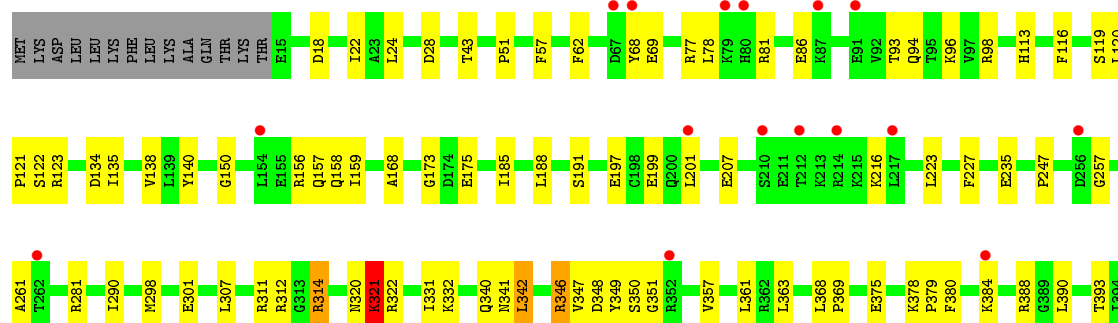


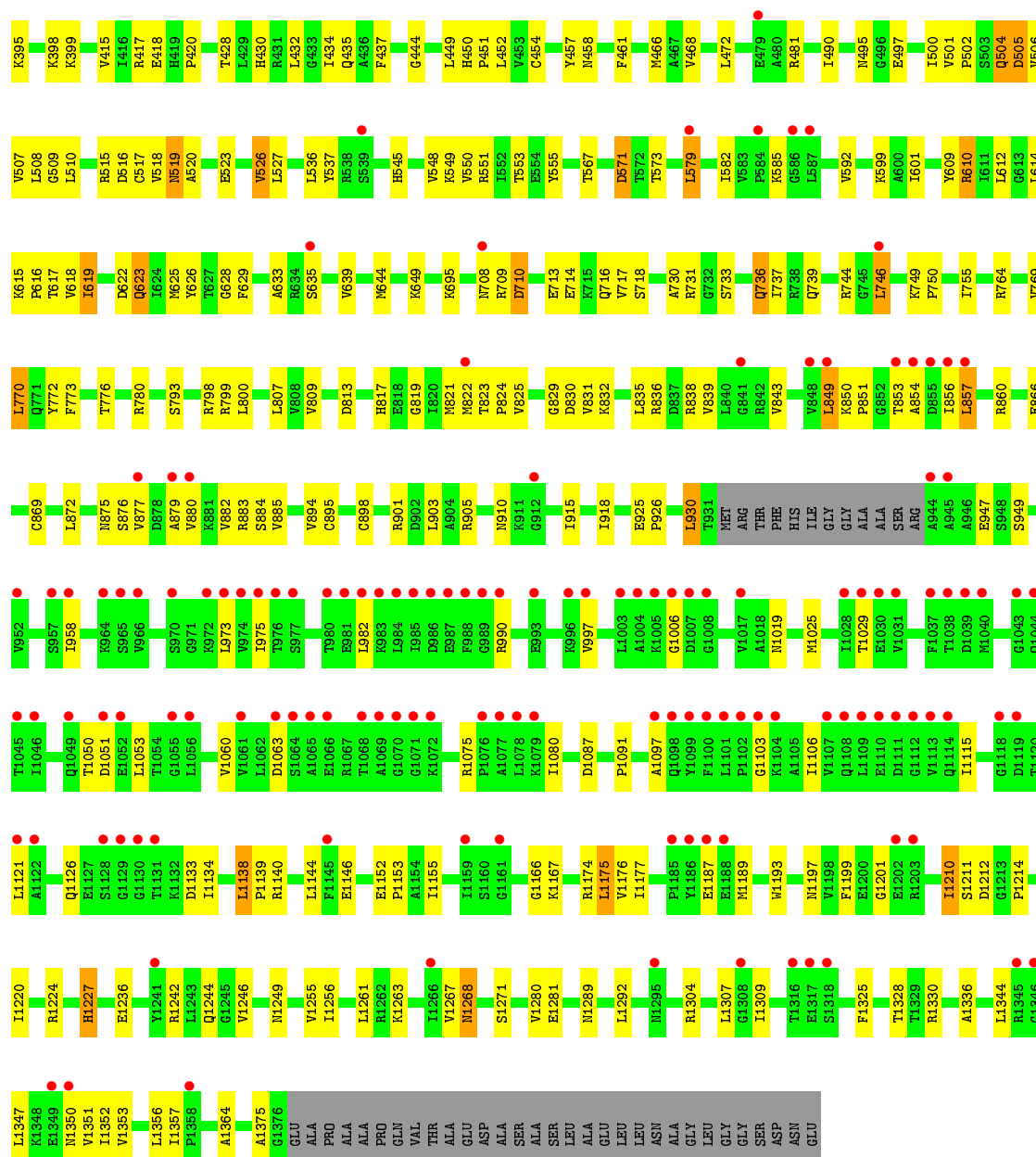
- Molecule 2: DNA-directed RNA polymerase subunit beta



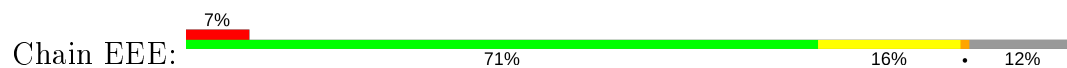


- Molecule 3: DNA-directed RNA polymerase subunit beta'

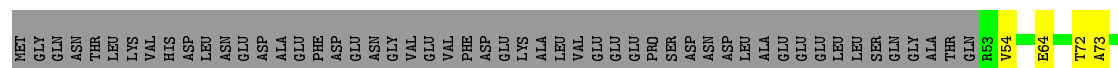


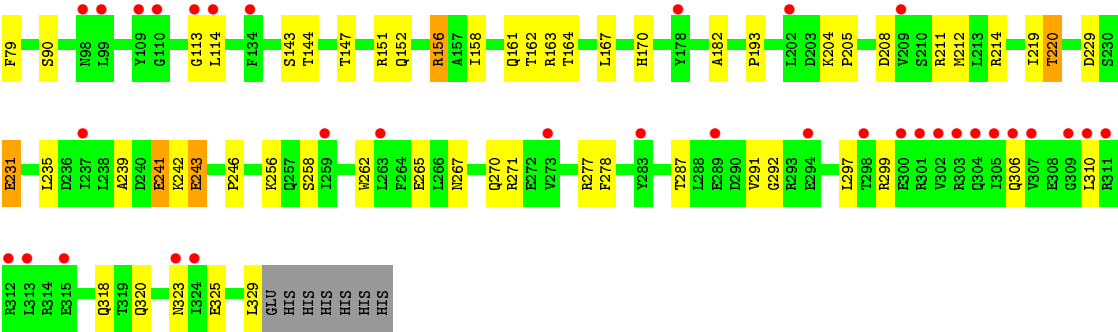


• Molecule 4: DNA-directed RNA polymerase subunit omega

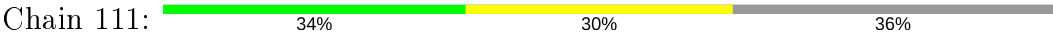


• Molecule 5: RNA polymerase sigma factor RpoS





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.94Å 154.99Å 233.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.90 – 3.96 38.88 – 3.96	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.90-3.96) 98.5 (38.88-3.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.303 , 0.375 0.296 , 0.361	Depositor DCC
R_{free} test set	2024 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	179.4	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 220.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28871	wwPDB-VP
Average B, all atoms (Å ²)	305.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	0.65	0/1809	0.72	0/2450
1	BBB	0.64	0/1789	0.70	0/2425
2	CCC	0.63	0/10739	0.72	0/14489
3	DDD	0.64	0/10636	0.72	0/14362
4	EEE	0.64	0/629	0.71	0/847
5	FFF	0.66	0/2282	0.65	0/3076
6	111	0.31	0/741	0.63	0/1143
7	222	0.29	0/779	0.61	0/1201
All	All	0.62	0/29404	0.71	0/39993

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	68	0
1	BBB	1767	0	1789	66	1
2	CCC	10570	0	10582	317	1
3	DDD	10478	0	10691	346	0
4	EEE	627	0	634	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	FFF	2253	0	2298	60	0
6	111	661	0	362	23	0
7	222	695	0	385	17	0
8	CCC	1	0	0	0	0
8	DDD	1	0	0	0	0
9	DDD	2	0	0	2	0
10	DDD	29	0	11	4	0
All	All	28871	0	28565	763	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 13.

All (763) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:27:LEU:CD1	2:CCC:524:ILE:HD11	1.15	1.62
3:DDD:490:ILE:HD11	3:DDD:614:LEU:CD1	1.45	1.46
2:CCC:27:LEU:CD1	2:CCC:524:ILE:CD1	1.75	1.39
2:CCC:27:LEU:HD13	2:CCC:524:ILE:CD1	0.87	1.35
3:DDD:898:CYS:SG	9:DDD:1502:ZN:ZN	1.24	1.25
3:DDD:515:ARG:NH2	3:DDD:717:VAL:HB	1.55	1.20
2:CCC:806:PRO:HG2	3:DDD:633:ALA:HA	1.26	1.14
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG21	1.30	1.10
1:BBB:67:GLU:CB	1:BBB:171:LEU:HD22	1.81	1.09
3:DDD:506:VAL:HG11	3:DDD:625:MET:HA	1.34	1.09
3:DDD:821:MET:HE3	3:DDD:879:ALA:HB1	1.32	1.07
3:DDD:490:ILE:HD11	3:DDD:614:LEU:HD13	1.08	1.05
2:CCC:27:LEU:CG	2:CCC:524:ILE:HD11	1.86	1.04
3:DDD:490:ILE:CD1	3:DDD:614:LEU:CD1	2.36	1.03
1:BBB:67:GLU:HB3	1:BBB:171:LEU:CD2	1.87	1.03
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.40	1.03
3:DDD:506:VAL:CG1	3:DDD:625:MET:HA	1.86	1.03
3:DDD:817:HIS:HB3	3:DDD:860:ARG:NH2	1.75	1.01
3:DDD:515:ARG:NH2	3:DDD:717:VAL:CB	2.23	1.01
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.44	1.00
3:DDD:490:ILE:CD1	3:DDD:614:LEU:HD13	1.92	0.99
2:CCC:27:LEU:HD12	2:CCC:711:ASP:HB2	1.43	0.98
1:BBB:65:LEU:O	1:BBB:169:GLY:HA2	1.65	0.97
3:DDD:821:MET:CE	3:DDD:879:ALA:HB1	1.94	0.95
2:CCC:563:THR:OG1	2:CCC:569:ILE:O	1.84	0.95
2:CCC:27:LEU:HD13	2:CCC:524:ILE:HD13	0.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	0.98	0.94
2:CCC:27:LEU:HD12	2:CCC:524:ILE:HD11	1.48	0.94
1:BBB:86:LYS:HG2	1:BBB:173:VAL:HG12	1.47	0.93
3:DDD:515:ARG:HH21	3:DDD:717:VAL:HB	1.34	0.92
1:BBB:86:LYS:HE2	1:BBB:174:ASP:H	1.34	0.92
7:222:13:DA:H4'	7:222:14:DC:OP2	1.69	0.91
3:DDD:490:ILE:HD11	3:DDD:614:LEU:HD11	1.53	0.91
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.54	0.90
2:CCC:888:THR:O	2:CCC:914:LYS:N	2.04	0.90
3:DDD:515:ARG:CZ	3:DDD:717:VAL:HB	2.01	0.90
2:CCC:517:GLN:OE1	2:CCC:760:ASN:N	2.06	0.89
2:CCC:1268:GLN:HE21	3:DDD:351:GLY:HA2	1.38	0.89
3:DDD:731:ARG:NH1	10:DDD:1504:UTP:O2G	2.06	0.89
1:BBB:67:GLU:N	1:BBB:171:LEU:HD21	1.87	0.89
2:CCC:516:ASP:HB2	2:CCC:522:SER:OG	1.72	0.89
1:AAA:82:LEU:HD22	1:AAA:173:VAL:CG2	2.02	0.88
3:DDD:481:ARG:NH1	4:EEE:3:ARG:O	2.05	0.88
3:DDD:610:ARG:HD3	3:DDD:866:GLU:OE1	1.72	0.88
1:AAA:235:ARG:HB2	1:BBB:13:LEU:HD23	1.56	0.88
3:DDD:517:CYS:HA	3:DDD:716:GLN:NE2	1.89	0.88
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.55	0.86
2:CCC:514:PHE:CZ	7:222:20:DG:H4'	2.11	0.86
3:DDD:452:LEU:HD21	3:DDD:625:MET:HB2	1.56	0.86
3:DDD:555:TYR:CD1	3:DDD:585:LYS:HD2	2.11	0.86
3:DDD:898:CYS:HG	9:DDD:1502:ZN:ZN	0.87	0.85
2:CCC:1342:GLU:HA	3:DDD:18:ASP:HB2	1.57	0.84
2:CCC:866:ASP:OD2	2:CCC:944:ARG:HB2	1.76	0.84
2:CCC:518:ASN:O	2:CCC:691:PRO:HD3	1.78	0.84
3:DDD:610:ARG:CD	3:DDD:866:GLU:OE1	2.26	0.83
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG22	1.58	0.83
2:CCC:806:PRO:HG2	3:DDD:633:ALA:CA	2.08	0.83
5:FFF:242:LYS:HG3	5:FFF:243:GLU:H	1.42	0.83
1:BBB:86:LYS:CG	1:BBB:173:VAL:HG12	2.09	0.82
2:CCC:28:LEU:HD21	2:CCC:527:LYS:HD3	1.61	0.82
3:DDD:615:LYS:HB2	3:DDD:616:PRO:HD3	1.61	0.82
2:CCC:28:LEU:HD13	2:CCC:133:ASN:O	1.79	0.82
3:DDD:515:ARG:NH2	3:DDD:717:VAL:C	2.32	0.82
3:DDD:555:TYR:CE1	3:DDD:585:LYS:HD2	2.15	0.81
1:BBB:56:VAL:O	1:BBB:175:ALA:HB2	1.81	0.81
2:CCC:27:LEU:HD12	2:CCC:524:ILE:CD1	2.04	0.80
2:CCC:764:CYS:HA	2:CCC:833:ILE:HD11	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:56:VAL:O	1:AAA:175:ALA:HB2	1.81	0.79
5:FFF:241:GLU:HG3	5:FFF:242:LYS:N	1.98	0.79
1:AAA:45:ARG:NE	1:BBB:38:THR:OG1	2.15	0.79
2:CCC:27:LEU:CB	2:CCC:524:ILE:HD11	2.14	0.78
2:CCC:901:LEU:O	2:CCC:905:ILE:HG13	1.82	0.77
5:FFF:262:TRP:HE1	5:FFF:320:GLN:HE22	1.32	0.77
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.18	0.77
2:CCC:27:LEU:CD1	2:CCC:711:ASP:HB2	2.14	0.77
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.18	0.77
3:DDD:452:LEU:HG	3:DDD:625:MET:SD	2.25	0.77
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.18	0.77
2:CCC:828:PHE:CE2	2:CCC:1066:MET:HE1	2.20	0.76
3:DDD:832:LYS:HG3	3:DDD:1242:ARG:HD3	1.67	0.76
3:DDD:505:ASP:HB2	3:DDD:629:PHE:HD1	1.51	0.75
2:CCC:88:ARG:HA	2:CCC:934:PHE:CE1	2.22	0.75
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.22	0.75
3:DDD:832:LYS:CG	3:DDD:1242:ARG:HD3	2.17	0.75
5:FFF:242:LYS:HG3	5:FFF:243:GLU:N	2.01	0.75
1:AAA:57:THR:HG23	1:AAA:158:ARG:NH2	2.02	0.74
2:CCC:516:ASP:CB	2:CCC:522:SER:OG	2.35	0.74
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.66	0.74
3:DDD:363:LEU:HD23	3:DDD:618:VAL:HG13	1.70	0.74
3:DDD:505:ASP:HB2	3:DDD:629:PHE:CD1	2.23	0.74
2:CCC:560:PRO:CB	3:DDD:776:THR:HG21	2.17	0.74
2:CCC:1269:ARG:NH2	3:DDD:340:GLN:O	2.20	0.74
3:DDD:363:LEU:CD2	3:DDD:618:VAL:HG13	2.18	0.73
3:DDD:821:MET:HA	3:DDD:880:VAL:O	1.88	0.73
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.70	0.73
3:DDD:518:VAL:N	3:DDD:716:GLN:HE22	1.86	0.73
6:111:56:DG:C2	7:222:8:DG:N2	2.57	0.72
2:CCC:550:VAL:HG21	3:DDD:776:THR:CG2	2.18	0.72
3:DDD:821:MET:CE	3:DDD:879:ALA:CB	2.65	0.72
3:DDD:822:MET:HE1	3:DDD:882:VAL:HG21	1.71	0.72
2:CCC:28:LEU:HD21	2:CCC:527:LYS:CD	2.20	0.72
3:DDD:822:MET:CE	3:DDD:882:VAL:HG21	2.20	0.71
2:CCC:514:PHE:CZ	7:222:20:DG:C4'	2.74	0.71
3:DDD:452:LEU:HB3	3:DDD:500:ILE:HG23	1.73	0.71
3:DDD:140:TYR:OH	3:DDD:312:ARG:HD2	1.91	0.70
3:DDD:378:LYS:H	3:DDD:379:PRO:HD2	1.56	0.70
2:CCC:528:ARG:NH2	2:CCC:576:SER:O	2.24	0.70
3:DDD:506:VAL:HG13	3:DDD:625:MET:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:822:MET:CE	3:DDD:882:VAL:HG11	2.22	0.70
2:CCC:764:CYS:HA	2:CCC:833:ILE:CD1	2.22	0.69
2:CCC:868:SER:OG	2:CCC:944:ARG:N	2.22	0.69
1:BBB:86:LYS:HE2	1:BBB:174:ASP:N	2.06	0.69
4:EEE:25:ARG:NH2	4:EEE:68:GLU:OE1	2.25	0.69
2:CCC:925:SER:O	2:CCC:1056:VAL:HG13	1.93	0.69
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.23	0.69
2:CCC:515:MET:HB2	2:CCC:526:HIS:ND1	2.08	0.69
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.07	0.69
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.75	0.68
2:CCC:547:VAL:HG22	6:111:49:DG:N1	2.07	0.68
3:DDD:395:LYS:HD3	5:FFF:329:LEU:HD13	1.74	0.68
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.76	0.68
3:DDD:134:ASP:HB3	3:DDD:159:ILE:HD11	1.76	0.68
3:DDD:515:ARG:NH2	3:DDD:717:VAL:CG1	2.56	0.68
3:DDD:1140:ARG:NH1	3:DDD:1144:LEU:HD11	2.09	0.68
3:DDD:518:VAL:H	3:DDD:716:GLN:HE22	1.42	0.68
1:AAA:49:SER:HB3	2:CCC:1083:GLU:OE2	1.94	0.67
3:DDD:817:HIS:HB3	3:DDD:860:ARG:HH21	1.58	0.67
2:CCC:1145:ILE:HG22	2:CCC:1161:LEU:HD11	1.76	0.67
2:CCC:118:LYS:NZ	2:CCC:485:ASP:O	2.28	0.67
2:CCC:1234:LYS:HE2	2:CCC:1238:LEU:HD21	1.77	0.67
2:CCC:1223:ARG:HG2	3:DDD:635:SER:O	1.94	0.67
3:DDD:361:LEU:O	3:DDD:626:TYR:OH	2.13	0.66
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD21	1.77	0.66
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.25	0.66
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.77	0.66
3:DDD:555:TYR:CE1	3:DDD:585:LYS:CD	2.79	0.66
3:DDD:515:ARG:CZ	3:DDD:717:VAL:CG1	2.73	0.66
2:CCC:27:LEU:CD1	2:CCC:524:ILE:HD13	1.79	0.66
2:CCC:1101:LEU:HD13	3:DDD:504:GLN:HG2	1.78	0.65
3:DDD:905:ARG:NH1	3:DDD:910:ASN:OD1	2.29	0.65
2:CCC:1268:GLN:HE21	3:DDD:351:GLY:CA	2.08	0.65
3:DDD:822:MET:HE2	3:DDD:882:VAL:HG11	1.78	0.65
5:FFF:262:TRP:HE1	5:FFF:320:GLN:NE2	1.94	0.65
2:CCC:842:ASP:O	5:FFF:214:ARG:CZ	2.45	0.65
3:DDD:515:ARG:CZ	3:DDD:717:VAL:CB	2.73	0.65
3:DDD:930:LEU:HB3	3:DDD:1134:ILE:HG13	1.79	0.65
2:CCC:241:LEU:HD23	2:CCC:277:LEU:HD21	1.78	0.64
2:CCC:517:GLN:OE1	2:CCC:759:SER:HA	1.96	0.64
3:DDD:342:LEU:HD21	3:DDD:1352:ILE:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:821:MET:HE1	3:DDD:879:ALA:CB	2.27	0.64
2:CCC:906:PHE:CZ	5:FFF:323:ASN:HA	2.32	0.64
2:CCC:27:LEU:HD13	2:CCC:524:ILE:HD11	0.73	0.64
2:CCC:46:GLN:HB2	2:CCC:51:ALA:HA	1.78	0.64
2:CCC:672:GLU:HG3	2:CCC:673:HIS:CD2	2.32	0.64
3:DDD:508:LEU:HD12	3:DDD:508:LEU:O	1.97	0.64
3:DDD:517:CYS:HA	3:DDD:716:GLN:HE22	1.61	0.64
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HG21	1.80	0.63
2:CCC:828:PHE:CZ	2:CCC:1066:MET:CE	2.82	0.63
2:CCC:821:ARG:HH11	2:CCC:1082:ILE:HD13	1.63	0.63
1:AAA:159:ILE:HD11	2:CCC:876:GLU:OE1	1.99	0.63
2:CCC:1318:GLY:O	2:CCC:1319:MET:HB2	1.98	0.62
2:CCC:898:GLU:HG2	5:FFF:256:LYS:HG2	1.81	0.62
2:CCC:397:LEU:O	2:CCC:398:SER:OG	2.11	0.62
5:FFF:235:LEU:O	5:FFF:235:LEU:HD12	1.98	0.62
3:DDD:451:PRO:HB2	3:DDD:625:MET:SD	2.39	0.62
2:CCC:906:PHE:HZ	5:FFF:323:ASN:HA	1.63	0.62
2:CCC:894:GLN:NE2	3:DDD:69:GLU:OE2	2.32	0.62
2:CCC:548:ARG:HB3	2:CCC:570:GLY:HA3	1.82	0.62
2:CCC:1294:LYS:HD3	3:DDD:347:VAL:HG13	1.81	0.62
5:FFF:265:GLU:O	5:FFF:265:GLU:HG2	1.99	0.62
2:CCC:812:PHE:CE1	3:DDD:629:PHE:HZ	2.17	0.62
2:CCC:812:PHE:CE1	3:DDD:629:PHE:CZ	2.88	0.62
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:CA	2.28	0.62
2:CCC:576:SER:OG	2:CCC:659:GLN:O	2.17	0.62
3:DDD:555:TYR:CD1	3:DDD:585:LYS:CD	2.82	0.62
2:CCC:1029:LEU:HG	2:CCC:1033:ARG:HD3	1.82	0.61
3:DDD:452:LEU:CD2	3:DDD:625:MET:SD	2.88	0.61
3:DDD:515:ARG:HH22	3:DDD:717:VAL:C	2.02	0.61
2:CCC:12:ARG:HG3	2:CCC:1181:PRO:HB2	1.83	0.61
2:CCC:28:LEU:CD1	2:CCC:133:ASN:O	2.48	0.61
2:CCC:28:LEU:CD2	2:CCC:527:LYS:HD3	2.30	0.61
2:CCC:27:LEU:HD11	2:CCC:708:VAL:HA	1.82	0.61
5:FFF:241:GLU:HG3	5:FFF:242:LYS:H	1.63	0.61
2:CCC:992:LEU:HB3	2:CCC:993:PRO:HD2	1.83	0.61
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.83	0.61
1:BBB:67:GLU:CB	1:BBB:171:LEU:CD2	2.61	0.61
1:AAA:150:ARG:HH12	1:BBB:7:GLU:HB2	1.65	0.61
3:DDD:332:LYS:HA	3:DDD:1328:THR:HG21	1.81	0.61
3:DDD:22:ILE:HG22	3:DDD:1336:ALA:HA	1.83	0.61
3:DDD:452:LEU:HB3	3:DDD:500:ILE:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:154:PRO:HD2	1:BBB:157:THR:HB	1.82	0.61
3:DDD:1140:ARG:HH12	3:DDD:1144:LEU:HD11	1.64	0.61
2:CCC:1123:GLY:HA3	2:CCC:1204:LEU:HD11	1.83	0.60
1:AAA:38:THR:HG21	1:BBB:46:ILE:HD11	1.82	0.60
3:DDD:793:SER:HB2	3:DDD:1138:LEU:HD12	1.83	0.60
2:CCC:88:ARG:NH1	2:CCC:1040:ASP:OD1	2.34	0.60
2:CCC:836:LEU:HD11	2:CCC:921:PRO:CD	2.31	0.60
3:DDD:1263:LYS:HB2	3:DDD:1307:LEU:HD11	1.83	0.60
3:DDD:644:MET:HB2	3:DDD:764:ARG:HD2	1.83	0.60
2:CCC:259:GLY:O	2:CCC:260:LYS:HB2	2.02	0.60
1:BBB:86:LYS:CG	1:BBB:173:VAL:CG1	2.80	0.60
2:CCC:812:PHE:CD1	3:DDD:629:PHE:CZ	2.90	0.60
1:AAA:45:ARG:NH2	1:BBB:34:GLY:O	2.28	0.59
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.65	0.59
5:FFF:277:ARG:CD	5:FFF:306:GLN:HE21	2.15	0.59
2:CCC:144:VAL:HG23	2:CCC:515:MET:HB3	1.85	0.59
1:AAA:35:PHE:CZ	1:BBB:50:SER:OG	2.51	0.59
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.33	0.59
3:DDD:614:LEU:O	3:DDD:617:THR:OG1	2.19	0.59
3:DDD:517:CYS:CA	3:DDD:716:GLN:HE22	2.16	0.59
3:DDD:501:VAL:HG13	3:DDD:502:PRO:HD2	1.84	0.59
2:CCC:560:PRO:HB2	3:DDD:776:THR:CG2	2.32	0.59
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG22	1.84	0.59
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:HG3	1.85	0.59
2:CCC:1290:MET:HG2	2:CCC:1294:LYS:HD2	1.85	0.59
2:CCC:27:LEU:HD12	2:CCC:711:ASP:CB	2.26	0.59
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.33	0.58
2:CCC:832:HIS:CD2	2:CCC:1058:ARG:HH11	2.21	0.58
3:DDD:822:MET:HE2	3:DDD:882:VAL:CG1	2.32	0.58
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.84	0.58
3:DDD:506:VAL:HA	3:DDD:628:GLY:HA3	1.85	0.58
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.34	0.58
1:AAA:165:GLU:O	1:AAA:167:PRO:HD3	2.04	0.58
2:CCC:1301:ARG:HG3	2:CCC:1302:THR:N	2.19	0.58
6:111:55:DC:H2"	6:111:56:DG:C8	2.39	0.58
2:CCC:841:ARG:CZ	3:DDD:257:GLY:HA2	2.34	0.58
3:DDD:517:CYS:SG	3:DDD:716:GLN:OE1	2.56	0.58
5:FFF:152:GLN:HE21	5:FFF:156:ARG:HH11	1.51	0.58
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.67	0.58
1:BBB:86:LYS:HG2	1:BBB:173:VAL:CG1	2.29	0.58
2:CCC:517:GLN:HG3	2:CCC:759:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1267:VAL:O	3:DDD:1268:ASN:CB	2.52	0.58
3:DDD:930:LEU:HD12	3:DDD:1134:ILE:HD11	1.86	0.57
1:BBB:152:TYR:CD2	3:DDD:536:LEU:HD21	2.39	0.57
5:FFF:267:ASN:HB2	5:FFF:270:GLN:HB2	1.85	0.57
2:CCC:518:ASN:HD22	2:CCC:761:GLN:HG2	1.70	0.57
2:CCC:547:VAL:HG22	6:111:49:DG:C6	2.40	0.57
2:CCC:1212:LEU:HD21	2:CCC:1227:VAL:HG21	1.87	0.57
2:CCC:842:ASP:O	5:FFF:214:ARG:NH2	2.38	0.57
3:DDD:301:GLU:HG3	3:DDD:312:ARG:HH22	1.68	0.57
3:DDD:500:ILE:HG22	3:DDD:500:ILE:O	2.03	0.57
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.31	0.57
2:CCC:186:PHE:CD1	2:CCC:196:VAL:HG22	2.40	0.57
2:CCC:207:THR:HG21	2:CCC:351:LEU:HG	1.87	0.57
3:DDD:1140:ARG:HH12	3:DDD:1236:GLU:HG3	1.68	0.57
3:DDD:895:CYS:SG	3:DDD:898:CYS:SG	3.02	0.57
2:CCC:638:SER:O	2:CCC:641:GLU:N	2.38	0.56
3:DDD:1063:ASP:HB3	3:DDD:1103:GLY:HA3	1.86	0.56
3:DDD:548:VAL:HG12	3:DDD:550:VAL:HG22	1.87	0.56
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.43	0.56
2:CCC:228:VAL:HB	2:CCC:335:THR:OG1	2.04	0.56
2:CCC:374:GLU:OE1	6:111:44:DG:N2	2.33	0.56
3:DDD:515:ARG:NH2	3:DDD:717:VAL:HG12	2.20	0.56
3:DDD:518:VAL:O	3:DDD:519:ASN:C	2.43	0.56
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.70	0.56
5:FFF:231:GLU:OE1	7:222:19:DA:N6	2.38	0.56
2:CCC:828:PHE:CZ	2:CCC:1066:MET:HE3	2.40	0.56
2:CCC:836:LEU:HD11	2:CCC:921:PRO:HD3	1.87	0.56
3:DDD:1080:ILE:HB	3:DDD:1097:ALA:HB3	1.86	0.56
2:CCC:1120:ALA:HA	2:CCC:1204:LEU:HD12	1.87	0.56
2:CCC:547:VAL:HG22	6:111:49:DG:H1	1.71	0.56
2:CCC:541:GLU:OE2	6:111:50:DT:C2	2.58	0.56
3:DDD:351:GLY:O	3:DDD:468:VAL:N	2.25	0.56
2:CCC:541:GLU:OE2	6:111:50:DT:N3	2.39	0.56
2:CCC:1268:GLN:NE2	3:DDD:351:GLY:HA2	2.14	0.56
3:DDD:495:ASN:O	3:DDD:497:GLU:N	2.37	0.56
2:CCC:211:ARG:NH1	2:CCC:357:ASN:O	2.39	0.56
2:CCC:868:SER:HB3	2:CCC:942:ASP:HB3	1.86	0.56
3:DDD:610:ARG:HH12	3:DDD:901:ARG:HH12	1.54	0.56
3:DDD:709:ARG:O	3:DDD:710:ASP:CB	2.54	0.56
2:CCC:807:TRP:CD1	2:CCC:817:LEU:HD22	2.41	0.56
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:713:GLU:HG2	3:DDD:714:GLU:N	2.21	0.56
3:DDD:122:SER:O	3:DDD:123:ARG:HB2	2.06	0.55
2:CCC:618:GLN:HE21	3:DDD:769:VAL:HG23	1.71	0.55
3:DDD:301:GLU:HG3	3:DDD:312:ARG:NH2	2.20	0.55
3:DDD:452:LEU:HD21	3:DDD:625:MET:CB	2.31	0.55
2:CCC:894:GLN:HB3	3:DDD:77:ARG:HH21	1.71	0.55
2:CCC:555:TYR:HA	3:DDD:773:PHE:HE1	1.70	0.55
1:BBB:163:GLU:O	1:BBB:163:GLU:HG3	2.07	0.55
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.89	0.55
1:AAA:44:ARG:NH2	2:CCC:1215:GLY:HA2	2.21	0.55
1:AAA:41:ASN:ND2	2:CCC:1217:THR:O	2.40	0.55
2:CCC:1247:SER:O	3:DDD:348:ASP:HB3	2.06	0.55
7:222:20:DG:O5'	7:222:20:DG:H8	1.89	0.55
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CE1	2.41	0.55
2:CCC:28:LEU:HD13	2:CCC:133:ASN:C	2.27	0.55
1:AAA:35:PHE:HZ	1:BBB:50:SER:CB	2.18	0.55
1:AAA:35:PHE:HZ	1:BBB:50:SER:HB3	1.71	0.55
2:CCC:828:PHE:HB3	2:CCC:1060:ILE:HG21	1.88	0.55
2:CCC:905:ILE:HG12	5:FFF:310:LEU:HD22	1.88	0.55
2:CCC:1253:LEU:HB3	5:FFF:235:LEU:CD1	2.36	0.54
5:FFF:114:LEU:HD21	5:FFF:161:GLN:HB2	1.88	0.54
2:CCC:906:PHE:HZ	5:FFF:323:ASN:OD1	1.91	0.54
2:CCC:1258:PRO:HG2	3:DDD:346:ARG:HB2	1.90	0.54
2:CCC:160:ASP:O	2:CCC:162:GLY:N	2.35	0.54
2:CCC:198:ILE:O	2:CCC:201:ARG:HG3	2.08	0.54
2:CCC:804:PHE:O	2:CCC:1225:VAL:HG13	2.07	0.54
3:DDD:515:ARG:HH21	3:DDD:717:VAL:C	2.10	0.54
3:DDD:849:LEU:HB3	3:DDD:856:ILE:HA	1.89	0.54
2:CCC:797:GLY:HA3	2:CCC:1233:LEU:HD23	1.88	0.54
2:CCC:519:ASN:HD21	2:CCC:796:LEU:HD22	1.73	0.54
2:CCC:1284:ALA:CA	3:DDD:1357:ILE:HD12	2.34	0.54
5:FFF:267:ASN:HB2	5:FFF:270:GLN:CG	2.37	0.54
3:DDD:235:GLU:OE2	3:DDD:235:GLU:N	2.36	0.54
1:AAA:199:ASP:OD1	1:AAA:199:ASP:N	2.41	0.54
2:CCC:4:SER:O	2:CCC:8:LYS:HG3	2.08	0.54
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.40	0.54
3:DDD:1267:VAL:O	3:DDD:1268:ASN:HB2	2.07	0.53
1:BBB:199:ASP:N	1:BBB:199:ASP:OD1	2.41	0.53
3:DDD:1167:LYS:HB2	3:DDD:1174:ARG:HD2	1.89	0.53
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:CG2	2.37	0.53
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:953:LEU:HG	2:CCC:1036:ILE:HG21	1.90	0.53
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HG12	1.90	0.53
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.38	0.53
2:CCC:812:PHE:HB3	3:DDD:357:VAL:HG11	1.89	0.53
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG13	1.89	0.53
3:DDD:836:ARG:HG3	3:DDD:869:CYS:HB3	1.90	0.53
2:CCC:828:PHE:CE2	2:CCC:1066:MET:CE	2.91	0.53
2:CCC:836:LEU:CD1	2:CCC:921:PRO:HD3	2.38	0.53
2:CCC:807:TRP:CD1	2:CCC:817:LEU:CD2	2.92	0.53
2:CCC:28:LEU:O	2:CCC:32:LEU:HD12	2.07	0.53
3:DDD:571:ASP:N	3:DDD:571:ASP:OD1	2.42	0.53
3:DDD:615:LYS:HE2	4:EEE:5:THR:HG21	1.91	0.53
3:DDD:832:LYS:HG2	3:DDD:1242:ARG:HD3	1.91	0.53
6:111:56:DG:N2	7:222:8:DG:N3	2.57	0.53
2:CCC:1042:LEU:HD13	2:CCC:1046:VAL:HG12	1.91	0.53
2:CCC:1253:LEU:HB3	5:FFF:235:LEU:HD13	1.91	0.52
2:CCC:494:ASN:ND2	7:222:25:DA:OP1	2.42	0.52
2:CCC:539:THR:O	2:CCC:543:ALA:N	2.42	0.52
2:CCC:88:ARG:HA	2:CCC:934:PHE:HE1	1.73	0.52
3:DDD:24:LEU:HD21	3:DDD:116:PHE:CZ	2.44	0.52
2:CCC:1061:GLN:NE2	2:CCC:1240:ASP:OD1	2.42	0.52
2:CCC:1247:SER:HB3	3:DDD:375:GLU:O	2.09	0.52
3:DDD:451:PRO:HA	3:DDD:454:CYS:SG	2.49	0.52
5:FFF:208:ASP:O	5:FFF:212:MET:HG2	2.09	0.52
2:CCC:547:VAL:CG2	6:111:49:DG:C6	2.93	0.52
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.92	0.52
3:DDD:393:THR:HG22	5:FFF:258:SER:OG	2.08	0.52
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.92	0.52
1:AAA:82:LEU:HD13	1:AAA:173:VAL:HG22	1.90	0.52
1:BBB:86:LYS:HD3	1:BBB:174:ASP:O	2.10	0.52
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.30	0.52
3:DDD:452:LEU:CG	3:DDD:625:MET:SD	2.94	0.52
3:DDD:1080:ILE:HD12	3:DDD:1115:ILE:HD11	1.92	0.52
2:CCC:828:PHE:HB2	2:CCC:1060:ILE:HD13	1.91	0.51
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.92	0.51
3:DDD:510:LEU:CD2	3:DDD:579:LEU:HD21	2.40	0.51
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.92	0.51
1:AAA:210:THR:HG22	1:AAA:211:ILE:N	2.26	0.51
2:CCC:517:GLN:OE1	2:CCC:759:SER:CA	2.59	0.51
3:DDD:1212:ASP:OD1	3:DDD:1212:ASP:N	2.42	0.51
3:DDD:582:ILE:HG23	3:DDD:623:GLN:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:564:PRO:HG2	2:CCC:568:ASN:O	2.10	0.51
2:CCC:635:THR:HG22	2:CCC:644:LEU:HD23	1.92	0.51
3:DDD:799:ARG:HB3	3:DDD:1309:ILE:HG21	1.91	0.51
3:DDD:507:VAL:HG13	3:DDD:601:ILE:HD12	1.91	0.51
2:CCC:241:LEU:CD2	2:CCC:277:LEU:HD21	2.40	0.51
2:CCC:68:LEU:HD12	2:CCC:475:VAL:HG13	1.92	0.51
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	1.93	0.51
6:111:56:DG:N2	7:222:8:DG:C2	2.78	0.51
3:DDD:1256:ILE:HD12	3:DDD:1256:ILE:N	2.26	0.51
3:DDD:347:VAL:O	3:DDD:350:SER:OG	2.19	0.51
1:AAA:82:LEU:CD2	1:AAA:173:VAL:HG21	2.21	0.51
3:DDD:363:LEU:HD22	3:DDD:618:VAL:HG13	1.91	0.51
3:DDD:519:ASN:ND2	3:DDD:710:ASP:CA	2.74	0.51
2:CCC:68:LEU:HD12	2:CCC:475:VAL:CG1	2.41	0.51
2:CCC:709:ALA:HB3	2:CCC:792:GLY:O	2.10	0.51
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.91	0.50
3:DDD:380:PHE:HB3	3:DDD:415:VAL:HG11	1.92	0.50
1:AAA:164:ASP:N	1:AAA:164:ASP:OD1	2.39	0.50
2:CCC:1255:THR:HG21	3:DDD:341:ASN:CG	2.32	0.50
2:CCC:576:SER:HB3	2:CCC:579:ALA:HB2	1.93	0.50
3:DDD:1140:ARG:NH1	3:DDD:1236:GLU:HG3	2.27	0.50
1:BBB:67:GLU:N	1:BBB:171:LEU:CD2	2.68	0.50
2:CCC:517:GLN:CD	2:CCC:760:ASN:H	2.14	0.50
2:CCC:821:ARG:NH1	2:CCC:1082:ILE:HD13	2.26	0.50
3:DDD:490:ILE:CD1	3:DDD:614:LEU:HD12	2.39	0.50
2:CCC:868:SER:CB	2:CCC:944:ARG:HB3	2.42	0.50
3:DDD:93:THR:HG22	3:DDD:94:GLN:H	1.75	0.50
5:FFF:158:ILE:O	5:FFF:162:THR:HB	2.12	0.50
3:DDD:822:MET:HE2	3:DDD:882:VAL:HG21	1.94	0.50
3:DDD:832:LYS:HG2	3:DDD:1242:ARG:CD	2.41	0.50
3:DDD:156:ARG:HH22	3:DDD:191:SER:HB2	1.77	0.50
3:DDD:876:SER:HB3	3:DDD:990:ARG:NH1	2.27	0.50
2:CCC:514:PHE:HZ	7:222:20:DG:H2"	1.77	0.49
3:DDD:331:ILE:O	3:DDD:331:ILE:HG22	2.12	0.49
3:DDD:506:VAL:CG1	3:DDD:625:MET:CA	2.76	0.49
1:AAA:153:VAL:CG2	1:AAA:177:TYR:HE2	2.24	0.49
2:CCC:1342:GLU:HA	3:DDD:18:ASP:CB	2.36	0.49
3:DDD:619:ILE:O	3:DDD:623:GLN:HG2	2.12	0.49
2:CCC:547:VAL:CG2	6:111:49:DG:N1	2.74	0.49
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	2.17	0.49
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:676:ALA:HA	3:DDD:772:TYR:OH	2.12	0.49
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.95	0.49
3:DDD:915:ILE:O	3:DDD:918:ILE:N	2.46	0.49
2:CCC:1066:MET:HG2	2:CCC:1234:LYS:HA	1.94	0.49
2:CCC:73:TYR:HB2	2:CCC:98:VAL:HG22	1.95	0.49
3:DDD:592:VAL:O	3:DDD:592:VAL:HG22	2.12	0.49
3:DDD:515:ARG:NH2	3:DDD:717:VAL:O	2.45	0.49
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.94	0.49
2:CCC:1184:THR:HG23	2:CCC:1189:GLY:HA3	1.94	0.49
2:CCC:812:PHE:CD1	3:DDD:629:PHE:CE1	3.01	0.49
3:DDD:793:SER:HB2	3:DDD:1138:LEU:CD1	2.43	0.49
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.30	0.49
1:BBB:158:ARG:HD2	1:BBB:172:LEU:HD21	1.93	0.49
2:CCC:668:ILE:HD11	2:CCC:683:ALA:HB2	1.95	0.49
3:DDD:1347:LEU:HD22	3:DDD:1357:ILE:HG23	1.93	0.49
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.28	0.49
2:CCC:984:VAL:O	2:CCC:984:VAL:HG13	2.12	0.49
2:CCC:1106:ARG:NH1	10:DDD:1504:UTP:O1G	2.45	0.48
3:DDD:1261:LEU:HB3	3:DDD:1304:ARG:HD3	1.94	0.48
3:DDD:872:LEU:HD22	3:DDD:877:VAL:HG21	1.95	0.48
3:DDD:290:ILE:CD1	5:FFF:64:GLU:HB3	2.42	0.48
3:DDD:1197:ASN:N	3:DDD:1210:ILE:O	2.46	0.48
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB2	1.95	0.48
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.43	0.48
2:CCC:882:ILE:HG12	2:CCC:919:ARG:HB3	1.96	0.48
3:DDD:1075:ARG:NH2	3:DDD:1193:TRP:CE3	2.81	0.48
3:DDD:1166:GLY:HA3	3:DDD:1176:VAL:HG23	1.93	0.48
3:DDD:457:TYR:O	3:DDD:458:ASN:HB3	2.12	0.48
2:CCC:1314:GLN:HA	4:EEE:28:ARG:NH2	2.29	0.48
3:DDD:506:VAL:HG13	3:DDD:625:MET:CA	2.42	0.48
2:CCC:185:ASP:HB2	2:CCC:197:ARG:HG3	1.96	0.48
3:DDD:119:SER:HA	3:DDD:311:ARG:HH21	1.78	0.48
2:CCC:836:LEU:HD12	2:CCC:883:LEU:CD1	2.43	0.48
1:BBB:33:ARG:HH22	2:CCC:1081:PRO:HB3	1.79	0.48
2:CCC:454:ARG:HG2	2:CCC:459:MET:HG3	1.96	0.48
3:DDD:458:ASN:ND2	10:DDD:1504:UTP:O3'	2.46	0.48
3:DDD:823:THR:HB	3:DDD:824:PRO:HD2	1.95	0.48
2:CCC:566:GLY:O	2:CCC:568:ASN:N	2.46	0.48
3:DDD:1271:SER:OG	3:DDD:1292:LEU:HD21	2.13	0.48
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.95	0.48
2:CCC:1269:ARG:HA	3:DDD:346:ARG:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:57:PHE:O	3:DDD:98:ARG:NH2	2.47	0.48
3:DDD:708:ASN:ND2	3:DDD:714:GLU:O	2.47	0.48
2:CCC:842:ASP:N	2:CCC:1045:GLY:O	2.47	0.48
2:CCC:225:PHE:CE1	2:CCC:345:PRO:HA	2.49	0.48
2:CCC:389:PHE:O	2:CCC:419:ILE:HG23	2.14	0.48
2:CCC:878:THR:HG22	2:CCC:879:GLY:N	2.29	0.48
3:DDD:1347:LEU:HD22	3:DDD:1357:ILE:CG2	2.44	0.48
3:DDD:822:MET:HE2	3:DDD:882:VAL:CG2	2.44	0.48
7:222:8:DG:H2'	7:222:9:DT:C6	2.48	0.47
2:CCC:836:LEU:HB3	2:CCC:918:LEU:HD11	1.96	0.47
3:DDD:1152:GLU:O	3:DDD:1214:PRO:HD2	2.14	0.47
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.49	0.47
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HG13	1.97	0.47
2:CCC:156:PHE:CE2	2:CCC:158:ASP:HB2	2.50	0.47
2:CCC:891:GLY:O	2:CCC:892:GLU:C	2.53	0.47
2:CCC:1105:SER:HB2	3:DDD:731:ARG:HG3	1.97	0.47
3:DDD:849:LEU:CD1	3:DDD:853:THR:HA	2.43	0.47
3:DDD:43:THR:HG21	5:FFF:164:THR:HG22	1.96	0.47
1:AAA:35:PHE:CZ	1:BBB:50:SER:CB	2.96	0.47
2:CCC:186:PHE:CE1	2:CCC:429:MET:HG2	2.50	0.47
1:BBB:174:ASP:OD1	1:BBB:174:ASP:N	2.46	0.47
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	1.96	0.47
3:DDD:615:LYS:HB2	3:DDD:616:PRO:CD	2.39	0.47
1:BBB:165:GLU:HG3	1:BBB:165:GLU:O	2.13	0.47
2:CCC:127:ILE:O	2:CCC:127:ILE:HG13	2.14	0.47
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.96	0.47
2:CCC:1004:ASP:OD1	2:CCC:1004:ASP:N	2.48	0.47
3:DDD:903:LEU:HD21	3:DDD:1249:ASN:HD22	1.79	0.47
3:DDD:157:GLN:HG2	3:DDD:188:LEU:HD21	1.95	0.47
3:DDD:368:LEU:HD12	3:DDD:369:PRO:HD2	1.97	0.47
3:DDD:515:ARG:NH2	3:DDD:717:VAL:CA	2.77	0.47
1:AAA:47:LEU:HD13	1:AAA:183:ILE:CD1	2.45	0.47
1:BBB:55:ALA:CB	1:BBB:175:ALA:HB1	2.45	0.47
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.15	0.47
1:AAA:57:THR:HG22	1:AAA:58:GLU:HG3	1.97	0.47
3:DDD:378:LYS:H	3:DDD:379:PRO:CD	2.23	0.47
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.45	0.47
1:BBB:55:ALA:HB3	1:BBB:175:ALA:HB1	1.96	0.47
2:CCC:1257:GLN:HB2	2:CCC:1258:PRO:HD2	1.96	0.47
3:DDD:430:HIS:CD2	3:DDD:432:LEU:HB2	2.50	0.47
3:DDD:857:LEU:HD13	3:DDD:875:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:519:ASN:HD21	3:DDD:710:ASP:N	2.13	0.47
3:DDD:623:GLN:HA	3:DDD:623:GLN:HE21	1.80	0.47
3:DDD:452:LEU:HD21	3:DDD:625:MET:SD	2.55	0.47
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG11	1.97	0.47
2:CCC:541:GLU:OE2	6:111:50:DT:C4	2.68	0.46
2:CCC:44:GLU:O	2:CCC:46:GLN:N	2.47	0.46
2:CCC:728:ASP:OD1	2:CCC:729:ALA:N	2.47	0.46
3:DDD:134:ASP:O	3:DDD:138:VAL:HG23	2.15	0.46
2:CCC:906:PHE:CZ	5:FFF:323:ASN:OD1	2.68	0.46
3:DDD:1140:ARG:NH2	3:DDD:1236:GLU:OE2	2.48	0.46
1:AAA:162:GLU:HG3	1:AAA:162:GLU:H	1.47	0.46
3:DDD:973:LEU:CD2	3:DDD:1006:GLY:HA2	2.46	0.46
3:DDD:357:VAL:HG12	3:DDD:461:PHE:CE2	2.51	0.46
3:DDD:527:LEU:HB2	3:DDD:550:VAL:CG1	2.27	0.46
3:DDD:506:VAL:HG13	3:DDD:625:MET:O	2.15	0.46
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.98	0.46
2:CCC:488:MET:HB3	2:CCC:489:PRO:HD2	1.96	0.46
2:CCC:1305:TYR:CZ	3:DDD:379:PRO:HB3	2.51	0.46
2:CCC:758:ARG:CD	2:CCC:835:GLU:HB2	2.46	0.46
3:DDD:363:LEU:HD23	3:DDD:618:VAL:CG1	2.43	0.46
3:DDD:452:LEU:CB	3:DDD:500:ILE:HG23	2.44	0.46
3:DDD:746:LEU:H	3:DDD:746:LEU:HD12	1.80	0.46
3:DDD:749:LYS:HB3	3:DDD:750:PRO:HD2	1.97	0.46
1:AAA:45:ARG:HE	1:BBB:38:THR:HG1	1.57	0.46
2:CCC:1257:GLN:HB3	2:CCC:1296:ASP:OD1	2.15	0.46
2:CCC:138:ILE:O	2:CCC:141:THR:OG1	2.31	0.46
3:DDD:1256:ILE:H	3:DDD:1256:ILE:HD12	1.81	0.46
5:FFF:162:THR:HG23	5:FFF:163:ARG:N	2.31	0.46
2:CCC:42:ASP:O	2:CCC:50:GLU:HG2	2.15	0.46
5:FFF:277:ARG:HD3	5:FFF:306:GLN:HE21	1.80	0.46
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.15	0.46
6:111:56:DG:N2	7:222:8:DG:N2	2.64	0.46
1:AAA:22:THR:OG1	1:AAA:207:THR:O	2.28	0.46
2:CCC:1252:SER:OG	2:CCC:1257:GLN:N	2.49	0.46
1:AAA:192:VAL:CG2	1:AAA:198:LEU:HD12	2.45	0.46
2:CCC:758:ARG:HD3	2:CCC:835:GLU:HB2	1.96	0.46
2:CCC:453:ILE:HD11	2:CCC:530:ILE:HD13	1.98	0.45
5:FFF:162:THR:HG23	5:FFF:163:ARG:HG3	1.98	0.45
2:CCC:1037:THR:HG22	2:CCC:1037:THR:O	2.17	0.45
3:DDD:793:SER:CB	3:DDD:1138:LEU:CD1	2.94	0.45
2:CCC:347:ILE:HD11	2:CCC:433:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:86:LYS:CE	1:AAA:174:ASP:HB2	2.46	0.45
1:AAA:184:ALA:CB	2:CCC:1091:GLY:HA3	2.45	0.45
3:DDD:1350:ASN:HA	3:DDD:1353:VAL:HG22	1.99	0.45
3:DDD:349:TYR:CE1	3:DDD:472:LEU:HD11	2.51	0.45
2:CCC:1103:VAL:HG11	3:DDD:639:VAL:HG11	1.98	0.45
1:AAA:165:GLU:C	1:AAA:167:PRO:HD3	2.37	0.45
1:AAA:38:THR:HG23	1:BBB:42:ALA:O	2.15	0.45
3:DDD:320:ASN:O	3:DDD:321:LYS:HG3	2.16	0.45
3:DDD:609:TYR:OH	3:DDD:905:ARG:O	2.33	0.45
2:CCC:91:THR:HG21	2:CCC:128:PRO:HG3	1.99	0.45
2:CCC:145:ILE:HD11	2:CCC:506:PHE:CD1	2.52	0.45
2:CCC:24:VAL:HG11	2:CCC:704:MET:SD	2.57	0.45
2:CCC:832:HIS:CE1	2:CCC:1238:LEU:HD12	2.51	0.45
3:DDD:1289:ASN:HA	3:DDD:1292:LEU:HD12	1.98	0.45
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.32	0.45
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.17	0.45
3:DDD:1050:THR:HG22	3:DDD:1051:ASP:N	2.32	0.45
3:DDD:369:PRO:HB3	3:DDD:444:GLY:O	2.17	0.45
3:DDD:150:GLY:N	3:DDD:175:GLU:O	2.50	0.45
3:DDD:515:ARG:NE	3:DDD:717:VAL:HB	2.31	0.45
3:DDD:1364:ALA:HB3	4:EEE:21:LEU:HD11	1.99	0.45
5:FFF:267:ASN:HB2	5:FFF:270:GLN:CB	2.47	0.45
2:CCC:557:ARG:NH1	2:CCC:611:GLU:OE1	2.50	0.45
3:DDD:1152:GLU:N	3:DDD:1153:PRO:HD3	2.31	0.45
3:DDD:1280:VAL:HG12	3:DDD:1281:GLU:N	2.32	0.45
3:DDD:321:LYS:O	3:DDD:321:LYS:HD2	2.16	0.45
3:DDD:926:PRO:O	3:DDD:930:LEU:N	2.50	0.45
1:AAA:112:ALA:HB1	1:AAA:123:ILE:HG21	1.99	0.44
3:DDD:1133:ASP:O	3:DDD:1244:GLN:NE2	2.50	0.44
2:CCC:229:ILE:HD12	2:CCC:240:GLU:CD	2.38	0.44
3:DDD:320:ASN:O	3:DDD:322:ARG:N	2.50	0.44
3:DDD:435:GLN:HB2	3:DDD:457:TYR:OH	2.17	0.44
3:DDD:509:GLY:HA3	3:DDD:628:GLY:O	2.16	0.44
3:DDD:755:ILE:HD12	3:DDD:755:ILE:H	1.82	0.44
3:DDD:1364:ALA:HB3	4:EEE:21:LEU:CD1	2.47	0.44
2:CCC:514:PHE:CE1	7:222:20:DG:H4'	2.49	0.44
2:CCC:706:ARG:HA	2:CCC:793:GLU:HA	2.00	0.44
3:DDD:519:ASN:HD22	3:DDD:710:ASP:HA	1.83	0.44
7:222:13:DA:C4'	7:222:14:DC:OP2	2.54	0.44
1:AAA:178:SER:HA	1:AAA:179:PRO:HD3	1.85	0.44
2:CCC:46:GLN:HB2	2:CCC:51:ALA:CA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1268:GLN:HG2	3:DDD:350:SER:HB2	1.98	0.44
5:FFF:267:ASN:HB2	5:FFF:270:GLN:CD	2.38	0.44
5:FFF:318:GLN:HA	5:FFF:323:ASN:HB2	2.00	0.44
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.98	0.44
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	1.99	0.44
1:AAA:234:LEU:HD23	1:BBB:13:LEU:N	2.32	0.44
2:CCC:232:ILE:O	2:CCC:331:LYS:HD3	2.18	0.44
2:CCC:660:VAL:HG11	3:DDD:769:VAL:CG1	2.48	0.44
3:DDD:713:GLU:HG2	3:DDD:714:GLU:H	1.83	0.44
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	2.00	0.44
5:FFF:163:ARG:HD3	5:FFF:167:LEU:HD12	1.99	0.44
3:DDD:508:LEU:HD12	3:DDD:508:LEU:C	2.38	0.44
2:CCC:60:GLN:HA	2:CCC:67:GLU:HA	1.98	0.44
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:HE1	2.36	0.44
5:FFF:72:THR:HG22	5:FFF:73:ALA:H	1.82	0.44
1:AAA:159:ILE:CD1	2:CCC:876:GLU:OE1	2.65	0.44
3:DDD:197:GLU:O	3:DDD:201:LEU:HG	2.18	0.44
3:DDD:515:ARG:HH22	3:DDD:718:SER:N	2.16	0.44
3:DDD:884:SER:OG	3:DDD:885:VAL:N	2.51	0.44
1:AAA:10:LYS:HA	1:BBB:227:GLN:OE1	2.17	0.43
2:CCC:693:LEU:HD12	2:CCC:831:ILE:HD11	2.01	0.43
5:FFF:170:HIS:NE2	6:111:31:DT:H2'	2.33	0.43
2:CCC:1318:GLY:O	2:CCC:1319:MET:CB	2.66	0.43
3:DDD:502:PRO:HB2	3:DDD:506:VAL:HB	2.00	0.43
1:AAA:181:GLU:O	2:CCC:821:ARG:NH2	2.51	0.43
2:CCC:1307:ASN:HB3	2:CCC:1312:ASN:O	2.17	0.43
2:CCC:989:LEU:HD13	2:CCC:1000:LEU:CD2	2.48	0.43
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	2.00	0.43
3:DDD:519:ASN:ND2	3:DDD:710:ASP:HA	2.32	0.43
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.18	0.43
4:EEE:5:THR:HG22	4:EEE:7:GLN:H	1.83	0.43
5:FFF:147:THR:O	5:FFF:151:ARG:HG2	2.18	0.43
2:CCC:100:LEU:HD22	2:CCC:493:ILE:HD11	2.00	0.43
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.48	0.43
3:DDD:612:LEU:HB3	3:DDD:616:PRO:HG2	2.01	0.43
3:DDD:930:LEU:CD1	3:DDD:1246:VAL:CG2	2.97	0.43
2:CCC:124:MET:HB2	2:CCC:498:ILE:HD12	2.00	0.43
2:CCC:757:THR:O	2:CCC:833:ILE:HD12	2.18	0.43
3:DDD:709:ARG:HB3	3:DDD:710:ASP:H	1.67	0.43
2:CCC:660:VAL:HG11	3:DDD:769:VAL:HG13	2.01	0.43
2:CCC:1285:TYR:O	2:CCC:1289:GLU:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:350:SER:HA	3:DDD:468:VAL:O	2.19	0.43
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.49	0.43
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	2.01	0.43
1:BBB:47:LEU:HD13	1:BBB:183:ILE:CD1	2.48	0.43
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.84	0.43
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:CE1	3.07	0.43
2:CCC:560:PRO:O	3:DDD:780:ARG:NH2	2.46	0.43
3:DDD:770:LEU:O	3:DDD:773:PHE:N	2.51	0.43
1:AAA:230:ALA:HB1	1:BBB:11:PRO:O	2.19	0.43
2:CCC:146:VAL:HG13	2:CCC:529:ARG:O	2.18	0.43
2:CCC:548:ARG:CB	2:CCC:570:GLY:HA3	2.47	0.43
3:DDD:553:THR:OG1	3:DDD:567:THR:HG23	2.18	0.43
1:AAA:45:ARG:NH1	2:CCC:1216:ARG:HA	2.33	0.43
2:CCC:161:LYS:H	2:CCC:161:LYS:HG2	1.67	0.43
2:CCC:555:TYR:HA	3:DDD:773:PHE:CE1	2.53	0.43
3:DDD:449:LEU:HD22	3:DDD:466:MET:SD	2.59	0.43
2:CCC:1222:GLU:OE2	3:DDD:537:TYR:HE1	2.02	0.43
3:DDD:813:ASP:OD1	3:DDD:883:ARG:NH2	2.42	0.43
5:FFF:182:ALA:HA	5:FFF:193:PRO:HG3	2.00	0.43
2:CCC:517:GLN:CG	2:CCC:760:ASN:H	2.32	0.42
3:DDD:1155:ILE:H	3:DDD:1211:SER:HB2	1.84	0.42
2:CCC:347:ILE:HD11	2:CCC:433:ILE:CD1	2.48	0.42
2:CCC:836:LEU:HD11	2:CCC:921:PRO:HD2	2.00	0.42
3:DDD:452:LEU:HD21	3:DDD:625:MET:CG	2.49	0.42
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	2.00	0.42
3:DDD:290:ILE:HD12	5:FFF:64:GLU:HB3	2.01	0.42
6:111:55:DC:C2'	6:111:56:DG:C8	3.03	0.42
2:CCC:184:LEU:HB2	2:CCC:389:PHE:CE1	2.54	0.42
2:CCC:397:LEU:O	2:CCC:398:SER:CB	2.67	0.42
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.49	0.42
5:FFF:144:THR:HA	6:111:40:DA:N7	2.35	0.42
1:AAA:47:LEU:HA	1:AAA:51:MET:HG2	2.01	0.42
1:BBB:112:ALA:HB1	1:BBB:123:ILE:HG21	2.02	0.42
3:DDD:68:TYR:CZ	3:DDD:78:LEU:HD21	2.54	0.42
5:FFF:220:THR:HG21	7:222:22:DA:N1	2.35	0.42
2:CCC:127:ILE:CG1	2:CCC:127:ILE:O	2.67	0.42
2:CCC:854:ILE:HB	2:CCC:857:VAL:HG21	2.00	0.42
3:DDD:1087:ASP:OD1	3:DDD:1087:ASP:N	2.52	0.42
3:DDD:1138:LEU:N	3:DDD:1139:PRO:CD	2.81	0.42
1:BBB:57:THR:HG22	1:BBB:58:GLU:HG3	2.02	0.42
2:CCC:550:VAL:HG22	3:DDD:780:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:802:VAL:HG12	2:CCC:803:ALA:N	2.35	0.42
2:CCC:812:PHE:CE2	2:CCC:813:GLU:HG3	2.55	0.42
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	2.00	0.42
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:HE21	1.84	0.42
3:DDD:519:ASN:O	3:DDD:520:ALA:HB3	2.20	0.42
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HH11	1.84	0.42
1:AAA:35:PHE:CE1	1:BBB:46:ILE:HG12	2.55	0.42
2:CCC:1292:THR:OG1	2:CCC:1293:VAL:N	2.52	0.42
2:CCC:812:PHE:HD1	3:DDD:629:PHE:CE1	2.37	0.42
3:DDD:502:PRO:HG2	3:DDD:601:ILE:HG21	2.01	0.42
1:BBB:152:TYR:CE2	3:DDD:536:LEU:HD21	2.55	0.42
2:CCC:199:ASP:HB2	2:CCC:201:ARG:HG3	2.00	0.42
2:CCC:125:GLY:HA2	2:CCC:499:SER:HB2	2.00	0.42
2:CCC:556:GLY:HA3	2:CCC:589:THR:HG21	2.01	0.42
2:CCC:832:HIS:HE1	2:CCC:1238:LEU:HD12	1.85	0.42
3:DDD:450:HIS:HA	3:DDD:451:PRO:HD3	1.84	0.42
1:BBB:67:GLU:CA	1:BBB:171:LEU:CD2	2.97	0.42
2:CCC:1064:ASP:OD1	2:CCC:1239:VAL:HG12	2.20	0.42
10:DDD:1504:UTP:O1A	10:DDD:1504:UTP:H4'	2.20	0.42
1:BBB:44:ARG:HA	1:BBB:183:ILE:HD13	2.02	0.41
2:CCC:163:LYS:HG2	2:CCC:164:THR:N	2.35	0.41
2:CCC:185:ASP:OD1	2:CCC:185:ASP:N	2.52	0.41
3:DDD:817:HIS:CB	3:DDD:860:ARG:NH2	2.65	0.41
1:AAA:86:LYS:NZ	1:AAA:174:ASP:HB2	2.36	0.41
2:CCC:98:VAL:HB	2:CCC:124:MET:HE2	2.01	0.41
3:DDD:903:LEU:HD12	3:DDD:903:LEU:H	1.84	0.41
2:CCC:1314:GLN:HG3	4:EEE:28:ARG:CZ	2.50	0.41
1:AAA:82:LEU:HB3	1:AAA:173:VAL:HG11	2.02	0.41
1:AAA:66:HIS:CE1	1:AAA:69:SER:HB3	2.56	0.41
1:BBB:159:ILE:HG13	1:BBB:166:ARG:NE	2.34	0.41
2:CCC:1119:MET:HE2	2:CCC:1204:LEU:HB3	2.02	0.41
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	2.02	0.41
2:CCC:338:THR:HG23	2:CCC:345:PRO:HG3	2.02	0.41
5:FFF:72:THR:HG22	5:FFF:73:ALA:N	2.35	0.41
2:CCC:557:ARG:HH12	2:CCC:611:GLU:CD	2.24	0.41
3:DDD:168:ALA:O	3:DDD:173:GLY:N	2.53	0.41
1:BBB:83:LEU:HD11	3:DDD:526:VAL:HB	2.02	0.41
3:DDD:516:ASP:HB3	3:DDD:573:THR:HG21	2.01	0.41
5:FFF:143:SER:HB3	6:111:41:DT:H73	2.02	0.41
6:111:59:DG:N2	7:222:5:DC:O2	2.53	0.41
1:BBB:67:GLU:CA	1:BBB:171:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:192:VAL:CG2	1:BBB:198:LEU:HD12	2.50	0.41
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD22	2.02	0.41
2:CCC:1337:ILE:HG23	2:CCC:1337:ILE:O	2.21	0.41
2:CCC:208:ILE:HG13	2:CCC:356:THR:HG21	2.02	0.41
2:CCC:625:GLU:O	2:CCC:626:GLU:HB3	2.20	0.41
3:DDD:793:SER:OG	3:DDD:1138:LEU:HD11	2.20	0.41
3:DDD:819:GLY:O	3:DDD:1227:HIS:CD2	2.73	0.41
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	2.03	0.41
6:111:47:DC:H4'	6:111:48:DA:OP1	2.20	0.41
2:CCC:245:ARG:C	2:CCC:247:ARG:H	2.24	0.41
2:CCC:811:ASN:HA	2:CCC:815:SER:O	2.20	0.41
3:DDD:1140:ARG:HG3	3:DDD:1140:ARG:HH11	1.86	0.41
3:DDD:1175:LEU:HD12	3:DDD:1177:ILE:CG1	2.51	0.41
3:DDD:135:ILE:HG23	3:DDD:185:ILE:HD13	2.02	0.41
6:111:51:DC:H2''	6:111:52:DT:C5	2.56	0.41
1:AAA:50:SER:O	1:AAA:150:ARG:HD2	2.21	0.41
1:AAA:166:ARG:NH2	2:CCC:863:SER:HB2	2.36	0.41
3:DDD:452:LEU:HD11	3:DDD:622:ASP:HA	2.03	0.41
3:DDD:825:VAL:HG12	3:DDD:832:LYS:HB3	2.01	0.41
1:BBB:66:HIS:CE1	1:BBB:69:SER:HB3	2.55	0.41
1:BBB:86:LYS:HG3	1:BBB:173:VAL:CG1	2.50	0.41
2:CCC:1234:LYS:CE	2:CCC:1238:LEU:HD21	2.49	0.41
2:CCC:389:PHE:HB3	2:CCC:420:LEU:HD12	2.02	0.41
2:CCC:30:ILE:CD1	2:CCC:575:LEU:HD22	2.50	0.41
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.54	0.41
1:AAA:152:TYR:OH	2:CCC:824:GLN:O	2.31	0.41
3:DDD:1175:LEU:O	3:DDD:1187:GLU:HA	2.21	0.41
3:DDD:314:ARG:HH11	3:DDD:314:ARG:HB2	1.85	0.41
3:DDD:388:ARG:HB3	3:DDD:390:LEU:HD13	2.02	0.41
3:DDD:519:ASN:HA	3:DDD:523:GLU:CG	2.51	0.41
2:CCC:1105:SER:CB	3:DDD:731:ARG:HD2	2.50	0.41
2:CCC:1302:THR:HG22	5:FFF:246:PRO:HA	2.01	0.41
3:DDD:733:SER:O	3:DDD:737:ILE:HG13	2.21	0.41
1:AAA:192:VAL:HG23	1:AAA:198:LEU:HD12	2.02	0.41
2:CCC:443:ASP:N	2:CCC:443:ASP:OD1	2.53	0.41
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.84	0.41
2:CCC:868:SER:CB	2:CCC:942:ASP:HB3	2.49	0.41
3:DDD:1220:ILE:HG12	3:DDD:1224:ARG:HH22	1.86	0.41
3:DDD:261:ALA:HA	5:FFF:219:ILE:CG2	2.51	0.41
3:DDD:420:PRO:HA	3:DDD:437:PHE:O	2.21	0.41
1:BBB:192:VAL:HG23	1:BBB:198:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:228:LEU:HA	1:BBB:231:PHE:HD2	1.86	0.41
2:CCC:390:PHE:HA	2:CCC:419:ILE:HG23	2.03	0.41
3:DDD:346:ARG:H	3:DDD:346:ARG:HG2	1.73	0.41
3:DDD:799:ARG:HD2	3:DDD:1146:GLU:OE2	2.21	0.41
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.38	0.41
5:FFF:204:LYS:HB3	5:FFF:205:PRO:HD2	2.02	0.41
5:FFF:156:ARG:NH2	6:111:34:DG:O6	2.54	0.40
1:AAA:234:LEU:HD23	1:BBB:13:LEU:H	1.86	0.40
2:CCC:1146:GLN:HB2	2:CCC:1161:LEU:HD12	2.03	0.40
2:CCC:635:THR:CG2	2:CCC:644:LEU:HD23	2.51	0.40
3:DDD:332:LYS:HA	3:DDD:1328:THR:CG2	2.49	0.40
1:AAA:44:ARG:HA	1:AAA:183:ILE:HD13	2.02	0.40
1:BBB:192:VAL:O	1:BBB:193:GLU:C	2.59	0.40
2:CCC:865:LEU:HD23	2:CCC:871:VAL:HG23	2.01	0.40
2:CCC:868:SER:HB2	2:CCC:944:ARG:HB3	2.02	0.40
3:DDD:113:HIS:CE1	3:DDD:307:LEU:HD13	2.56	0.40
3:DDD:832:LYS:HE2	3:DDD:1242:ARG:HG2	2.03	0.40
3:DDD:417:ARG:C	3:DDD:418:GLU:HG2	2.41	0.40
6:111:32:DA:C2	7:222:32:DA:C6	3.09	0.40
1:AAA:134:THR:HB	2:CCC:773:LEU:HD22	2.02	0.40
1:AAA:29:GLU:CB	1:AAA:30:PRO:HA	2.44	0.40
2:CCC:1274:GLU:HA	3:DDD:428:THR:HG21	2.03	0.40
2:CCC:28:LEU:HD21	2:CCC:527:LYS:HD2	2.01	0.40
3:DDD:502:PRO:CG	3:DDD:601:ILE:HG21	2.51	0.40
3:DDD:508:LEU:HB2	3:DDD:730:ALA:HB2	2.03	0.40
3:DDD:926:PRO:O	3:DDD:930:LEU:HG	2.21	0.40
1:BBB:67:GLU:CG	1:BBB:171:LEU:HD22	2.46	0.40
2:CCC:1157:GLN:O	2:CCC:1157:GLN:HG3	2.22	0.40
2:CCC:1311:GLY:O	4:EEE:31:GLN:NE2	2.44	0.40
2:CCC:805:MET:HG2	2:CCC:1225:VAL:HG11	2.03	0.40
3:DDD:1330:ARG:HD2	3:DDD:1330:ARG:N	2.36	0.40
3:DDD:709:ARG:O	3:DDD:710:ASP:HB3	2.22	0.40
2:CCC:618:GLN:NE2	3:DDD:769:VAL:HG23	2.36	0.40
4:EEE:59:ILE:HG23	4:EEE:64:LEU:HD11	2.04	0.40
1:AAA:192:VAL:O	1:AAA:193:GLU:C	2.60	0.40
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	2.20	0.40
3:DDD:43:THR:HG21	5:FFF:164:THR:CG2	2.52	0.40
3:DDD:615:LYS:N	3:DDD:616:PRO:CD	2.84	0.40
3:DDD:736:GLN:HA	3:DDD:736:GLN:HE21	1.87	0.40
3:DDD:807:LEU:CD2	3:DDD:1255:VAL:HG13	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:160:HIS:ND1	2:CCC:272:ARG:NH2[4_445]	2.08	0.12

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%)	201 (88%)	20 (9%)	7 (3%)	4	31
1	BBB	226/242 (93%)	205 (91%)	18 (8%)	3 (1%)	12	47
2	CCC	1338/1342 (100%)	1197 (90%)	123 (9%)	18 (1%)	12	47
3	DDD	1346/1407 (96%)	1210 (90%)	119 (9%)	17 (1%)	12	47
4	EEE	77/90 (86%)	70 (91%)	7 (9%)	0	100	100
5	FFF	275/336 (82%)	249 (90%)	25 (9%)	1 (0%)	34	70
All	All	3490/3659 (95%)	3132 (90%)	312 (9%)	46 (1%)	12	47

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CCC	161	LYS
2	CCC	1319	MET
3	DDD	519	ASN
3	DDD	710	ASP
3	DDD	1268	ASN
2	CCC	45	GLY
2	CCC	398	SER
2	CCC	567	PRO
2	CCC	1004	ASP
2	CCC	1297	ASP
2	CCC	1318	GLY
3	DDD	207	GLU
3	DDD	1053	LEU

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Mol	Chain	Res	Type
3	DDD	1201	GLY
5	FFF	113	GLY
1	AAA	164	ASP
1	BBB	232	VAL
2	CCC	201	ARG
2	CCC	234	ASP
2	CCC	260	LYS
2	CCC	1103	VAL
2	CCC	1224	PRO
3	DDD	342	LEU
1	AAA	161	SER
1	AAA	208	ASN
1	AAA	210	THR
2	CCC	812	PHE
3	DDD	321	LYS
3	DDD	1344	LEU
2	CCC	110	PRO
2	CCC	1153	ALA
3	DDD	81	ARG
3	DDD	96	LYS
3	DDD	854	ALA
3	DDD	947	GLU
3	DDD	1325	PHE
3	DDD	1375	ALA
3	DDD	829	GLY
1	AAA	211	ILE
1	BBB	14	VAL
1	AAA	14	VAL
1	AAA	40	GLY
1	BBB	40	GLY
2	CCC	627	GLY
3	DDD	1091	PRO
2	CCC	1185	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	198/208 (95%)	190 (96%)	8 (4%)	31	57
1	BBB	196/208 (94%)	188 (96%)	8 (4%)	30	57
2	CCC	1155/1157 (100%)	1119 (97%)	36 (3%)	40	63
3	DDD	1127/1168 (96%)	1082 (96%)	45 (4%)	31	57
4	EEE	67/74 (90%)	65 (97%)	2 (3%)	41	64
5	FFF	240/292 (82%)	229 (95%)	11 (5%)	27	54
All	All	2983/3107 (96%)	2873 (96%)	110 (4%)	34	59

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	13	LEU
1	AAA	28	LEU
1	AAA	157	THR
1	AAA	159	ILE
1	AAA	162	GLU
1	AAA	164	ASP
1	AAA	165	GLU
1	AAA	166	ARG
1	BBB	13	LEU
1	BBB	28	LEU
1	BBB	159	ILE
1	BBB	160	HIS
1	BBB	162	GLU
1	BBB	165	GLU
1	BBB	174	ASP
1	BBB	233	ASP
2	CCC	12	ARG
2	CCC	23	ASP
2	CCC	47	TYR
2	CCC	185	ASP
2	CCC	202	ARG
2	CCC	234	ASP
2	CCC	320	ASP
2	CCC	332	ARG
2	CCC	423	ASP
2	CCC	443	ASP
2	CCC	514	PHE
2	CCC	515	MET
2	CCC	541	GLU
2	CCC	553	THR

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Mol	Chain	Res	Type
2	CCC	561	ILE
2	CCC	609	ILE
2	CCC	628	HIS
2	CCC	635	THR
2	CCC	660	VAL
2	CCC	694	ARG
2	CCC	700	VAL
2	CCC	757	THR
2	CCC	764	CYS
2	CCC	788	SER
2	CCC	828	PHE
2	CCC	876	GLU
2	CCC	888	THR
2	CCC	913	VAL
2	CCC	914	LYS
2	CCC	994	ARG
2	CCC	1006	GLU
2	CCC	1069	ARG
2	CCC	1224	PRO
2	CCC	1240	ASP
2	CCC	1241	ASP
2	CCC	1272	GLU
3	DDD	28	ASP
3	DDD	86	GLU
3	DDD	158	GLN
3	DDD	199	GLU
3	DDD	216	LYS
3	DDD	281	ARG
3	DDD	298	MET
3	DDD	314	ARG
3	DDD	321	LYS
3	DDD	346	ARG
3	DDD	384	LYS
3	DDD	398	LYS
3	DDD	399	LYS
3	DDD	504	GLN
3	DDD	505	ASP
3	DDD	526	VAL
3	DDD	549	LYS
3	DDD	551	ARG
3	DDD	571	ASP
3	DDD	579	LEU

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Mol	Chain	Res	Type
3	DDD	599	LYS
3	DDD	610	ARG
3	DDD	619	ILE
3	DDD	623	GLN
3	DDD	649	LYS
3	DDD	695	LYS
3	DDD	736	GLN
3	DDD	746	LEU
3	DDD	770	LEU
3	DDD	798	ARG
3	DDD	830	ASP
3	DDD	831	VAL
3	DDD	835	LEU
3	DDD	838	ARG
3	DDD	843	VAL
3	DDD	849	LEU
3	DDD	857	LEU
3	DDD	930	LEU
3	DDD	1138	LEU
3	DDD	1175	LEU
3	DDD	1189	MET
3	DDD	1199	PHE
3	DDD	1210	ILE
3	DDD	1227	HIS
3	DDD	1356	LEU
4	EEE	5	THR
4	EEE	43	ASN
5	FFF	54	VAL
5	FFF	156	ARG
5	FFF	211	ARG
5	FFF	220	THR
5	FFF	229	ASP
5	FFF	231	GLU
5	FFF	241	GLU
5	FFF	243	GLU
5	FFF	271	ARG
5	FFF	299	ARG
5	FFF	325	GLU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
10	UTP	DDD	1504	8	26,30,30	1.85	4 (15%)	34,47,47	1.06	1 (2%)

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
10	UTP	DDD	1504	8	-	3/22/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	DDD	1504	UTP	C6-C5	-6.70	1.34	1.52
10	DDD	1504	UTP	C6-N1	-4.93	1.38	1.47
10	DDD	1504	UTP	C5-C4	-2.63	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	DDD	1504	UTP	C2-N1	2.41	1.39	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	DDD	1504	UTP	C5-C6-N1	3.33	122.59	111.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

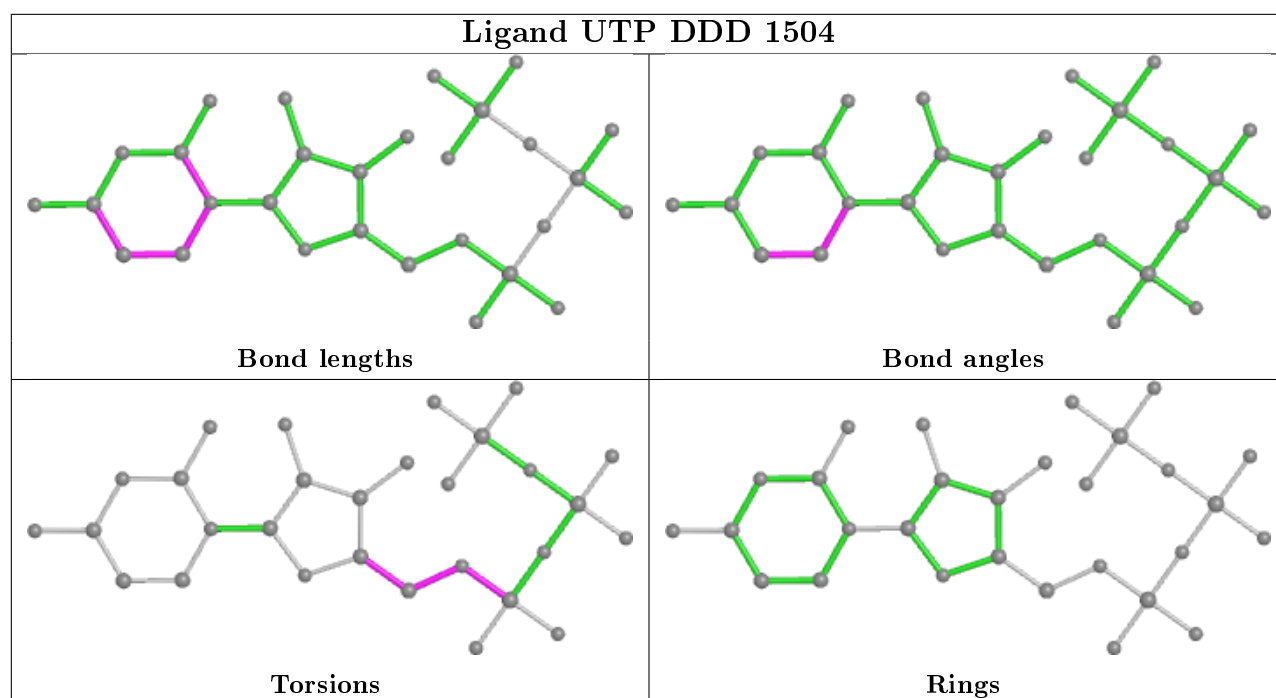
Mol	Chain	Res	Type	Atoms
10	DDD	1504	UTP	C4'-C5'-O5'-PA
10	DDD	1504	UTP	O4'-C4'-C5'-O5'
10	DDD	1504	UTP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	DDD	1504	UTP	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	AAA	230/242 (95%)	0.33	16 (6%) 16 13	183, 315, 405, 447	0
1	BBB	228/242 (94%)	0.49	26 (11%) 5 5	253, 351, 413, 450	0
2	CCC	1340/1342 (99%)	0.16	74 (5%) 25 22	152, 278, 401, 490	0
3	DDD	1350/1407 (95%)	0.48	150 (11%) 5 5	144, 294, 409, 509	0
4	EEE	79/90 (87%)	0.04	6 (7%) 13 11	261, 342, 445, 500	0
5	FFF	277/336 (82%)	0.45	34 (12%) 4 5	201, 327, 412, 459	0
6	111	32/50 (64%)	-0.20	0 100 100	288, 337, 424, 451	0
7	222	34/50 (68%)	0.28	3 (8%) 10 9	265, 333, 436, 477	0
All	All	3570/3759 (94%)	0.33	309 (8%) 10 9	144, 301, 411, 509	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	976	THR	10.5
5	FFF	310	LEU	10.0
3	DDD	1078	LEU	9.9
3	DDD	1098	GLN	9.3
3	DDD	1068	THR	9.2
5	FFF	306	GLN	9.0
3	DDD	1065	ALA	8.9
3	DDD	879	ALA	8.9
3	DDD	1101	LEU	8.7
3	DDD	1130	GLY	8.7
3	DDD	1007	ASP	8.6
3	DDD	989	GLY	8.2
3	DDD	1099	TYR	7.9
1	AAA	213	PRO	7.3
3	DDD	1066	GLU	7.3
3	DDD	982	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
3	DDD	1030	GLU	6.6
2	CCC	850	ILE	6.0
2	CCC	1003	THR	6.0
2	CCC	1004	ASP	6.0
2	CCC	869	GLY	6.0
3	DDD	1203	ARG	6.0
5	FFF	263	LEU	5.9
3	DDD	974	VAL	5.8
3	DDD	988	PHE	5.8
3	DDD	1129	GLY	5.8
3	DDD	1055	GLY	5.6
3	DDD	965	SER	5.5
1	BBB	164	ASP	5.5
3	DDD	1121	LEU	5.5
3	DDD	1064	SER	5.3
5	FFF	113	GLY	5.3
3	DDD	841	GLY	5.2
3	DDD	966	VAL	5.1
3	DDD	1004	ALA	5.1
3	DDD	1038	THR	5.1
2	CCC	311	CYS	5.1
3	DDD	1317	GLU	5.1
3	DDD	975	ILE	5.0
5	FFF	311	ARG	5.0
3	DDD	1028	ILE	4.9
2	CCC	983	GLY	4.9
3	DDD	1077	ALA	4.9
2	CCC	911	SER	4.8
3	DDD	857	LEU	4.7
3	DDD	997	VAL	4.7
2	CCC	906	PHE	4.7
3	DDD	977	SER	4.7
4	EEE	78	ALA	4.6
2	CCC	102	LEU	4.5
3	DDD	880	VAL	4.5
5	FFF	301	ARG	4.5
3	DDD	848	VAL	4.4
3	DDD	1076	PRO	4.4
3	DDD	1161	GLY	4.4
3	DDD	944	ALA	4.4
2	CCC	103	VAL	4.4
3	DDD	1029	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	107	ILE	4.3
3	DDD	984	LEU	4.3
2	CCC	984	VAL	4.3
1	BBB	165	GLU	4.2
3	DDD	1100	PHE	4.2
5	FFF	324	ILE	4.2
3	DDD	877	VAL	4.1
3	DDD	1187	GLU	4.1
3	DDD	1063	ASP	4.1
3	DDD	856	ILE	4.0
4	EEE	80	LEU	4.0
3	DDD	1112	GLY	4.0
2	CCC	1002	LEU	4.0
2	CCC	1054	LEU	3.9
3	DDD	973	LEU	3.9
3	DDD	1110	GLU	3.9
2	CCC	113	THR	3.9
2	CCC	1180	MET	3.9
3	DDD	958	ILE	3.9
3	DDD	1202	GLU	3.9
1	BBB	26	VAL	3.9
3	DDD	986	ASP	3.8
7	222	21	DG	3.8
2	CCC	912	ASP	3.8
3	DDD	1111	ASP	3.8
2	CCC	1055	ALA	3.8
3	DDD	1109	LEU	3.8
4	EEE	79	GLU	3.8
3	DDD	79	LYS	3.7
1	AAA	172	LEU	3.6
7	222	22	DA	3.6
3	DDD	1069	ALA	3.6
7	222	23	DT	3.6
5	FFF	305	ILE	3.5
1	BBB	90	VAL	3.5
3	DDD	1005	LYS	3.5
1	AAA	135	ASP	3.5
1	BBB	101	THR	3.5
3	DDD	983	LYS	3.5
3	DDD	1040	MET	3.5
3	DDD	1008	GLY	3.5
2	CCC	1284	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
5	FFF	309	GLY	3.5
2	CCC	883	LEU	3.4
5	FFF	303	ARG	3.4
3	DDD	1118	GLY	3.4
3	DDD	1345	ARG	3.4
3	DDD	87	LYS	3.4
1	AAA	171	LEU	3.4
3	DDD	587	LEU	3.4
3	DDD	256	ASP	3.4
1	BBB	98	VAL	3.4
3	DDD	1003	LEU	3.4
1	BBB	151	GLY	3.3
3	DDD	586	GLY	3.3
1	BBB	13	LEU	3.3
3	DDD	993	GLU	3.3
1	AAA	144	ILE	3.3
3	DDD	1122	ALA	3.3
5	FFF	312	ARG	3.3
3	DDD	154	LEU	3.3
3	DDD	1102	PRO	3.3
3	DDD	990	ARG	3.3
2	CCC	104	ILE	3.3
1	AAA	76	GLU	3.2
2	CCC	124	MET	3.2
1	AAA	34	GLY	3.2
3	DDD	1266	ILE	3.2
3	DDD	1079	LYS	3.2
3	DDD	539	SER	3.2
3	DDD	1346	GLY	3.2
3	DDD	1039	ASP	3.2
3	DDD	584	PRO	3.2
2	CCC	885	GLY	3.2
2	CCC	239	MET	3.2
2	CCC	870	ILE	3.1
3	DDD	985	ILE	3.1
3	DDD	1071	GLY	3.1
3	DDD	972	LYS	3.1
3	DDD	1113	VAL	3.1
3	DDD	1188	GLU	3.1
3	DDD	1046	ILE	3.1
2	CCC	169	LYS	3.1
2	CCC	722	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	DDD	708	ASN	3.1
1	BBB	181	GLU	3.1
1	AAA	133	LEU	3.1
1	BBB	205	MET	3.0
3	DDD	217	LEU	3.0
3	DDD	945	ALA	3.0
2	CCC	1188	ASP	3.0
1	AAA	173	VAL	3.0
5	FFF	259	ILE	3.0
3	DDD	1006	GLY	3.0
3	DDD	1031	VAL	3.0
1	BBB	100	LEU	3.0
2	CCC	1282	GLY	2.9
2	CCC	1005	GLU	2.9
2	CCC	905	ILE	2.9
2	CCC	231	GLU	2.9
3	DDD	746	LEU	2.9
3	DDD	987	GLU	2.9
2	CCC	105	TYR	2.9
3	DDD	1316	THR	2.8
1	BBB	93	GLN	2.8
3	DDD	1114	GLN	2.8
1	AAA	70	THR	2.8
1	BBB	89	ALA	2.8
2	CCC	982	GLY	2.8
3	DDD	1037	PHE	2.8
2	CCC	67	GLU	2.8
2	CCC	533	LEU	2.8
3	DDD	201	LEU	2.8
3	DDD	1241	TYR	2.8
1	AAA	214	GLU	2.8
1	BBB	166	ARG	2.8
2	CCC	871	VAL	2.8
2	CCC	990	ASP	2.8
1	BBB	198	LEU	2.8
2	CCC	171	LEU	2.8
5	FFF	294	GLU	2.8
5	FFF	307	VAL	2.7
2	CCC	926	GLY	2.7
3	DDD	1051	ASP	2.7
2	CCC	1001	GLY	2.7
5	FFF	109	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
3	DDD	980	THR	2.7
3	DDD	1044	GLN	2.7
2	CCC	374	GLU	2.7
3	DDD	1186	TYR	2.7
5	FFF	300	GLU	2.7
2	CCC	282	VAL	2.7
1	AAA	19	VAL	2.7
2	CCC	1217	THR	2.7
2	CCC	232	ILE	2.7
3	DDD	67	ASP	2.6
5	FFF	237	ILE	2.6
3	DDD	855	ASP	2.6
1	AAA	92	VAL	2.6
3	DDD	479	GLU	2.6
5	FFF	283	TYR	2.6
1	BBB	211	ILE	2.6
1	BBB	144	ILE	2.6
5	FFF	302	VAL	2.6
1	BBB	25	LYS	2.6
3	DDD	635	SER	2.6
2	CCC	629	PHE	2.6
2	CCC	378	ARG	2.5
5	FFF	202	LEU	2.5
1	AAA	51	MET	2.5
2	CCC	927	THR	2.5
3	DDD	91	GLU	2.5
3	DDD	912	GLY	2.5
3	DDD	1043	GLY	2.5
3	DDD	964	LYS	2.5
5	FFF	289	GLU	2.5
1	BBB	24	ALA	2.5
5	FFF	313	LEU	2.5
3	DDD	957	SER	2.5
4	EEE	75	GLN	2.5
3	DDD	1052	GLU	2.5
3	DDD	1107	VAL	2.5
3	DDD	1145	PHE	2.5
3	DDD	1097	ALA	2.4
2	CCC	721	GLY	2.4
2	CCC	849	GLU	2.4
3	DDD	1049	GLN	2.4
4	EEE	76	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	DDD	1104	LYS	2.4
1	BBB	133	LEU	2.4
3	DDD	1070	GLY	2.4
3	DDD	1103	GLY	2.4
5	FFF	273	VAL	2.4
2	CCC	385	PHE	2.4
3	DDD	212	THR	2.4
2	CCC	861	ALA	2.3
5	FFF	304	GLN	2.3
3	DDD	80	HIS	2.3
2	CCC	650	VAL	2.3
3	DDD	952	VAL	2.3
2	CCC	163	LYS	2.3
2	CCC	116	ASP	2.3
2	CCC	1185	PRO	2.3
2	CCC	310	ILE	2.3
2	CCC	1189	GLY	2.3
5	FFF	114	LEU	2.3
2	CCC	991	LYS	2.3
5	FFF	134	PHE	2.3
3	DDD	1045	THR	2.3
5	FFF	99	LEU	2.3
4	EEE	15	ASN	2.3
3	DDD	1358	PRO	2.3
2	CCC	657	THR	2.3
5	FFF	315	GLU	2.3
3	DDD	1017	VAL	2.3
3	DDD	1185	PRO	2.3
2	CCC	695	ALA	2.3
3	DDD	854	ALA	2.3
1	BBB	201	LEU	2.3
2	CCC	28	LEU	2.3
1	AAA	75	GLN	2.3
3	DDD	1119	ASP	2.2
5	FFF	298	THR	2.2
3	DDD	1318	SER	2.2
2	CCC	114	VAL	2.2
5	FFF	209	VAL	2.2
5	FFF	178	TYR	2.2
3	DDD	1061	VAL	2.2
3	DDD	1308	GLY	2.2
3	DDD	1350	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	DDD	210	SER	2.2
3	DDD	579	LEU	2.2
5	FFF	110	GLY	2.2
5	FFF	323	ASN	2.2
2	CCC	215	TYR	2.2
2	CCC	1124	ILE	2.2
3	DDD	1349	GLU	2.2
2	CCC	884	VAL	2.2
1	BBB	187	VAL	2.1
3	DDD	1072	LYS	2.1
2	CCC	986	ALA	2.1
2	CCC	1142	ARG	2.1
3	DDD	1128	SER	2.1
3	DDD	822	MET	2.1
3	DDD	262	THR	2.1
2	CCC	240	GLU	2.1
5	FFF	98	ASN	2.1
2	CCC	101	ARG	2.1
2	CCC	506	PHE	2.1
3	DDD	970	SER	2.1
3	DDD	1159	ILE	2.1
1	AAA	193	GLU	2.1
1	BBB	174	ASP	2.1
2	CCC	985	GLU	2.1
3	DDD	853	THR	2.1
1	BBB	220	ALA	2.1
3	DDD	384	LYS	2.0
3	DDD	981	GLU	2.0
1	BBB	49	SER	2.0
3	DDD	352	ARG	2.0
2	CCC	1141	LEU	2.0
3	DDD	1056	LEU	2.0
2	CCC	117	ILE	2.0
3	DDD	214	ARG	2.0
3	DDD	849	LEU	2.0
3	DDD	1131	THR	2.0
3	DDD	1108	GLN	2.0
2	CCC	777	VAL	2.0
3	DDD	68	TYR	2.0
3	DDD	996	LYS	2.0
3	DDD	1295	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

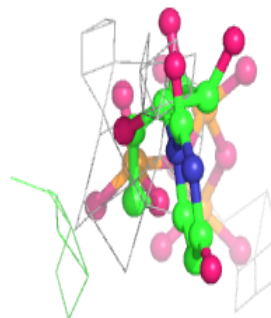
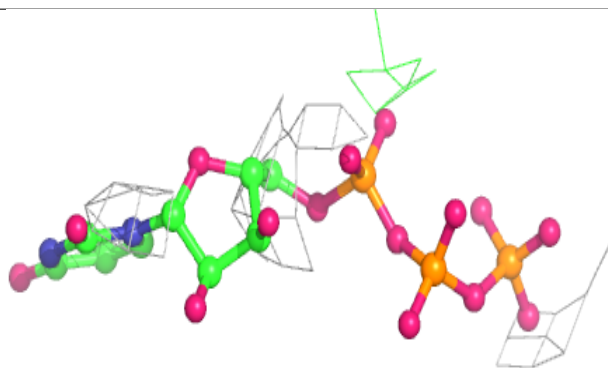
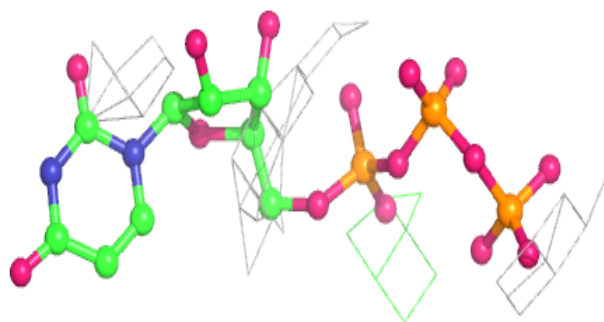
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	UTP	DDD	1504	29/29	0.78	0.47	222,339,384,387	0
9	ZN	DDD	1501	1/1	0.82	0.11	395,395,395,395	0
8	MG	CCC	1401	1/1	0.92	0.25	174,174,174,174	0
8	MG	DDD	1503	1/1	0.92	0.30	125,125,125,125	0
9	ZN	DDD	1502	1/1	0.98	0.09	255,255,255,255	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 UTP DDD 1504:

$2mF_o-DF_c$ (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.