



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:07 PM BST

PDB ID : 6UTZ  
Title : E. coli sigma-S transcription initiation complex with a 6-nt RNA ("Fresh" crystal soaked with CTP and UTP for 30 minutes)  
Authors : Zuo, Y.; De, S.; Steitz, T.A.  
Deposited on : 2019-10-30  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

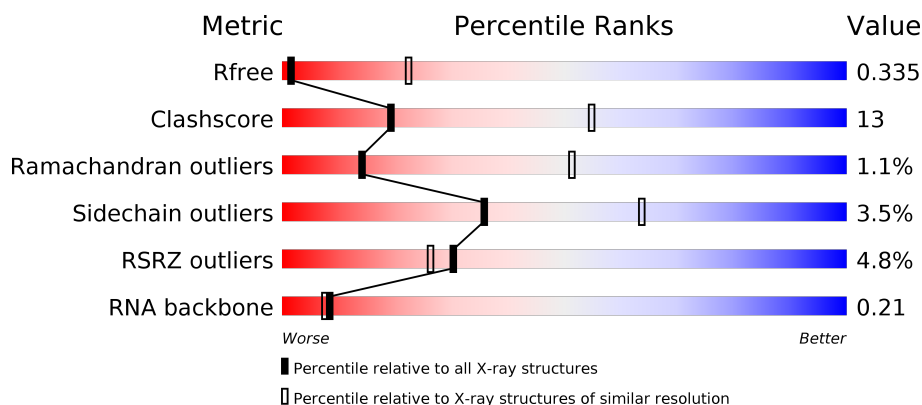
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





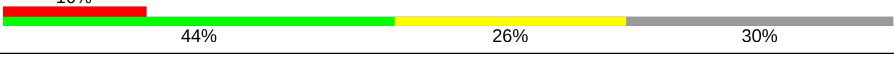

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	AAA	242	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>• 5%</div> </div> </div>
1	BBB	242	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>• 6%</div> </div> </div>
2	CCC	1342	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
3	DDD	1407	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>••</div> </div> </div>

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

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29063 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 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
2	CCC	1341	Total	C	N	O	S	0	0	0
			10577	6636	1842	2056	43			

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	30	Total	C	N	O	P	0	0	0
			618	294	111	183	30			

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

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

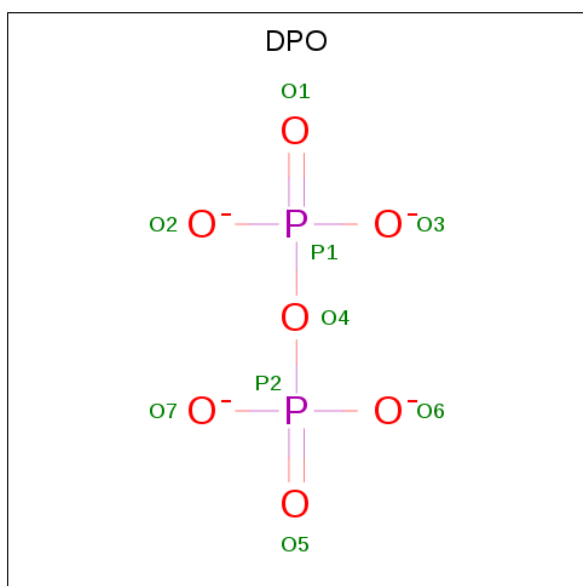
- Molecule 8 is a RNA chain called RNA 6-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	6	Total	C	N	O	P	0	0	0
			137	57	22	50	8			

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

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

- Molecule 10 is DIPHOSPHATE (three-letter code: DPO) (formula: O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	CCC	1	Total	O	P	0	0
			9	7	2		

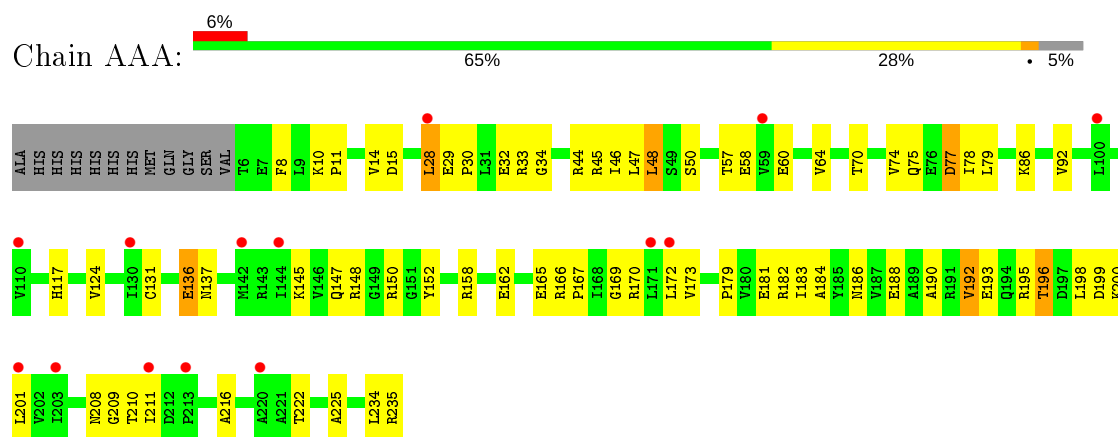
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

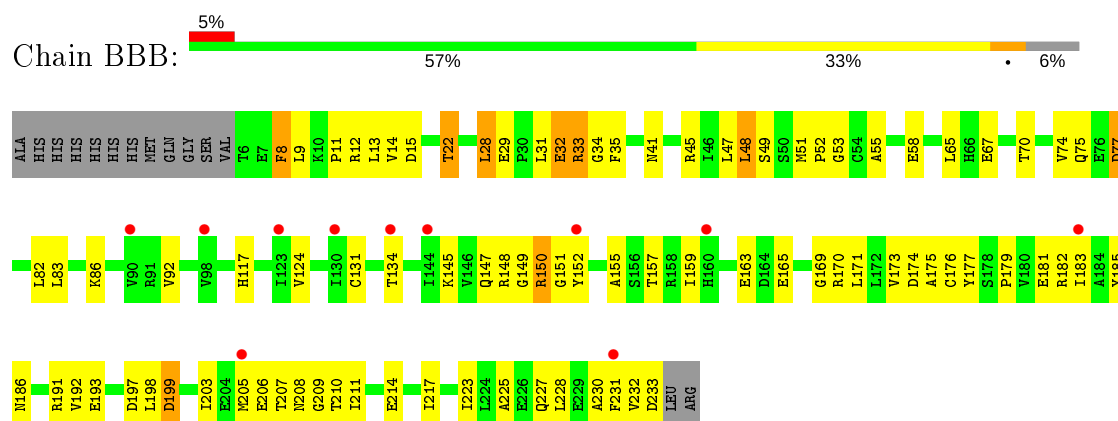
### 3 Residue-property plots [i](#)

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

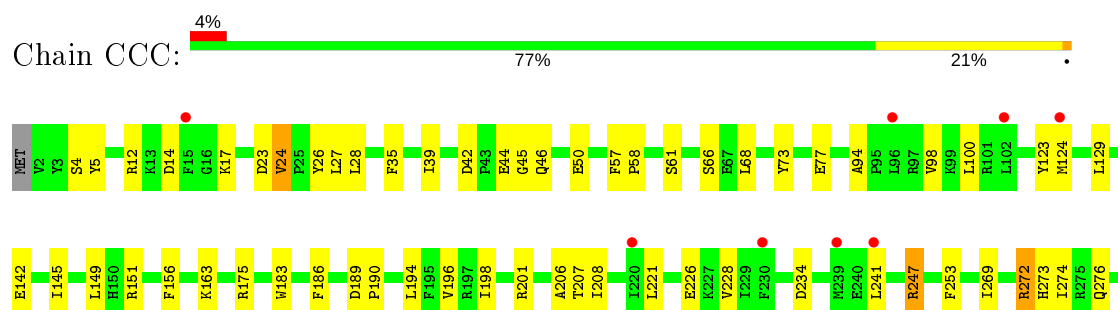
- Molecule 1: DNA-directed RNA polymerase subunit alpha

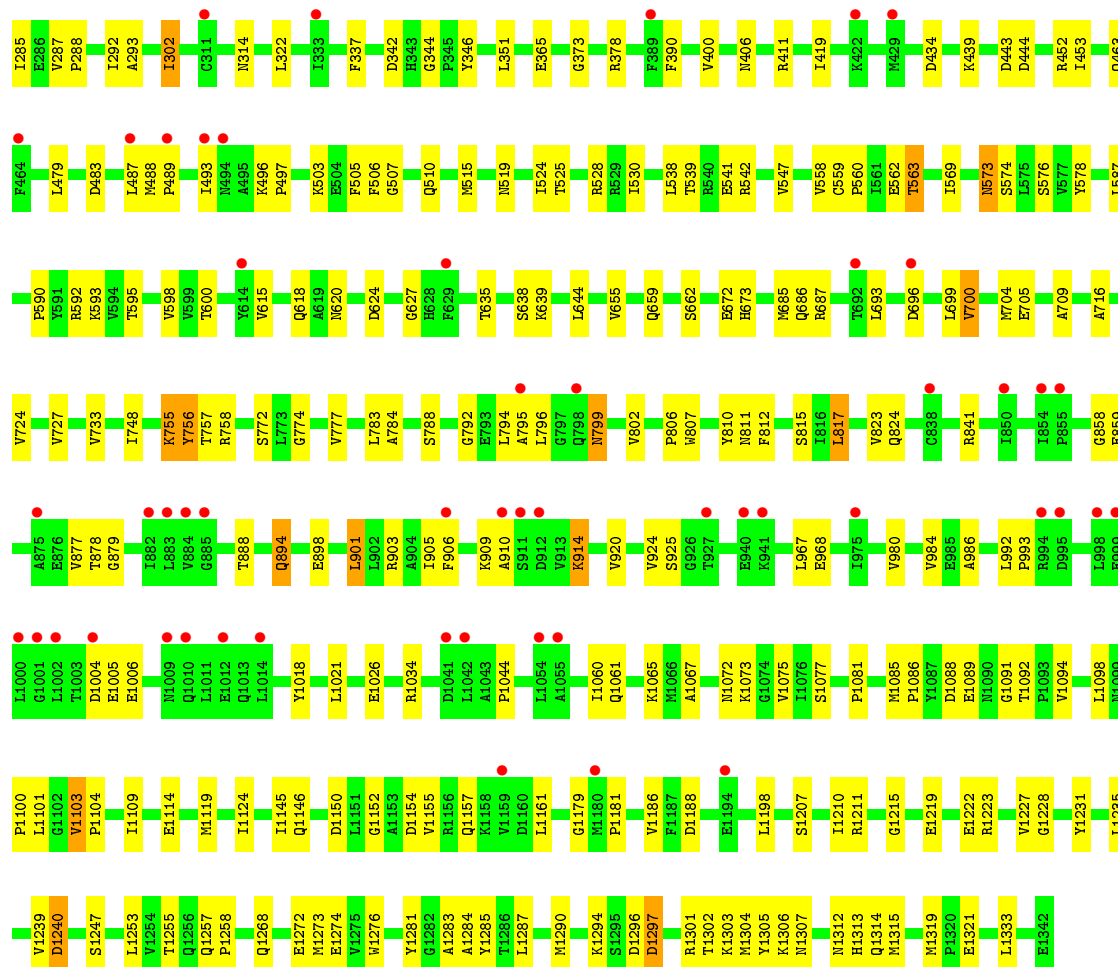


- Molecule 1: DNA-directed RNA polymerase subunit alpha

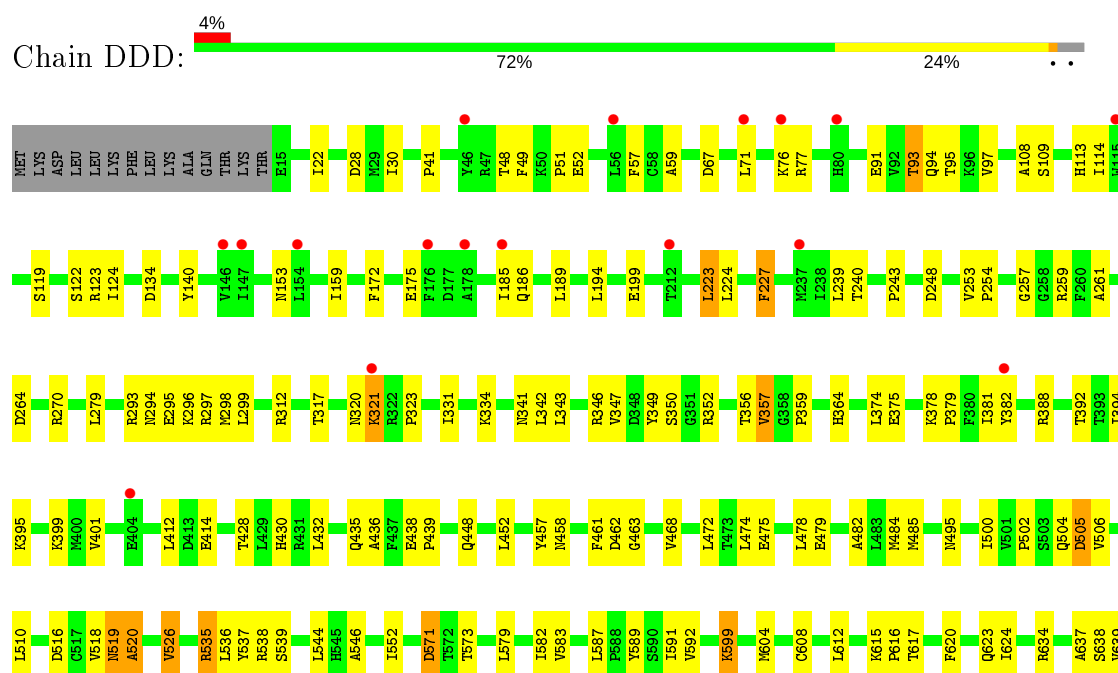


- Molecule 2: DNA-directed RNA polymerase subunit beta

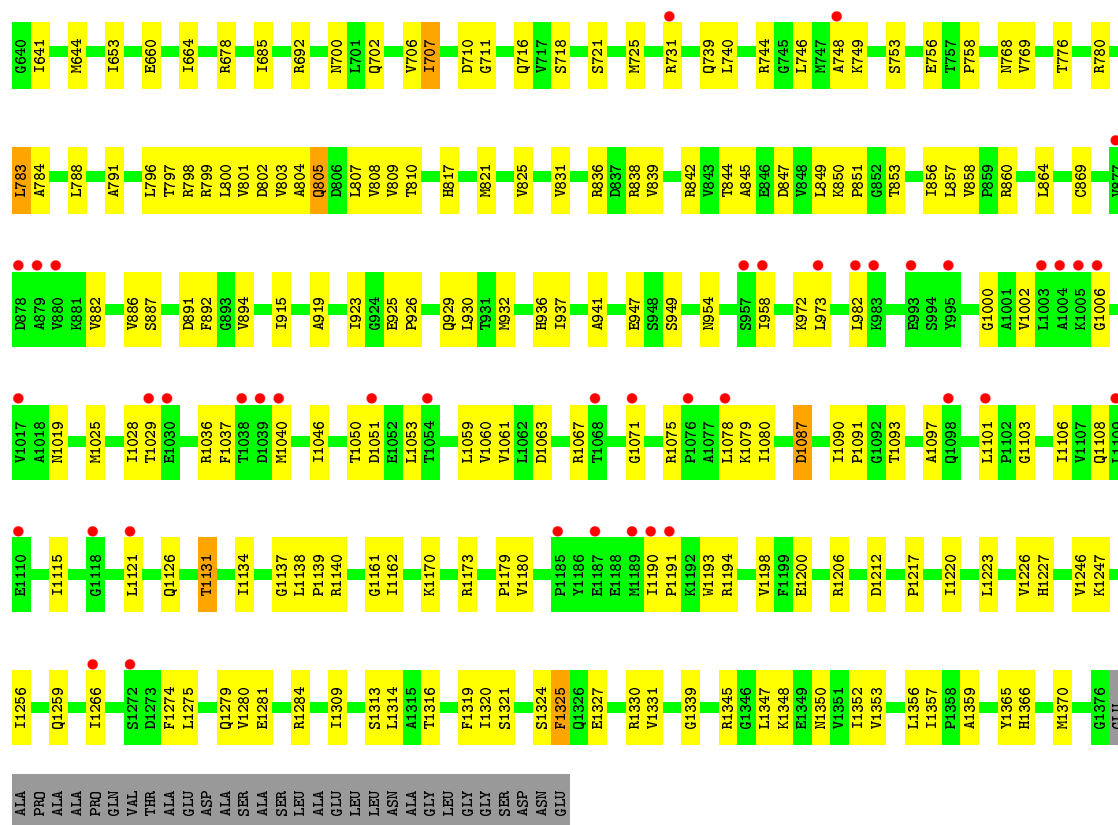




• Molecule 3: DNA-directed RNA polymerase subunit beta'



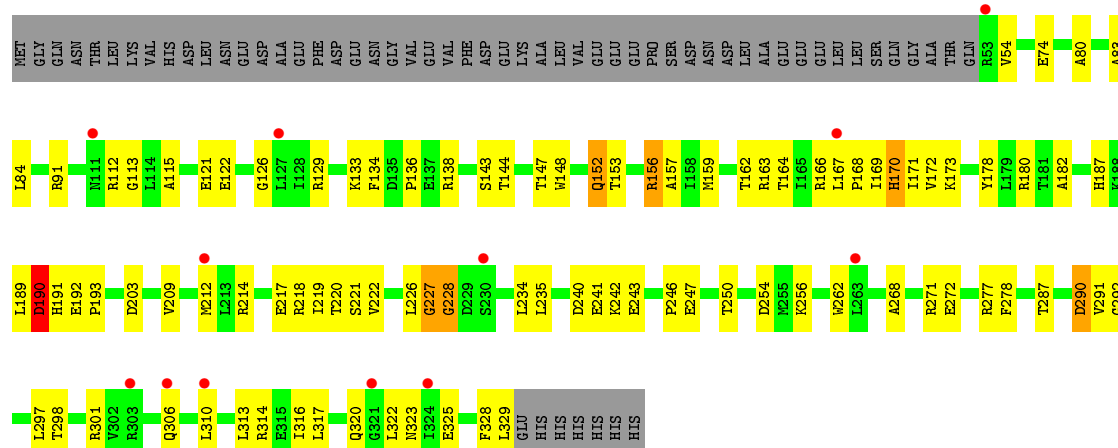




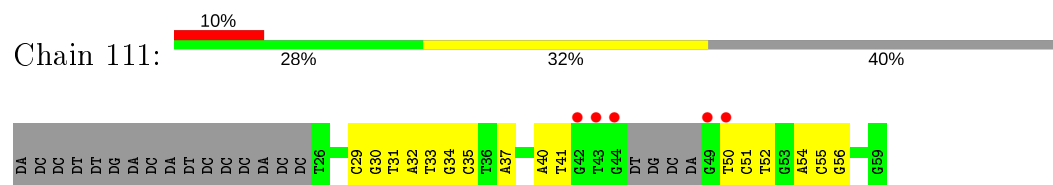
- Molecule 4: DNA-directed RNA polymerase subunit omega



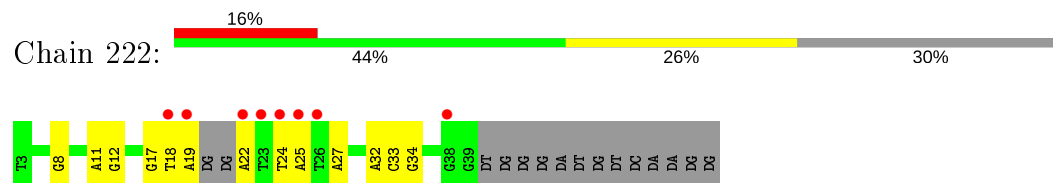
- Molecule 5: RNA polymerase sigma factor RpoS



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



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



- Molecule 8: RNA 6-mer



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.93Å 155.99Å 233.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 3.80 49.44 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.40-3.80) 99.0 (49.44-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.274 , 0.343 0.270 , 0.335	Depositor DCC
$R_{free}$ test set	2301 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	153.3	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 176.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	29063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	255.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AAA	0.66	0/1809	0.74	0/2450
1	BBB	0.68	0/1789	0.77	0/2425
2	CCC	0.65	0/10746	0.79	0/14499
3	DDD	0.65	0/10729	0.78	0/14487
4	EEE	0.64	0/629	0.79	0/847
5	FFF	0.66	0/2282	0.69	0/3076
6	111	0.32	0/691	0.64	0/1063
7	222	0.38	0/802	0.66	0/1234
8	333	0.36	0/116	0.61	0/178
All	All	0.64	0/29593	0.77	0/40259

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	71	0
1	BBB	1767	0	1789	102	0
2	CCC	10577	0	10591	257	0
3	DDD	10568	0	10780	303	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EEE	627	0	634	22	0
5	FFF	2253	0	2298	93	0
6	111	618	0	341	28	0
7	222	716	0	397	27	1
8	333	137	0	65	10	0
9	CCC	1	0	0	0	0
9	DDD	1	0	0	0	0
10	CCC	9	0	0	1	0
11	DDD	2	0	0	0	0
All	All	29063	0	28708	741	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 (741) 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)
1:BBB:49:SER:O	1:BBB:151:GLY:HA3	1.42	1.18
3:DDD:817:HIS:HB3	3:DDD:860:ARG:NH2	1.62	1.13
6:111:54:DA:H2"	6:111:55:DC:C5	1.93	1.04
1:BBB:179:PRO:HG2	1:BBB:211:ILE:HD12	1.41	1.03
2:CCC:1005:GLU:HG2	2:CCC:1006:GLU:H	1.24	1.02
2:CCC:624:ASP:OD1	2:CCC:624:ASP:O	1.78	1.00
3:DDD:1266:ILE:HD13	3:DDD:1274:PHE:HB3	1.43	0.99
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	1.43	0.99
3:DDD:849:LEU:HD12	3:DDD:850:LYS:O	1.65	0.97
1:BBB:205:MET:CE	1:BBB:217:ILE:HG13	1.96	0.96
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.44	0.96
2:CCC:1222:GLU:OE2	3:DDD:537:TYR:OH	1.83	0.95
6:111:54:DA:H2"	6:111:55:DC:C6	2.01	0.94
1:AAA:45:ARG:NH2	1:BBB:34:GLY:O	2.00	0.94
1:AAA:60:GLU:HG3	1:AAA:169:GLY:O	1.68	0.94
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:CD1	1.98	0.93
5:FFF:234:LEU:HD21	7:222:19:DA:H61	1.33	0.92
1:BBB:179:PRO:HG2	1:BBB:211:ILE:CD1	1.98	0.92
3:DDD:458:ASN:ND2	3:DDD:929:GLN:OE1	2.03	0.91
5:FFF:227:GLY:O	8:333:14:GTP:N7	2.05	0.90
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.51	0.90
3:DDD:844:THR:O	3:DDD:860:ARG:O	1.91	0.89
5:FFF:262:TRP:HE1	5:FFF:320:GLN:HE22	1.16	0.87
1:BBB:11:PRO:HG3	1:BBB:31:LEU:CD2	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1333:LEU:O	3:DDD:113:HIS:NE2	2.08	0.86
2:CCC:1124:ILE:HD11	2:CCC:1198:LEU:HD11	1.58	0.85
1:BBB:11:PRO:HG3	1:BBB:31:LEU:HD21	1.56	0.85
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG23	1.61	0.83
2:CCC:1313:HIS:HB2	3:DDD:474:LEU:HG	1.61	0.82
3:DDD:849:LEU:CD1	3:DDD:850:LYS:O	2.27	0.81
1:AAA:192:VAL:HG12	1:AAA:193:GLU:N	1.95	0.81
5:FFF:156:ARG:NH2	6:111:34:DG:N7	2.28	0.81
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.09	0.81
3:DDD:392:THR:CG2	5:FFF:320:GLN:O	2.28	0.80
2:CCC:755:LYS:O	2:CCC:757:THR:OG1	2.01	0.79
3:DDD:817:HIS:HB3	3:DDD:860:ARG:HH22	1.41	0.79
1:BBB:155:ALA:O	1:BBB:159:ILE:HG22	1.82	0.79
2:CCC:1333:LEU:HD11	3:DDD:331:ILE:HD12	1.64	0.79
2:CCC:528:ARG:NH2	2:CCC:576:SER:O	2.15	0.79
1:BBB:49:SER:O	1:BBB:151:GLY:CA	2.27	0.79
3:DDD:839:VAL:HG12	3:DDD:864:LEU:CD1	2.13	0.79
2:CCC:1302:THR:HG22	5:FFF:246:PRO:HA	1.65	0.78
3:DDD:615:LYS:HE2	4:EEE:5:THR:HB	1.66	0.77
3:DDD:817:HIS:HB3	3:DDD:860:ARG:HH21	1.49	0.77
3:DDD:172:PHE:HB3	3:DDD:175:GLU:HB2	1.65	0.77
3:DDD:817:HIS:CB	3:DDD:860:ARG:NH2	2.47	0.77
1:AAA:32:GLU:HA	1:AAA:198:LEU:CD2	2.14	0.76
3:DDD:343:LEU:HD11	3:DDD:1324:SER:HB2	1.68	0.76
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.68	0.76
3:DDD:134:ASP:HB3	3:DDD:159:ILE:HD11	1.68	0.76
3:DDD:519:ASN:O	3:DDD:520:ALA:HB3	1.86	0.76
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.68	0.75
1:AAA:28:LEU:HD21	1:BBB:231:PHE:HE1	1.51	0.75
1:BBB:86:LYS:HG2	1:BBB:173:VAL:HG12	1.66	0.75
2:CCC:1281:TYR:CD2	3:DDD:484:MET:HG2	2.22	0.74
5:FFF:227:GLY:O	8:333:14:GTP:C8	2.41	0.74
1:BBB:205:MET:HE3	1:BBB:217:ILE:HG13	1.70	0.74
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:HD13	1.70	0.73
2:CCC:563:THR:OG1	2:CCC:569:ILE:O	2.06	0.73
2:CCC:453:ILE:HD12	2:CCC:587:LEU:HD21	1.70	0.73
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.69	0.73
3:DDD:664:ILE:HD11	3:DDD:685:ILE:HD11	1.71	0.73
1:AAA:235:ARG:HB3	1:BBB:214:GLU:OE2	1.89	0.73
1:BBB:152:TYR:CE2	3:DDD:536:LEU:HD21	2.23	0.73
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:CA	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1257:GLN:HG2	2:CCC:1296:ASP:OD1	1.89	0.73
1:AAA:188:GLU:O	1:AAA:199:ASP:HB2	1.89	0.73
2:CCC:186:PHE:CD1	2:CCC:196:VAL:HG22	2.23	0.73
5:FFF:228:GLY:HA3	8:333:14:GTP:O1A	1.87	0.73
3:DDD:842:ARG:HD3	3:DDD:882:VAL:HG11	1.70	0.72
6:111:54:DA:C2'	6:111:55:DC:C5	2.72	0.71
2:CCC:562:GLU:HG2	2:CCC:574:SER:HB2	1.71	0.71
1:BBB:179:PRO:HG2	1:BBB:211:ILE:CG1	2.20	0.71
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	1.72	0.71
2:CCC:292:ILE:HB	2:CCC:322:LEU:HD11	1.73	0.71
2:CCC:247:ARG:HA	2:CCC:274:ILE:HD11	1.71	0.71
1:AAA:124:VAL:HG11	1:AAA:209:GLY:HA3	1.71	0.70
2:CCC:1005:GLU:HG2	2:CCC:1006:GLU:N	2.01	0.70
1:AAA:50:SER:HG	1:BBB:35:PHE:HZ	1.39	0.70
1:BBB:205:MET:HE1	1:BBB:217:ILE:HG13	1.72	0.70
3:DDD:849:LEU:HD12	3:DDD:850:LYS:N	2.07	0.70
2:CCC:1273:MET:HG3	7:222:12:DG:H4'	1.73	0.70
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.06	0.70
1:BBB:65:LEU:O	1:BBB:169:GLY:HA2	1.92	0.69
1:AAA:75:GLN:HE22	2:CCC:772:SER:HA	1.57	0.69
3:DDD:259:ARG:NH2	7:222:22:DA:OP2	2.24	0.69
2:CCC:100:LEU:HD22	2:CCC:493:ILE:HD11	1.75	0.69
3:DDD:140:TYR:OH	3:DDD:312:ARG:HD2	1.93	0.69
2:CCC:183:TRP:CH2	6:111:51:DC:H2'	2.28	0.69
1:AAA:184:ALA:CB	2:CCC:1091:GLY:HA3	2.24	0.68
1:AAA:192:VAL:HG12	1:AAA:193:GLU:H	1.57	0.68
1:AAA:34:GLY:O	1:BBB:45:ARG:NH2	2.26	0.68
3:DDD:295:GLU:OE1	5:FFF:121:GLU:HG3	1.93	0.68
1:BBB:14:VAL:HG21	1:BBB:29:GLU:CG	2.23	0.68
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG22	1.75	0.68
1:BBB:83:LEU:HD11	3:DDD:526:VAL:HB	1.76	0.68
2:CCC:894:GLN:HB3	3:DDD:77:ARG:HH22	1.58	0.68
1:BBB:14:VAL:HG21	1:BBB:29:GLU:HG2	1.76	0.67
3:DDD:122:SER:O	3:DDD:123:ARG:HB2	1.95	0.67
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.76	0.67
1:BBB:51:MET:C	1:BBB:150:ARG:HB2	2.14	0.67
5:FFF:222:VAL:CG1	5:FFF:235:LEU:HB2	2.25	0.67
3:DDD:357:VAL:HB	3:DDD:359:PRO:HD3	1.75	0.67
3:DDD:620:PHE:O	3:DDD:624:ILE:HG13	1.95	0.66
1:BBB:22:THR:O	1:BBB:207:THR:HG22	1.96	0.66
5:FFF:277:ARG:CD	5:FFF:306:GLN:HE21	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:807:LEU:HD11	3:DDD:894:VAL:CG2	2.26	0.66
1:AAA:32:GLU:HG3	1:AAA:198:LEU:HD21	1.78	0.66
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.60	0.66
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	1.93	0.66
3:DDD:1330:ARG:NH2	7:222:8:DG:OP1	2.29	0.65
2:CCC:1333:LEU:CD1	3:DDD:331:ILE:HD12	2.25	0.65
3:DDD:844:THR:HG21	3:DDD:858:VAL:HG11	1.78	0.65
1:BBB:51:MET:O	1:BBB:150:ARG:HA	1.97	0.65
2:CCC:253:PHE:CZ	2:CCC:287:VAL:HG12	2.31	0.65
1:BBB:67:GLU:N	1:BBB:171:LEU:HD21	2.12	0.65
5:FFF:218:ARG:HD3	7:222:24:DT:O4	1.97	0.65
2:CCC:186:PHE:CE1	2:CCC:196:VAL:HG22	2.31	0.65
1:AAA:74:VAL:HG13	1:AAA:131:CYS:SG	2.37	0.65
1:BBB:182:ARG:H	1:BBB:206:GLU:HB3	1.61	0.65
3:DDD:615:LYS:HB2	3:DDD:616:PRO:HD3	1.79	0.64
1:AAA:32:GLU:HA	1:AAA:198:LEU:HD22	1.79	0.64
2:CCC:980:VAL:HG13	2:CCC:984:VAL:HG23	1.78	0.64
5:FFF:234:LEU:CD2	7:222:19:DA:H61	2.08	0.64
2:CCC:373:GLY:HA3	5:FFF:54:VAL:HG21	1.79	0.64
2:CCC:903:ARG:HB3	2:CCC:909:LYS:HG2	1.80	0.64
2:CCC:1306:LYS:HG2	5:FFF:250:THR:OG1	1.98	0.64
2:CCC:1101:LEU:HD23	3:DDD:725:MET:HE2	1.78	0.64
3:DDD:932:MET:SD	8:333:19:U:H2'	2.37	0.64
1:BBB:86:LYS:HE2	1:BBB:174:ASP:H	1.63	0.64
3:DDD:1217:PRO:HA	3:DDD:1220:ILE:HD12	1.79	0.64
1:AAA:165:GLU:HG3	1:AAA:165:GLU:O	1.98	0.63
1:BBB:11:PRO:HB2	1:BBB:28:LEU:HD12	1.81	0.63
3:DDD:842:ARG:HB3	3:DDD:882:VAL:CG1	2.29	0.63
1:AAA:234:LEU:HD23	1:BBB:13:LEU:H	1.63	0.63
2:CCC:635:THR:HG22	2:CCC:644:LEU:CD2	2.28	0.63
3:DDD:579:LEU:HB3	3:DDD:592:VAL:HG21	1.81	0.62
4:EEE:2:ALA:N	4:EEE:5:THR:O	2.31	0.62
2:CCC:672:GLU:HG3	2:CCC:673:HIS:CD2	2.33	0.62
3:DDD:800:LEU:CD2	3:DDD:1309:ILE:CD1	2.76	0.62
2:CCC:901:LEU:HG	5:FFF:278:PHE:CD2	2.35	0.62
3:DDD:153:ASN:ND2	3:DDD:172:PHE:CZ	2.67	0.62
5:FFF:133:LYS:HE3	6:111:35:DC:OP1	1.98	0.62
5:FFF:170:HIS:NE2	6:111:31:DT:H2'	2.15	0.62
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.81	0.62
2:CCC:968:GLU:HB2	2:CCC:1018:TYR:HE1	1.64	0.62
2:CCC:558:VAL:HG12	2:CCC:573:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:777:VAL:HG11	2:CCC:783:LEU:HD21	1.81	0.61
2:CCC:400:VAL:HG11	2:CCC:452:ARG:HD3	1.82	0.61
3:DDD:1347:LEU:HD22	3:DDD:1357:ILE:HG23	1.82	0.61
1:BBB:74:VAL:HG13	1:BBB:131:CYS:SG	2.41	0.61
1:BBB:179:PRO:CG	1:BBB:211:ILE:HD12	2.25	0.61
3:DDD:847:ASP:OD1	3:DDD:860:ARG:HB2	2.00	0.61
2:CCC:1306:LYS:HE2	5:FFF:250:THR:HA	1.82	0.61
1:AAA:182:ARG:CD	2:CCC:1092:THR:HG22	2.31	0.61
3:DDD:842:ARG:CD	3:DDD:882:VAL:HG11	2.31	0.61
4:EEE:41:GLU:HG3	4:EEE:42:GLU:H	1.65	0.61
2:CCC:724:VAL:O	2:CCC:774:GLY:HA2	2.00	0.61
3:DDD:748:ALA:HB2	3:DDD:941:ALA:HB2	1.80	0.61
1:AAA:46:ILE:HG12	1:BBB:35:PHE:HE1	1.66	0.61
1:BBB:205:MET:CE	1:BBB:217:ILE:CG1	2.75	0.61
3:DDD:615:LYS:HG2	4:EEE:5:THR:HG21	1.83	0.61
2:CCC:620:ASN:HD21	3:DDD:768:ASN:HB2	1.65	0.61
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.66	0.61
2:CCC:17:LYS:N	2:CCC:1188:ASP:OD2	2.29	0.61
5:FFF:189:LEU:O	5:FFF:191:HIS:N	2.34	0.61
2:CCC:858:GLY:HA3	5:FFF:328:PHE:HE1	1.65	0.61
2:CCC:906:PHE:HZ	5:FFF:323:ASN:HA	1.66	0.60
3:DDD:1266:ILE:HD13	3:DDD:1274:PHE:CB	2.25	0.60
3:DDD:261:ALA:HA	5:FFF:220:THR:O	2.01	0.60
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CG2	2.31	0.60
3:DDD:1036:ARG:HB3	3:DDD:1079:LYS:HB3	1.84	0.60
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD22	1.82	0.60
3:DDD:519:ASN:O	3:DDD:520:ALA:CB	2.49	0.60
3:DDD:1050:THR:HG22	3:DDD:1051:ASP:N	2.17	0.60
2:CCC:618:GLN:NE2	3:DDD:769:VAL:HB	2.17	0.60
1:BBB:157:THR:O	1:BBB:157:THR:HG22	2.01	0.60
3:DDD:320:ASN:O	3:DDD:321:LYS:HB2	2.01	0.60
2:CCC:1305:TYR:CZ	5:FFF:247:GLU:HG2	2.37	0.59
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.32	0.59
3:DDD:707:ILE:HD11	3:DDD:716:GLN:HG2	1.84	0.59
2:CCC:906:PHE:CZ	5:FFF:323:ASN:HA	2.36	0.59
6:111:31:DT:H1'	6:111:32:DA:H5'	1.82	0.59
5:FFF:226:LEU:O	7:222:17:DG:N2	2.35	0.59
2:CCC:496:LYS:HB3	7:222:24:DT:OP1	2.02	0.59
6:111:29:DC:H2''	6:111:30:DG:C8	2.38	0.59
5:FFF:143:SER:CB	6:111:41:DT:H72	2.31	0.59
1:BBB:208:ASN:OD1	1:BBB:209:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1313:SER:O	3:DDD:1316:THR:HG22	2.02	0.59
3:DDD:392:THR:HG21	5:FFF:320:GLN:HB3	1.84	0.59
1:AAA:48:LEU:CD2	1:AAA:183:ILE:HG22	2.32	0.59
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD11	1.86	0.58
5:FFF:226:LEU:HD21	7:222:19:DA:H61	1.67	0.58
2:CCC:525:THR:CG2	2:CCC:687:ARG:CD	2.81	0.58
3:DDD:941:ALA:HB1	3:DDD:1131:THR:HG21	1.84	0.58
5:FFF:178:TYR:CE1	5:FFF:209:VAL:HG22	2.37	0.58
1:AAA:75:GLN:NE2	2:CCC:772:SER:HA	2.18	0.58
2:CCC:624:ASP:O	2:CCC:624:ASP:CG	2.42	0.58
2:CCC:434:ASP:O	2:CCC:439:LYS:O	2.20	0.58
2:CCC:705:GLU:HB3	2:CCC:794:LEU:H	1.69	0.58
2:CCC:1294:LYS:HD3	3:DDD:347:VAL:HG13	1.84	0.58
3:DDD:1080:ILE:HB	3:DDD:1097:ALA:HB3	1.86	0.58
2:CCC:1077:SER:HA	3:DDD:356:THR:OG1	2.03	0.58
5:FFF:162:THR:HG23	5:FFF:163:ARG:HG3	1.86	0.58
3:DDD:108:ALA:HB3	3:DDD:279:LEU:HD23	1.85	0.58
2:CCC:1154:ASP:OD1	2:CCC:1154:ASP:N	2.35	0.58
1:AAA:29:GLU:HB3	1:AAA:200:LYS:HB3	1.86	0.57
3:DDD:317:THR:HA	3:DDD:323:PRO:HA	1.86	0.57
3:DDD:784:ALA:O	3:DDD:788:LEU:HG	2.04	0.57
5:FFF:268:ALA:O	5:FFF:272:GLU:HG3	2.05	0.57
2:CCC:186:PHE:CE1	2:CCC:196:VAL:CG2	2.87	0.57
1:BBB:225:ALA:HA	1:BBB:228:LEU:HD12	1.85	0.57
3:DDD:334:LYS:NZ	7:222:11:DA:OP1	2.37	0.56
1:BBB:205:MET:HE3	1:BBB:217:ILE:CG1	2.34	0.56
2:CCC:272:ARG:O	2:CCC:276:GLN:HG2	2.04	0.56
4:EEE:41:GLU:HG3	4:EEE:42:GLU:N	2.20	0.56
1:BBB:33:ARG:HH22	2:CCC:1081:PRO:HB3	1.71	0.56
5:FFF:163:ARG:HD2	5:FFF:167:LEU:HB2	1.87	0.56
3:DDD:1198:VAL:HG12	3:DDD:1200:GLU:H	1.70	0.56
2:CCC:618:GLN:HE21	3:DDD:769:VAL:CG2	2.18	0.56
3:DDD:1138:LEU:N	3:DDD:1139:PRO:CD	2.69	0.56
6:111:56:DG:C2	7:222:8:DG:C2	2.94	0.56
1:AAA:222:THR:OG1	1:BBB:233:ASP:CB	2.53	0.56
2:CCC:1253:LEU:HA	5:FFF:240:ASP:HB2	1.88	0.55
3:DDD:248:ASP:OD2	5:FFF:242:LYS:NZ	2.39	0.55
3:DDD:707:ILE:HD12	3:DDD:707:ILE:H	1.72	0.55
2:CCC:1044:PRO:HB2	5:FFF:214:ARG:HG2	1.89	0.55
3:DDD:1080:ILE:HD12	3:DDD:1115:ILE:HD11	1.89	0.55
3:DDD:279:LEU:HD22	3:DDD:299:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:166:ARG:HH12	5:FFF:168:PRO:HA	1.71	0.55
5:FFF:298:THR:HG21	5:FFF:301:ARG:HD3	1.87	0.55
1:AAA:182:ARG:HD3	2:CCC:1092:THR:HG22	1.89	0.55
3:DDD:320:ASN:O	3:DDD:321:LYS:CB	2.54	0.55
3:DDD:518:VAL:HG21	3:DDD:707:ILE:HD13	1.88	0.55
5:FFF:148:TRP:O	5:FFF:152:GLN:HB3	2.06	0.55
2:CCC:1100:PRO:HB3	3:DDD:639:VAL:HG23	1.88	0.55
7:222:17:DG:H2'	7:222:18:DT:C6	2.42	0.55
2:CCC:686:GLN:HG2	2:CCC:796:LEU:HD13	1.89	0.55
3:DDD:1350:ASN:HA	3:DDD:1353:VAL:HG22	1.88	0.55
3:DDD:845:ALA:O	3:DDD:860:ARG:HG3	2.07	0.55
5:FFF:138:ARG:NH1	6:111:37:DA:C8	2.75	0.54
3:DDD:799:ARG:HB3	3:DDD:1309:ILE:HG21	1.89	0.54
3:DDD:644:MET:HE1	3:DDD:740:LEU:HB3	1.89	0.54
2:CCC:1101:LEU:HD23	3:DDD:725:MET:CE	2.37	0.54
2:CCC:145:ILE:HD11	2:CCC:506:PHE:CD1	2.42	0.54
2:CCC:984:VAL:O	2:CCC:984:VAL:HG13	2.07	0.54
3:DDD:124:ILE:HG13	3:DDD:189:LEU:HD11	1.90	0.54
2:CCC:1284:ALA:CB	3:DDD:1357:ILE:HB	2.38	0.54
1:AAA:152:TYR:CD2	2:CCC:824:GLN:HG2	2.43	0.54
2:CCC:519:ASN:HD21	2:CCC:796:LEU:HD22	1.72	0.54
3:DDD:615:LYS:HE2	4:EEE:5:THR:CB	2.36	0.54
3:DDD:678:ARG:NH1	3:DDD:756:GLU:OE2	2.41	0.54
2:CCC:123:TYR:CE2	5:FFF:190:ASP:O	2.61	0.54
1:BBB:179:PRO:HG2	1:BBB:211:ILE:HG13	1.90	0.54
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:HG3	1.90	0.54
3:DDD:1087:ASP:OD1	3:DDD:1087:ASP:N	2.41	0.54
1:AAA:234:LEU:HD22	1:BBB:12:ARG:HG2	1.89	0.54
5:FFF:163:ARG:CD	5:FFF:167:LEU:HD12	2.38	0.54
1:BBB:47:LEU:HA	1:BBB:51:MET:HG2	1.90	0.54
3:DDD:1327:GLU:O	3:DDD:1331:VAL:HG23	2.07	0.54
1:AAA:29:GLU:HB3	1:AAA:200:LYS:CB	2.38	0.53
5:FFF:262:TRP:HZ2	5:FFF:320:GLN:OE1	1.90	0.53
5:FFF:147:THR:HG21	6:111:40:DA:C6	2.43	0.53
3:DDD:972:LYS:HB3	3:DDD:1002:VAL:HG13	1.90	0.53
3:DDD:571:ASP:N	3:DDD:571:ASP:OD1	2.40	0.53
1:BBB:11:PRO:HB3	1:BBB:31:LEU:HG	1.91	0.53
2:CCC:142:GLU:OE1	2:CCC:515:MET:HE1	2.08	0.53
4:EEE:25:ARG:NH2	4:EEE:68:GLU:OE1	2.41	0.53
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.42	0.53
2:CCC:1124:ILE:CD1	2:CCC:1198:LEU:HD11	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1304:MET:SD	2:CCC:1314:GLN:O	2.67	0.53
2:CCC:151:ARG:HH21	2:CCC:156:PHE:HB2	1.73	0.53
2:CCC:888:THR:O	2:CCC:914:LYS:N	2.41	0.53
2:CCC:1285:TYR:HD2	3:DDD:479:GLU:OE2	1.91	0.53
1:BBB:67:GLU:HB3	1:BBB:171:LEU:CD2	2.28	0.53
2:CCC:878:THR:HG22	2:CCC:879:GLY:N	2.24	0.53
3:DDD:264:ASP:OD1	5:FFF:221:SER:OG	2.19	0.53
2:CCC:1333:LEU:CD1	3:DDD:331:ILE:CD1	2.86	0.53
5:FFF:234:LEU:HD21	7:222:19:DA:N6	2.14	0.53
2:CCC:1146:GLN:NE2	2:CCC:1150:ASP:OD2	2.42	0.53
2:CCC:226:GLU:HB2	2:CCC:337:PHE:HB3	1.91	0.53
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.72	0.53
5:FFF:277:ARG:HD3	5:FFF:306:GLN:HE21	1.73	0.53
6:111:29:DC:O2	7:222:34:DG:N2	2.38	0.53
2:CCC:562:GLU:HG2	2:CCC:574:SER:CB	2.36	0.53
3:DDD:1090:ILE:O	3:DDD:1093:THR:OG1	2.27	0.53
3:DDD:1280:VAL:HG12	3:DDD:1281:GLU:N	2.24	0.53
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.39	0.53
1:AAA:182:ARG:HD2	2:CCC:1092:THR:HG22	1.91	0.53
2:CCC:1223:ARG:HD2	3:DDD:637:ALA:HA	1.91	0.52
3:DDD:796:LEU:O	3:DDD:800:LEU:HG	2.09	0.52
2:CCC:638:SER:C	2:CCC:639:LYS:HG2	2.29	0.52
3:DDD:1330:ARG:HH21	7:222:8:DG:P	2.32	0.52
3:DDD:836:ARG:HG3	3:DDD:869:CYS:HB3	1.89	0.52
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.74	0.52
3:DDD:1314:LEU:HD11	3:DDD:1327:GLU:HG3	1.90	0.52
5:FFF:143:SER:HB2	6:111:41:DT:H72	1.90	0.52
1:AAA:195:ARG:CG	1:AAA:198:LEU:HD12	2.39	0.52
2:CCC:61:SER:HB3	2:CCC:479:LEU:HB3	1.92	0.52
2:CCC:463:GLN:HG3	2:CCC:505:PHE:HB2	1.92	0.52
3:DDD:930:LEU:HB3	3:DDD:1134:ILE:HG13	1.91	0.52
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.43	0.52
2:CCC:576:SER:OG	2:CCC:659:GLN:O	2.23	0.52
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.09	0.52
1:BBB:51:MET:O	1:BBB:150:ARG:CA	2.57	0.52
2:CCC:1257:GLN:CG	2:CCC:1296:ASP:OD1	2.58	0.52
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	1.92	0.52
6:111:52:DT:C2'	6:111:52:DT:O2	2.58	0.52
1:AAA:77:ASP:OD2	2:CCC:756:TYR:HE2	1.92	0.52
5:FFF:164:THR:HB	5:FFF:219:ILE:CD1	2.40	0.52
1:AAA:136:GLU:HG2	1:AAA:137:ASN:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB3	1.92	0.51
2:CCC:269:ILE:HG23	2:CCC:273:HIS:HB2	1.91	0.51
1:BBB:183:ILE:HD12	1:BBB:205:MET:HG3	1.92	0.51
2:CCC:142:GLU:OE1	2:CCC:515:MET:CE	2.57	0.51
2:CCC:241:LEU:HD22	2:CCC:285:ILE:CD1	2.39	0.51
5:FFF:133:LYS:HE3	6:111:35:DC:P	2.50	0.51
2:CCC:1290:MET:HG2	2:CCC:1294:LYS:HD2	1.92	0.51
2:CCC:924:VAL:HG12	2:CCC:925:SER:N	2.24	0.51
2:CCC:1273:MET:HB3	3:DDD:428:THR:HB	1.92	0.51
2:CCC:815:SER:OG	3:DDD:461:PHE:HB2	2.10	0.51
1:AAA:225:ALA:HB2	1:BBB:228:LEU:HD13	1.91	0.51
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.92	0.51
3:DDD:1078:LEU:HG	3:DDD:1101:LEU:HD11	1.92	0.51
2:CCC:558:VAL:CG1	2:CCC:573:ASN:ND2	2.73	0.51
3:DDD:518:VAL:O	3:DDD:519:ASN:C	2.49	0.51
2:CCC:207:THR:HG21	2:CCC:351:LEU:HG	1.93	0.51
2:CCC:73:TYR:HB2	2:CCC:98:VAL:HG22	1.93	0.51
6:111:32:DA:C2	7:222:32:DA:C2	2.99	0.51
1:BBB:33:ARG:HH22	2:CCC:1081:PRO:CG	2.24	0.51
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:CG1	2.41	0.51
3:DDD:478:LEU:HG	4:EEE:47:THR:CG2	2.39	0.51
3:DDD:582:ILE:HD12	3:DDD:623:GLN:HB3	1.92	0.51
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	1.89	0.51
5:FFF:169:ILE:HG22	5:FFF:173:LYS:HD2	1.92	0.51
1:BBB:124:VAL:HG21	1:BBB:210:THR:HG22	1.92	0.50
1:BBB:51:MET:O	1:BBB:151:GLY:N	2.43	0.50
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.92	0.50
3:DDD:153:ASN:ND2	3:DDD:172:PHE:CE2	2.79	0.50
3:DDD:475:GLU:O	3:DDD:479:GLU:HG3	2.10	0.50
2:CCC:905:ILE:HG13	5:FFF:310:LEU:HD22	1.92	0.50
2:CCC:23:ASP:N	2:CCC:23:ASP:OD1	2.43	0.50
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	2.11	0.50
3:DDD:1279:GLN:O	3:DDD:1279:GLN:HG3	2.10	0.50
2:CCC:510:GLN:HG2	8:333:14:GTP:O1G	2.11	0.50
1:AAA:14:VAL:HG21	1:AAA:29:GLU:HG2	1.93	0.50
1:BBB:51:MET:O	1:BBB:150:ARG:HB2	2.12	0.50
3:DDD:1281:GLU:HB3	3:DDD:1284:ARG:HG3	1.93	0.50
2:CCC:1258:PRO:HD2	3:DDD:346:ARG:HB2	1.92	0.50
7:222:11:DA:H2''	7:222:12:DG:H5'	1.94	0.50
2:CCC:1073:LYS:HB2	3:DDD:462:ASP:HB2	1.94	0.50
5:FFF:122:GLU:OE2	5:FFF:157:ALA:HB1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:226:LEU:HD21	7:222:19:DA:N6	2.26	0.50
1:BBB:86:LYS:HD3	1:BBB:174:ASP:HB2	1.92	0.50
2:CCC:538:LEU:CD1	2:CCC:547:VAL:HG11	2.42	0.50
3:DDD:516:ASP:HB3	3:DDD:573:THR:HG21	1.93	0.50
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.42	0.50
1:AAA:192:VAL:CG1	1:AAA:193:GLU:N	2.67	0.50
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.42	0.50
3:DDD:1037:PHE:CD2	3:DDD:1040:MET:SD	3.05	0.50
2:CCC:593:LYS:HG2	2:CCC:595:THR:HG23	1.94	0.50
3:DDD:114:ILE:CD1	3:DDD:312:ARG:HB2	2.42	0.50
3:DDD:294:ASN:O	3:DDD:298:MET:HG3	2.12	0.50
3:DDD:849:LEU:HB3	3:DDD:856:ILE:HA	1.94	0.50
5:FFF:84:LEU:HD11	5:FFF:136:PRO:HD3	1.94	0.50
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.94	0.49
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.75	0.49
2:CCC:57:PHE:HB3	2:CCC:58:PRO:HA	1.94	0.49
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.45	0.49
1:BBB:47:LEU:HD13	1:BBB:183:ILE:CD1	2.42	0.49
3:DDD:1191:PRO:HG2	3:DDD:1194:ARG:HG3	1.94	0.49
1:AAA:158:ARG:CD	1:AAA:172:LEU:HD11	2.42	0.49
3:DDD:973:LEU:CD2	3:DDD:1006:GLY:HA2	2.42	0.49
3:DDD:1280:VAL:HG12	3:DDD:1281:GLU:H	1.77	0.49
1:BBB:163:GLU:O	1:BBB:163:GLU:HG3	2.12	0.49
2:CCC:1306:LYS:CE	5:FFF:250:THR:HA	2.42	0.49
3:DDD:804:ALA:O	3:DDD:805:GLN:C	2.51	0.49
3:DDD:932:MET:SD	8:333:19:U:H3'	2.53	0.49
2:CCC:525:THR:CG2	2:CCC:687:ARG:HD2	2.42	0.49
3:DDD:502:PRO:HB3	3:DDD:506:VAL:HG11	1.94	0.49
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD13	1.95	0.49
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.94	0.49
1:BBB:33:ARG:CB	1:BBB:197:ASP:O	2.61	0.49
2:CCC:1290:MET:HG2	2:CCC:1294:LYS:CD	2.43	0.49
3:DDD:644:MET:CE	3:DDD:740:LEU:HB3	2.42	0.49
5:FFF:84:LEU:HD11	5:FFF:134:PHE:O	2.12	0.49
2:CCC:558:VAL:CG1	2:CCC:573:ASN:CG	2.81	0.49
1:AAA:48:LEU:CD2	1:AAA:183:ILE:CG2	2.90	0.49
3:DDD:1025:MET:CB	3:DDD:1126:GLN:HE21	2.25	0.49
3:DDD:482:ALA:O	4:EEE:16:ARG:NH1	2.46	0.49
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB2	2.13	0.48
2:CCC:1219:GLU:OE2	3:DDD:634:ARG:NH1	2.42	0.48
3:DDD:114:ILE:HD11	3:DDD:312:ARG:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:374:LEU:HD11	3:DDD:401:VAL:HG13	1.95	0.48
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB3	2.12	0.48
2:CCC:1284:ALA:HB1	3:DDD:1357:ILE:HB	1.95	0.48
5:FFF:262:TRP:CZ2	5:FFF:320:GLN:OE1	2.66	0.48
1:BBB:185:TYR:HA	1:BBB:203:ILE:HA	1.94	0.48
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.95	0.48
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD21	1.94	0.48
3:DDD:930:LEU:CB	3:DDD:1134:ILE:HG13	2.44	0.48
3:DDD:1161:GLY:HA3	3:DDD:1179:PRO:HA	1.94	0.48
3:DDD:516:ASP:HB3	3:DDD:573:THR:CG2	2.43	0.48
3:DDD:810:THR:HG21	3:DDD:892:PHE:HB2	1.95	0.48
6:111:56:DG:N2	7:222:8:DG:C2	2.82	0.48
1:BBB:11:PRO:HG3	1:BBB:31:LEU:HD23	1.90	0.48
2:CCC:253:PHE:CE1	2:CCC:287:VAL:HG12	2.48	0.48
3:DDD:700:ASN:CG	3:DDD:700:ASN:O	2.51	0.48
5:FFF:226:LEU:HD21	5:FFF:234:LEU:HD21	1.94	0.48
2:CCC:823:VAL:HG22	2:CCC:1060:ILE:HG13	1.96	0.48
3:DDD:122:SER:O	3:DDD:123:ARG:CB	2.60	0.48
3:DDD:395:LYS:HD3	5:FFF:329:LEU:HD13	1.96	0.48
4:EEE:29:GLN:HB3	4:EEE:35:LYS:CG	2.44	0.48
1:BBB:185:TYR:HB2	1:BBB:203:ILE:HG12	1.96	0.48
2:CCC:1146:GLN:HB2	2:CCC:1161:LEU:HD12	1.95	0.48
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.29	0.48
3:DDD:660:GLU:HG3	3:DDD:685:ILE:HD13	1.95	0.48
5:FFF:152:GLN:HG3	5:FFF:153:THR:N	2.29	0.48
1:BBB:33:ARG:HH22	2:CCC:1081:PRO:HG3	1.79	0.48
3:DDD:495:ASN:ND2	3:DDD:1247:LYS:HB2	2.28	0.48
1:BBB:33:ARG:HB2	1:BBB:197:ASP:O	2.14	0.47
2:CCC:149:LEU:HB2	2:CCC:530:ILE:CG2	2.44	0.47
2:CCC:992:LEU:HB3	2:CCC:993:PRO:HD2	1.96	0.47
3:DDD:1212:ASP:OD1	3:DDD:1212:ASP:N	2.47	0.47
2:CCC:287:VAL:HB	2:CCC:288:PRO:HD2	1.96	0.47
3:DDD:1266:ILE:CD1	3:DDD:1274:PHE:HB3	2.30	0.47
2:CCC:859:GLU:HA	2:CCC:859:GLU:OE1	2.14	0.47
3:DDD:194:LEU:HD22	3:DDD:224:LEU:HD23	1.96	0.47
1:BBB:48:LEU:CD2	1:BBB:183:ILE:CG2	2.92	0.47
2:CCC:558:VAL:HG11	2:CCC:573:ASN:CG	2.35	0.47
2:CCC:592:ARG:HG3	2:CCC:655:VAL:HG22	1.96	0.47
3:DDD:710:ASP:OD1	3:DDD:710:ASP:N	2.47	0.47
2:CCC:811:ASN:HA	2:CCC:815:SER:O	2.14	0.47
2:CCC:709:ALA:HB3	2:CCC:792:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:546:ALA:O	3:DDD:573:THR:HA	2.15	0.47
3:DDD:591:ILE:HG12	3:DDD:604:MET:HG2	1.95	0.47
1:AAA:145:LYS:HD3	1:AAA:147:GLN:HE21	1.80	0.47
1:BBB:205:MET:HE3	1:BBB:217:ILE:CD1	2.45	0.47
2:CCC:1124:ILE:HD11	2:CCC:1198:LEU:CD1	2.36	0.47
2:CCC:1073:LYS:NZ	8:333:18:C:OP1	2.41	0.47
1:BBB:145:LYS:HD3	1:BBB:147:GLN:HE21	1.80	0.47
2:CCC:42:ASP:O	2:CCC:50:GLU:HG2	2.14	0.47
2:CCC:66:SER:OG	2:CCC:479:LEU:HD22	2.14	0.47
5:FFF:133:LYS:CE	6:111:35:DC:OP1	2.62	0.47
8:333:18:C:H2'	8:333:19:U:O4'	2.14	0.47
2:CCC:14:ASP:O	2:CCC:1155:VAL:HG13	2.15	0.47
2:CCC:1257:GLN:HE22	3:DDD:341:ASN:HA	1.79	0.47
2:CCC:1333:LEU:HD12	3:DDD:331:ILE:CD1	2.44	0.47
3:DDD:495:ASN:HD22	3:DDD:1247:LYS:HB2	1.78	0.47
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:HA	1.97	0.47
3:DDD:253:VAL:HB	3:DDD:254:PRO:HD2	1.96	0.47
3:DDD:350:SER:HA	3:DDD:468:VAL:O	2.15	0.47
2:CCC:903:ARG:NH1	2:CCC:910:ALA:HB3	2.30	0.46
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:HG22	1.97	0.46
1:AAA:167:PRO:HG2	1:AAA:170:ARG:HD2	1.96	0.46
2:CCC:539:THR:HB	2:CCC:542:ARG:HG3	1.96	0.46
4:EEE:44:ASP:OD2	4:EEE:52:ARG:NH2	2.48	0.46
1:BBB:52:PRO:HA	1:BBB:150:ARG:HB3	1.97	0.46
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.97	0.46
2:CCC:1307:ASN:HB3	2:CCC:1312:ASN:O	2.16	0.46
2:CCC:898:GLU:HG2	5:FFF:256:LYS:HG2	1.97	0.46
3:DDD:1067:ARG:HD3	3:DDD:1071:GLY:O	2.16	0.46
3:DDD:1356:LEU:HD23	3:DDD:1365:TYR:CD2	2.50	0.46
3:DDD:452:LEU:HB3	3:DDD:500:ILE:HG23	1.97	0.46
1:BBB:152:TYR:CZ	3:DDD:536:LEU:HD21	2.50	0.46
2:CCC:183:TRP:CZ3	6:111:51:DC:C2'	2.99	0.46
1:BBB:22:THR:O	1:BBB:207:THR:CG2	2.62	0.46
3:DDD:653:ILE:HG12	3:DDD:692:ARG:HD2	1.98	0.46
3:DDD:849:LEU:CD1	3:DDD:850:LYS:N	2.75	0.46
3:DDD:381:ILE:HD11	3:DDD:412:LEU:HD13	1.96	0.46
2:CCC:186:PHE:CD1	2:CCC:196:VAL:CG2	2.96	0.46
2:CCC:618:GLN:HE21	3:DDD:769:VAL:HB	1.79	0.46
2:CCC:817:LEU:HD23	2:CCC:817:LEU:HA	1.76	0.46
3:DDD:186:GLN:HE22	3:DDD:240:THR:HG23	1.81	0.46
3:DDD:749:LYS:HB2	3:DDD:753:SER:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1050:THR:HG22	3:DDD:1051:ASP:H	1.79	0.46
3:DDD:500:ILE:HG22	3:DDD:500:ILE:O	2.14	0.46
3:DDD:394:ILE:HD12	5:FFF:254:ASP:HB2	1.98	0.46
2:CCC:24:VAL:HG11	2:CCC:704:MET:SD	2.56	0.46
3:DDD:1078:LEU:HD12	3:DDD:1121:LEU:HB3	1.98	0.46
3:DDD:1162:ILE:HG13	3:DDD:1180:VAL:HG13	1.97	0.46
3:DDD:93:THR:HG22	3:DDD:94:GLN:H	1.81	0.46
7:222:17:DG:C2'	7:222:18:DT:O4'	2.64	0.46
5:FFF:180:ARG:NH1	7:222:27:DA:OP1	2.49	0.46
3:DDD:923:ILE:HD12	3:DDD:1256:ILE:HD12	1.98	0.46
2:CCC:390:PHE:HA	2:CCC:419:ILE:HG23	1.98	0.46
3:DDD:1206:ARG:NH2	3:DDD:1223:LEU:O	2.46	0.46
3:DDD:223:LEU:O	3:DDD:227:PHE:N	2.48	0.46
3:DDD:41:PRO:O	3:DDD:270:ARG:HD3	2.16	0.46
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.15	0.46
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	1.99	0.46
5:FFF:182:ALA:HA	5:FFF:193:PRO:HG3	1.97	0.46
2:CCC:1305:TYR:CD2	5:FFF:250:THR:HG21	2.51	0.46
5:FFF:80:ALA:HA	5:FFF:83:ALA:HB3	1.98	0.46
1:AAA:48:LEU:HD23	1:AAA:183:ILE:CG2	2.46	0.45
1:BBB:48:LEU:CD2	1:BBB:183:ILE:HG22	2.46	0.45
2:CCC:578:TYR:HB3	2:CCC:590:PRO:HG2	1.98	0.45
3:DDD:1366:HIS:O	3:DDD:1370:MET:HG2	2.16	0.45
3:DDD:378:LYS:HE3	3:DDD:382:TYR:OH	2.16	0.45
1:BBB:83:LEU:CD1	3:DDD:526:VAL:HB	2.44	0.45
3:DDD:638:SER:OG	3:DDD:639:VAL:N	2.50	0.45
2:CCC:1303:LYS:HA	2:CCC:1303:LYS:HD2	1.82	0.45
2:CCC:4:SER:OG	2:CCC:5:TYR:N	2.49	0.45
3:DDD:1134:ILE:HG22	3:DDD:1138:LEU:HG	1.97	0.45
2:CCC:1274:GLU:HA	3:DDD:428:THR:HG21	1.98	0.45
3:DDD:623:GLN:HA	3:DDD:623:GLN:NE2	2.32	0.45
2:CCC:1240:ASP:OD1	2:CCC:1240:ASP:N	2.49	0.45
3:DDD:1000:GLY:HA2	3:DDD:1028:ILE:HD12	1.98	0.45
2:CCC:1268:GLN:OE1	3:DDD:352:ARG:HD2	2.16	0.45
3:DDD:516:ASP:CB	3:DDD:573:THR:HG21	2.46	0.45
2:CCC:894:GLN:HE22	3:DDD:76:LYS:HD3	1.81	0.45
2:CCC:794:LEU:HD21	2:CCC:796:LEU:HD21	1.97	0.45
3:DDD:510:LEU:HD22	3:DDD:579:LEU:HD11	1.98	0.45
3:DDD:849:LEU:C	3:DDD:849:LEU:HD12	2.36	0.45
1:AAA:50:SER:OG	1:BBB:35:PHE:HZ	1.96	0.45
3:DDD:973:LEU:HD23	3:DDD:1006:GLY:HA2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:746:LEU:HD23	3:DDD:758:PRO:HB3	1.99	0.45
3:DDD:842:ARG:HB3	3:DDD:882:VAL:HG11	1.98	0.45
3:DDD:932:MET:SD	8:333:19:U:C3'	3.05	0.45
5:FFF:171:ILE:HG23	5:FFF:212:MET:SD	2.57	0.45
1:AAA:44:ARG:NH2	2:CCC:1215:GLY:HA2	2.32	0.45
2:CCC:503:LYS:HG3	2:CCC:503:LYS:O	2.16	0.45
2:CCC:68:LEU:CD2	2:CCC:489:PRO:HB3	2.47	0.45
1:BBB:48:LEU:HD12	3:DDD:539:SER:OG	2.16	0.45
10:CCC:1402:DPO:O6	3:DDD:937:ILE:HD11	2.17	0.45
1:AAA:186:ASN:O	1:AAA:201:LEU:HD12	2.17	0.45
1:BBB:182:ARG:O	1:BBB:206:GLU:N	2.49	0.45
1:BBB:33:ARG:HH22	2:CCC:1081:PRO:CB	2.29	0.45
2:CCC:807:TRP:CZ3	2:CCC:1086:PRO:HD3	2.51	0.45
3:DDD:1046:ILE:HG22	3:DDD:1061:VAL:HA	1.98	0.45
2:CCC:560:PRO:O	3:DDD:780:ARG:NH2	2.50	0.45
1:AAA:190:ALA:HB2	1:AAA:199:ASP:HA	1.98	0.45
1:AAA:47:LEU:HD13	1:AAA:183:ILE:CD1	2.46	0.45
2:CCC:123:TYR:CZ	5:FFF:190:ASP:O	2.70	0.45
1:AAA:234:LEU:O	1:AAA:235:ARG:HB2	2.17	0.45
2:CCC:27:LEU:HB2	2:CCC:524:ILE:HD11	1.99	0.45
3:DDD:1037:PHE:HE2	3:DDD:1059:LEU:HD13	1.82	0.45
3:DDD:552:ILE:HG21	3:DDD:589:TYR:CD1	2.52	0.44
3:DDD:608:CYS:SG	3:DDD:617:THR:HG22	2.57	0.44
4:EEE:30:MET:SD	4:EEE:49:ILE:HG21	2.57	0.44
6:111:32:DA:N3	7:222:32:DA:C2	2.86	0.44
2:CCC:1145:ILE:HG22	2:CCC:1161:LEU:HD11	1.99	0.44
2:CCC:1179:GLY:O	2:CCC:1181:PRO:HD3	2.17	0.44
2:CCC:1304:MET:HE3	2:CCC:1315:MET:HA	1.99	0.44
2:CCC:241:LEU:HD22	2:CCC:285:ILE:HD11	1.98	0.44
3:DDD:59:ALA:HB3	3:DDD:71:LEU:HD11	1.99	0.44
1:AAA:11:PRO:O	1:BBB:230:ALA:HB2	2.17	0.44
2:CCC:685:MET:HE2	2:CCC:1067:ALA:CB	2.47	0.44
3:DDD:478:LEU:CG	4:EEE:47:THR:HG23	2.46	0.44
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.99	0.44
6:111:50:DT:H2"	6:111:51:DC:H5"	1.99	0.44
2:CCC:1004:ASP:OD1	2:CCC:1004:ASP:N	2.46	0.44
2:CCC:569:ILE:HD11	3:DDD:783:LEU:HB3	2.00	0.44
3:DDD:802:ASP:OD1	3:DDD:1325:PHE:HB2	2.17	0.44
1:AAA:75:GLN:HE21	2:CCC:727:VAL:HG11	1.83	0.44
1:BBB:77:ASP:OD1	1:BBB:77:ASP:N	2.50	0.44
2:CCC:733:VAL:CG1	2:CCC:748:ILE:CG2	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:9:LEU:HB2	1:BBB:32:GLU:OE1	2.17	0.44
2:CCC:1287:LEU:CD2	3:DDD:1357:ILE:HD11	2.48	0.44
3:DDD:919:ALA:O	3:DDD:923:ILE:HG13	2.17	0.44
1:BBB:74:VAL:CG1	1:BBB:131:CYS:SG	3.06	0.44
2:CCC:806:PRO:HA	2:CCC:811:ASN:HD21	1.82	0.44
3:DDD:67:ASP:OD1	3:DDD:95:THR:HG22	2.17	0.44
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	2.00	0.44
1:AAA:58:GLU:HB2	1:AAA:145:LYS:HB3	2.00	0.44
2:CCC:44:GLU:O	2:CCC:46:GLN:N	2.51	0.44
2:CCC:618:GLN:NE2	3:DDD:769:VAL:CG2	2.80	0.44
3:DDD:435:GLN:HB2	3:DDD:457:TYR:OH	2.18	0.44
1:BBB:185:TYR:CB	1:BBB:203:ILE:HG12	2.48	0.43
1:AAA:79:LEU:HD13	2:CCC:693:LEU:HD11	2.00	0.43
1:BBB:9:LEU:CB	1:BBB:32:GLU:OE1	2.66	0.43
2:CCC:1157:GLN:O	2:CCC:1157:GLN:HG3	2.17	0.43
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	2.17	0.43
3:DDD:1075:ARG:NH2	3:DDD:1193:TRP:CE3	2.86	0.43
3:DDD:510:LEU:HD11	3:DDD:624:ILE:HG23	2.01	0.43
3:DDD:364:HIS:HB3	4:EEE:4:VAL:HG13	1.99	0.43
2:CCC:123:TYR:HB3	5:FFF:187:HIS:HA	2.00	0.43
2:CCC:189:ASP:HB2	2:CCC:190:PRO:HD2	1.99	0.43
2:CCC:100:LEU:CD2	2:CCC:493:ILE:HD11	2.45	0.43
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	1.99	0.43
3:DDD:510:LEU:HD11	3:DDD:624:ILE:CG2	2.48	0.43
3:DDD:608:CYS:SG	3:DDD:617:THR:CG2	3.06	0.43
5:FFF:222:VAL:HG11	5:FFF:235:LEU:HB2	1.99	0.43
3:DDD:436:ALA:HB3	3:DDD:485:MET:HA	2.00	0.43
5:FFF:170:HIS:CE1	6:111:31:DT:C6	3.06	0.43
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HG13	2.00	0.43
2:CCC:777:VAL:HG11	2:CCC:783:LEU:CD2	2.48	0.43
3:DDD:430:HIS:CE1	3:DDD:432:LEU:HB2	2.54	0.43
2:CCC:1075:VAL:CG2	3:DDD:463:GLY:N	2.82	0.43
2:CCC:569:ILE:HD13	3:DDD:784:ALA:HA	2.01	0.43
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	2.01	0.43
3:DDD:807:LEU:HD13	3:DDD:1259:GLN:HE22	1.83	0.43
2:CCC:1257:GLN:NE2	3:DDD:341:ASN:HB3	2.34	0.43
3:DDD:342:LEU:HD12	3:DDD:342:LEU:HA	1.83	0.43
3:DDD:48:THR:O	3:DDD:48:THR:OG1	2.36	0.43
3:DDD:599:LYS:H	3:DDD:599:LYS:HD2	1.83	0.43
3:DDD:91:GLU:HG2	3:DDD:93:THR:OG1	2.19	0.43
5:FFF:287:THR:H	5:FFF:290:ASP:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.99	0.43
2:CCC:878:THR:CG2	2:CCC:879:GLY:N	2.82	0.43
3:DDD:702:GLN:O	3:DDD:718:SER:N	2.42	0.43
4:EEE:5:THR:HG22	4:EEE:7:GLN:H	1.84	0.43
5:FFF:126:GLY:HA3	5:FFF:153:THR:HG21	2.00	0.43
2:CCC:228:VAL:HG23	2:CCC:337:PHE:HB2	2.01	0.43
3:DDD:1321:SER:HA	3:DDD:1348:LYS:HE3	2.01	0.43
3:DDD:537:TYR:CE1	3:DDD:544:LEU:HG	2.54	0.43
2:CCC:503:LYS:HE2	7:222:22:DA:H4'	2.00	0.43
3:DDD:22:ILE:HG13	3:DDD:1319:PHE:CZ	2.53	0.43
3:DDD:293:ARG:O	3:DDD:297:ARG:HG3	2.19	0.43
3:DDD:51:PRO:HG2	3:DDD:71:LEU:HD21	2.01	0.43
3:DDD:797:THR:O	3:DDD:801:VAL:HG23	2.19	0.43
3:DDD:844:THR:HG21	3:DDD:858:VAL:CG1	2.49	0.43
3:DDD:932:MET:SD	8:333:19:U:C2'	3.07	0.43
1:AAA:195:ARG:O	1:AAA:196:THR:OG1	2.37	0.42
1:AAA:195:ARG:HG3	1:AAA:198:LEU:HD12	2.01	0.42
2:CCC:183:TRP:CZ3	6:111:51:DC:H2''	2.54	0.42
2:CCC:198:ILE:O	2:CCC:201:ARG:CG	2.66	0.42
2:CCC:269:ILE:HG23	2:CCC:273:HIS:CB	2.48	0.42
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	2.01	0.42
5:FFF:182:ALA:CA	5:FFF:193:PRO:HG3	2.49	0.42
1:BBB:52:PRO:HA	1:BBB:149:GLY:O	2.19	0.42
1:BBB:53:GLY:O	1:BBB:177:TYR:HB3	2.18	0.42
2:CCC:685:MET:CE	2:CCC:1067:ALA:CB	2.97	0.42
2:CCC:26:TYR:CE2	2:CCC:28:LEU:HB2	2.54	0.42
2:CCC:1301:ARG:NH1	5:FFF:243:GLU:OE2	2.52	0.42
5:FFF:112:ARG:CZ	7:222:25:DA:H4'	2.49	0.42
2:CCC:488:MET:HE3	2:CCC:489:PRO:HD2	2.00	0.42
3:DDD:1063:ASP:HB3	3:DDD:1103:GLY:HA3	2.02	0.42
3:DDD:1320:ILE:CG2	3:DDD:1352:ILE:HD13	2.49	0.42
1:AAA:211:ILE:HG22	1:AAA:216:ALA:HB2	2.01	0.42
2:CCC:810:TYR:HB3	2:CCC:817:LEU:HG	2.01	0.42
3:DDD:388:ARG:HH21	3:DDD:414:GLU:HG2	1.85	0.42
3:DDD:502:PRO:HB3	3:DDD:506:VAL:CG1	2.49	0.42
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HH11	1.84	0.42
3:DDD:842:ARG:HB3	3:DDD:882:VAL:HG13	2.02	0.42
5:FFF:159:MET:HG2	5:FFF:172:VAL:HG11	2.01	0.42
1:AAA:77:ASP:OD2	2:CCC:756:TYR:CE2	2.72	0.42
2:CCC:598:VAL:HG13	2:CCC:627:GLY:O	2.19	0.42
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:22:ILE:O	3:DDD:1339:GLY:HA2	2.20	0.42
3:DDD:438:GLU:HA	3:DDD:439:PRO:HD3	1.90	0.42
2:CCC:1276:TRP:CE2	3:DDD:801:VAL:HG11	2.53	0.42
2:CCC:901:LEU:HD23	5:FFF:310:LEU:HD21	2.01	0.42
2:CCC:559:CYS:CB	2:CCC:662:SER:HB3	2.49	0.42
3:DDD:349:TYR:CD2	3:DDD:472:LEU:HD11	2.55	0.42
3:DDD:612:LEU:HB3	3:DDD:616:PRO:HG2	2.01	0.42
3:DDD:808:VAL:HG21	3:DDD:1359:ALA:HB2	2.01	0.42
1:BBB:182:ARG:N	1:BBB:206:GLU:HB3	2.30	0.42
2:CCC:1152:GLY:HA3	2:CCC:1155:VAL:CG2	2.49	0.42
3:DDD:583:VAL:HG13	3:DDD:587:LEU:HD12	2.02	0.42
4:EEE:42:GLU:HB2	4:EEE:52:ARG:HH12	1.85	0.42
2:CCC:1109:ILE:HG22	2:CCC:1109:ILE:O	2.19	0.42
2:CCC:1314:GLN:HG3	4:EEE:28:ARG:NH2	2.35	0.42
3:DDD:825:VAL:HG23	3:DDD:838:ARG:NE	2.34	0.42
3:DDD:364:HIS:CG	4:EEE:4:VAL:HG22	2.54	0.42
1:BBB:223:ILE:O	1:BBB:227:GLN:HG2	2.20	0.42
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.58	0.42
2:CCC:483:ASP:O	2:CCC:487:LEU:HB2	2.19	0.42
2:CCC:877:VAL:HB	2:CCC:920:VAL:HG21	2.01	0.42
3:DDD:592:VAL:O	3:DDD:592:VAL:HG22	2.20	0.42
1:BBB:75:GLN:HG3	1:BBB:134:THR:CG2	2.49	0.42
2:CCC:406:ASN:HB3	2:CCC:411:ARG:HB2	2.02	0.42
3:DDD:1191:PRO:HG2	3:DDD:1194:ARG:CG	2.50	0.42
3:DDD:505:ASP:N	3:DDD:505:ASP:OD1	2.53	0.42
3:DDD:535:ARG:O	3:DDD:539:SER:HB2	2.20	0.42
2:CCC:1072:ASN:N	2:CCC:1072:ASN:OD1	2.47	0.41
3:DDD:109:SER:OG	3:DDD:296:LYS:HE2	2.19	0.41
5:FFF:144:THR:HA	6:111:40:DA:N7	2.35	0.41
1:BBB:199:ASP:N	1:BBB:199:ASP:OD1	2.53	0.41
2:CCC:1085:MET:HE2	2:CCC:1094:VAL:O	2.20	0.41
2:CCC:716:ALA:HB3	2:CCC:784:ALA:HB3	2.02	0.41
3:DDD:1137:GLY:O	3:DDD:1140:ARG:HB3	2.21	0.41
3:DDD:802:ASP:OD2	3:DDD:1313:SER:HB2	2.20	0.41
1:BBB:176:CYS:HB3	3:DDD:535:ARG:HH22	1.85	0.41
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CE2	2.55	0.41
3:DDD:124:ILE:HD11	3:DDD:185:ILE:CG2	2.49	0.41
6:111:50:DT:H1'	6:111:51:DC:O4'	2.19	0.41
2:CCC:841:ARG:HD3	3:DDD:257:GLY:HA2	2.01	0.41
3:DDD:973:LEU:HD22	3:DDD:1006:GLY:HA3	2.02	0.41
3:DDD:1050:THR:CG2	3:DDD:1051:ASP:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:113:HIS:CD2	3:DDD:239:LEU:HD11	2.55	0.41
3:DDD:800:LEU:CD2	3:DDD:1309:ILE:HD11	2.50	0.41
1:AAA:28:LEU:O	1:AAA:200:LYS:HB2	2.20	0.41
1:AAA:86:LYS:HG2	1:AAA:173:VAL:HG12	2.01	0.41
1:BBB:49:SER:C	1:BBB:151:GLY:HA3	2.32	0.41
2:CCC:699:LEU:HD23	2:CCC:699:LEU:HA	1.93	0.41
3:DDD:925:GLU:N	3:DDD:926:PRO:HD2	2.36	0.41
5:FFF:313:LEU:HA	5:FFF:316:ILE:HD12	2.02	0.41
1:BBB:55:ALA:HB3	1:BBB:175:ALA:HB1	2.02	0.41
1:BBB:48:LEU:HD23	1:BBB:183:ILE:CG2	2.51	0.41
2:CCC:967:LEU:CD2	2:CCC:1021:LEU:HD22	2.49	0.41
2:CCC:1319:MET:HB2	2:CCC:1319:MET:HE2	1.98	0.41
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	2.01	0.41
3:DDD:94:GLN:O	3:DDD:97:VAL:HG22	2.21	0.41
4:EEE:64:LEU:HD23	4:EEE:64:LEU:HA	1.95	0.41
6:111:33:DT:H1'	6:111:34:DG:H5'	2.03	0.41
1:BBB:58:GLU:CD	1:BBB:170:ARG:HE	2.23	0.41
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:NE2	2.35	0.41
5:FFF:235:LEU:HD12	5:FFF:235:LEU:O	2.21	0.41
1:BBB:52:PRO:HA	1:BBB:150:ARG:CB	2.51	0.41
2:CCC:802:VAL:HG11	2:CCC:1098:LEU:HD12	2.03	0.41
3:DDD:356:THR:O	3:DDD:448:GLN:HA	2.21	0.41
3:DDD:887:SER:HB3	3:DDD:1227:HIS:HE1	1.86	0.41
7:222:22:DA:OP1	7:222:22:DA:H3'	2.21	0.41
2:CCC:292:ILE:CB	2:CCC:322:LEU:HD11	2.48	0.41
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:CD2	2.50	0.41
2:CCC:1281:TYR:CE2	3:DDD:484:MET:HG2	2.56	0.41
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	2.02	0.41
3:DDD:364:HIS:CD2	4:EEE:4:VAL:HG22	2.55	0.41
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CB	2.51	0.41
2:CCC:1061:GLN:HE21	2:CCC:1239:VAL:CG1	2.34	0.41
2:CCC:1247:SER:HB3	3:DDD:375:GLU:O	2.21	0.41
1:BBB:41:ASN:HB2	1:BBB:185:TYR:OH	2.21	0.40
2:CCC:1065:LYS:HG2	2:CCC:1235:LEU:HD12	2.02	0.40
2:CCC:573:ASN:HD22	2:CCC:574:SER:N	2.19	0.40
3:DDD:1029:THR:HG23	3:DDD:1121:LEU:HG	2.03	0.40
5:FFF:277:ARG:CD	5:FFF:306:GLN:NE2	2.82	0.40
2:CCC:858:GLY:CA	5:FFF:328:PHE:HE1	2.33	0.40
1:AAA:74:VAL:CG1	1:AAA:131:CYS:SG	3.08	0.40
2:CCC:1088:ASP:OD1	2:CCC:1088:ASP:N	2.54	0.40
2:CCC:194:LEU:HD12	2:CCC:194:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:302:ILE:H	2:CCC:302:ILE:HG12	1.76	0.40
3:DDD:1037:PHE:CE2	3:DDD:1059:LEU:HD13	2.55	0.40
3:DDD:1173:ARG:HB2	3:DDD:1190:ILE:HB	2.03	0.40
3:DDD:30:ILE:HG23	3:DDD:243:PRO:HB3	2.03	0.40
5:FFF:317:LEU:CD2	5:FFF:322:LEU:HD12	2.51	0.40
3:DDD:791:ALA:HB2	7:222:11:DA:C8	2.57	0.40
1:AAA:57:THR:O	1:AAA:172:LEU:HD12	2.21	0.40
1:AAA:77:ASP:N	1:AAA:77:ASP:OD1	2.55	0.40
2:CCC:802:VAL:O	2:CCC:1227:VAL:HA	2.21	0.40
2:CCC:198:ILE:O	2:CCC:201:ARG:HG2	2.21	0.40
3:DDD:664:ILE:CD1	3:DDD:685:ILE:HD11	2.44	0.40
3:DDD:973:LEU:HD22	3:DDD:1006:GLY:CA	2.51	0.40
5:FFF:169:ILE:CG2	5:FFF:173:LYS:HD2	2.51	0.40
5:FFF:226:LEU:HD13	7:222:18:DT:O4	2.22	0.40
2:CCC:757:THR:HG22	2:CCC:758:ARG:N	2.35	0.40
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.35	0.40
2:CCC:35:PHE:CE2	2:CCC:39:ILE:HD12	2.57	0.40
2:CCC:1284:ALA:HB2	3:DDD:1357:ILE:HB	2.02	0.40
3:DDD:886:VAL:CG1	3:DDD:1226:VAL:CG1	2.99	0.40
5:FFF:167:LEU:HA	5:FFF:168:PRO:HD3	1.89	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)
3:DDD:1170:LYS:NZ	7:222:33:DC:OP1[3_644]	1.96	0.24

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	228/242 (94%)	207 (91%)	15 (7%)	6 (3%)	5	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	226/242 (93%)	211 (93%)	12 (5%)	3 (1%)	12	48
2	CCC	1339/1342 (100%)	1235 (92%)	90 (7%)	14 (1%)	15	52
3	DDD	1360/1407 (97%)	1256 (92%)	93 (7%)	11 (1%)	19	57
4	EEE	77/90 (86%)	74 (96%)	3 (4%)	0	100	100
5	FFF	275/336 (82%)	252 (92%)	18 (6%)	5 (2%)	8	42
All	All	3505/3659 (96%)	3235 (92%)	231 (7%)	39 (1%)	14	51

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	192	VAL
3	DDD	519	ASN
3	DDD	1053	LEU
5	FFF	190	ASP
1	AAA	210	THR
1	BBB	232	VAL
2	CCC	45	GLY
2	CCC	756	TYR
3	DDD	520	ALA
3	DDD	711	GLY
3	DDD	805	GLN
3	DDD	1275	LEU
5	FFF	113	GLY
1	AAA	8	PHE
1	AAA	162	GLU
2	CCC	342	ASP
2	CCC	812	PHE
2	CCC	914	LYS
3	DDD	49	PHE
5	FFF	115	ALA
1	AAA	196	THR
1	AAA	208	ASN
1	BBB	8	PHE
2	CCC	293	ALA
2	CCC	894	GLN
2	CCC	1103	VAL
2	CCC	1283	ALA
2	CCC	1297	ASP
3	DDD	321	LYS
2	CCC	234	ASP

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Mol	Chain	Res	Type
3	DDD	119	SER
3	DDD	1325	PHE
5	FFF	227	GLY
2	CCC	507	GLY
2	CCC	986	ALA
1	BBB	192	VAL
3	DDD	1091	PRO
2	CCC	1186	VAL
5	FFF	228	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	186 (94%)	12 (6%)	18	50
1	BBB	196/208 (94%)	179 (91%)	17 (9%)	10	38
2	CCC	1156/1157 (100%)	1127 (98%)	29 (2%)	47	70
3	DDD	1135/1168 (97%)	1103 (97%)	32 (3%)	43	68
4	EEE	67/74 (90%)	66 (98%)	1 (2%)	65	81
5	FFF	240/292 (82%)	225 (94%)	15 (6%)	18	49
All	All	2992/3107 (96%)	2886 (96%)	106 (4%)	36	64

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	10	LYS
1	AAA	15	ASP
1	AAA	28	LEU
1	AAA	33	ARG
1	AAA	48	LEU
1	AAA	70	THR
1	AAA	77	ASP
1	AAA	117	HIS
1	AAA	136	GLU

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Mol	Chain	Res	Type
1	AAA	150	ARG
1	AAA	166	ARG
1	AAA	181	GLU
1	BBB	8	PHE
1	BBB	15	ASP
1	BBB	22	THR
1	BBB	28	LEU
1	BBB	32	GLU
1	BBB	33	ARG
1	BBB	48	LEU
1	BBB	70	THR
1	BBB	77	ASP
1	BBB	117	HIS
1	BBB	150	ARG
1	BBB	181	GLU
1	BBB	186	ASN
1	BBB	191	ARG
1	BBB	193	GLU
1	BBB	198	LEU
1	BBB	199	ASP
2	CCC	12	ARG
2	CCC	24	VAL
2	CCC	77	GLU
2	CCC	124	MET
2	CCC	163	LYS
2	CCC	175	ARG
2	CCC	247	ARG
2	CCC	272	ARG
2	CCC	302	ILE
2	CCC	378	ARG
2	CCC	443	ASP
2	CCC	444	ASP
2	CCC	541	GLU
2	CCC	563	THR
2	CCC	573	ASN
2	CCC	600	THR
2	CCC	700	VAL
2	CCC	755	LYS
2	CCC	788	SER
2	CCC	799	ASN
2	CCC	817	LEU
2	CCC	901	LEU

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Mol	Chain	Res	Type
2	CCC	1026	GLU
2	CCC	1034	ARG
2	CCC	1089	GLU
2	CCC	1207	SER
2	CCC	1240	ASP
2	CCC	1255	THR
2	CCC	1272	GLU
3	DDD	28	ASP
3	DDD	52	GLU
3	DDD	93	THR
3	DDD	199	GLU
3	DDD	223	LEU
3	DDD	227	PHE
3	DDD	357	VAL
3	DDD	399	LYS
3	DDD	504	GLN
3	DDD	505	ASP
3	DDD	526	VAL
3	DDD	535	ARG
3	DDD	538	ARG
3	DDD	571	ASP
3	DDD	599	LYS
3	DDD	641	ILE
3	DDD	706	VAL
3	DDD	707	ILE
3	DDD	721	SER
3	DDD	731	ARG
3	DDD	783	LEU
3	DDD	798	ARG
3	DDD	821	MET
3	DDD	831	VAL
3	DDD	891	ASP
3	DDD	936	HIS
3	DDD	947	GLU
3	DDD	954	ASN
3	DDD	1087	ASP
3	DDD	1108	GLN
3	DDD	1131	THR
3	DDD	1345	ARG
4	EEE	45	LYS
5	FFF	74	GLU
5	FFF	91	ARG

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Mol	Chain	Res	Type
5	FFF	129	ARG
5	FFF	152	GLN
5	FFF	156	ARG
5	FFF	170	HIS
5	FFF	190	ASP
5	FFF	192	GLU
5	FFF	203	ASP
5	FFF	217	GLU
5	FFF	241	GLU
5	FFF	271	ARG
5	FFF	290	ASP
5	FFF	314	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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	4/6 (66%)	2 (50%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	18	C
8	333	19	U

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	DPO	CCC	1402	9	6,8,8	0.60	0	13,13,13	0.87	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
10	DPO	CCC	1402	9	-	2/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	CCC	1402	DPO	P2-O4-P1-O2
10	CCC	1402	DPO	P2-O4-P1-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	CCC	1402	DPO	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	230/242 (95%)	0.27	14 (6%) 21 17	203, 281, 334, 387	0
1	BBB	228/242 (94%)	0.09	11 (4%) 30 26	200, 266, 334, 384	0
2	CCC	1341/1342 (99%)	0.10	60 (4%) 33 28	123, 234, 335, 438	0
3	DDD	1362/1407 (96%)	0.11	59 (4%) 35 30	123, 247, 342, 403	0
4	EEE	79/90 (87%)	-0.21	3 (3%) 40 33	211, 286, 389, 411	0
5	FFF	277/336 (82%)	0.16	12 (4%) 35 30	205, 271, 363, 423	0
6	111	30/50 (60%)	0.11	5 (16%) 1 2	238, 288, 392, 433	0
7	222	35/50 (70%)	0.48	8 (22%) 0 0	187, 271, 417, 465	0
8	333	5/6 (83%)	0.59	0 100 100	219, 220, 242, 249	0
All	All	3587/3765 (95%)	0.12	172 (4%) 30 26	123, 251, 349, 465	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	CCC	1004	ASP	5.7
2	CCC	1055	ALA	5.6
3	DDD	1110	GLU	5.5
3	DDD	880	VAL	5.2
1	AAA	144	ILE	5.2
3	DDD	147	ILE	5.1
5	FFF	263	LEU	5.0
2	CCC	124	MET	4.8
6	111	49	DG	4.8
6	111	44	DG	4.6
3	DDD	1078	LEU	4.6
1	AAA	211	ILE	4.3
2	CCC	1041	ASP	4.2
3	DDD	973	LEU	3.9
2	CCC	494	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
3	DDD	1003	LEU	3.9
3	DDD	1040	MET	3.9
3	DDD	1121	LEU	3.9
5	FFF	53	ARG	3.9
2	CCC	850	ILE	3.9
3	DDD	46	TYR	3.8
2	CCC	998	LEU	3.8
3	DDD	71	LEU	3.8
1	BBB	152	TYR	3.7
2	CCC	1001	GLY	3.7
2	CCC	241	LEU	3.7
2	CCC	1042	LEU	3.5
1	BBB	205	MET	3.4
5	FFF	324	ILE	3.4
1	AAA	142	MET	3.4
1	AAA	201	LEU	3.4
2	CCC	464	PHE	3.3
7	222	38	DG	3.3
5	FFF	310	LEU	3.2
2	CCC	1159	VAL	3.2
2	CCC	941	LYS	3.2
2	CCC	1002	LEU	3.2
3	DDD	1190	ILE	3.2
1	BBB	144	ILE	3.2
1	AAA	213	PRO	3.2
3	DDD	115	TRP	3.2
3	DDD	1189	MET	3.2
3	DDD	1039	ASP	3.1
3	DDD	1017	VAL	3.1
2	CCC	493	ILE	3.1
3	DDD	1030	GLU	3.0
2	CCC	696	ASP	3.0
2	CCC	389	PHE	3.0
2	CCC	1180	MET	3.0
2	CCC	975	ILE	3.0
2	CCC	885	GLY	3.0
2	CCC	884	VAL	3.0
3	DDD	877	VAL	2.9
1	BBB	123	ILE	2.9
1	AAA	130	ILE	2.9
2	CCC	1054	LEU	2.9
2	CCC	239	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	CCC	487	LEU	2.8
2	CCC	906	PHE	2.8
3	DDD	982	LEU	2.8
2	CCC	912	ASP	2.8
4	EEE	80	LEU	2.8
3	DDD	237	MET	2.8
3	DDD	76	LYS	2.8
2	CCC	855	PRO	2.8
7	222	22	DA	2.8
2	CCC	1009	ASN	2.8
2	CCC	1014	LEU	2.8
5	FFF	303	ARG	2.7
3	DDD	748	ALA	2.7
3	DDD	879	ALA	2.7
1	BBB	160	HIS	2.7
1	AAA	100	LEU	2.7
2	CCC	911	SER	2.7
1	AAA	171	LEU	2.7
2	CCC	102	LEU	2.7
5	FFF	321	GLY	2.7
2	CCC	220	ILE	2.7
7	222	19	DA	2.7
7	222	24	DT	2.6
3	DDD	1054	THR	2.6
3	DDD	958	ILE	2.6
3	DDD	1187	GLU	2.6
3	DDD	56	LEU	2.6
3	DDD	1005	LYS	2.6
7	222	26	DT	2.6
1	AAA	59	VAL	2.6
2	CCC	854	ILE	2.6
3	DDD	1076	PRO	2.6
3	DDD	1029	THR	2.5
3	DDD	983	LYS	2.5
3	DDD	1101	LEU	2.5
2	CCC	838	CYS	2.5
1	AAA	203	ILE	2.5
1	BBB	98	VAL	2.5
1	BBB	231	PHE	2.5
2	CCC	999	GLU	2.5
2	CCC	692	THR	2.5
3	DDD	1068	THR	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	CCC	1000	LEU	2.5
3	DDD	1185	PRO	2.4
7	222	25	DA	2.4
2	CCC	614	TYR	2.4
2	CCC	940	GLU	2.4
3	DDD	80	HIS	2.4
3	DDD	1051	ASP	2.4
3	DDD	1006	GLY	2.4
5	FFF	111	ASN	2.4
3	DDD	404	GLU	2.4
2	CCC	883	LEU	2.4
3	DDD	154	LEU	2.4
3	DDD	1098	GLN	2.4
3	DDD	212	THR	2.3
2	CCC	1012	GLU	2.3
2	CCC	882	ILE	2.3
1	BBB	130	ILE	2.3
2	CCC	489	PRO	2.3
3	DDD	878	ASP	2.3
1	AAA	220	ALA	2.3
2	CCC	311	CYS	2.3
2	CCC	1194	GLU	2.3
3	DDD	1266	ILE	2.3
2	CCC	995	ASP	2.3
6	111	42	DG	2.3
2	CCC	96	LEU	2.3
2	CCC	1010	GLN	2.3
3	DDD	995	TYR	2.3
1	AAA	28	LEU	2.2
1	BBB	90	VAL	2.2
4	EEE	78	ALA	2.2
1	BBB	134	THR	2.2
3	DDD	1004	ALA	2.2
5	FFF	127	LEU	2.2
5	FFF	212	MET	2.2
3	DDD	1191	PRO	2.2
1	AAA	110	VAL	2.2
2	CCC	15	PHE	2.2
3	DDD	176	PHE	2.2
2	CCC	333	ILE	2.2
3	DDD	993	GLU	2.2
2	CCC	875	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	DDD	178	ALA	2.2
1	AAA	172	LEU	2.2
2	CCC	422	LYS	2.2
6	111	43	DT	2.2
2	CCC	910	ALA	2.1
5	FFF	167	LEU	2.1
3	DDD	1109	LEU	2.1
3	DDD	1038	THR	2.1
3	DDD	957	SER	2.1
6	111	50	DT	2.1
2	CCC	629	PHE	2.1
3	DDD	321	LYS	2.1
2	CCC	994	ARG	2.1
5	FFF	230	SER	2.1
3	DDD	382	TYR	2.1
3	DDD	1272	SER	2.1
2	CCC	429	MET	2.1
1	BBB	183	ILE	2.0
3	DDD	731	ARG	2.0
2	CCC	230	PHE	2.0
5	FFF	306	GLN	2.0
3	DDD	185	ILE	2.0
2	CCC	927	THR	2.0
3	DDD	1118	GLY	2.0
3	DDD	1071	GLY	2.0
2	CCC	795	ALA	2.0
2	CCC	798	GLN	2.0
3	DDD	146	VAL	2.0
4	EEE	76	GLU	2.0
7	222	18	DT	2.0
7	222	23	DT	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	ZN	DDD	1501	1/1	0.70	0.09	395,395,395,395	0
10	DPO	CCC	1402	9/9	0.93	0.57	230,239,254,258	0
9	MG	DDD	1503	1/1	0.95	0.29	177,177,177,177	0
11	ZN	DDD	1502	1/1	0.97	0.16	223,223,223,223	0
9	MG	CCC	1401	1/1	0.98	0.41	163,163,163,163	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.