



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 09:04 PM EDT

PDB ID : 6UU6
Title : E. coli sigma-S transcription initiation complex with a 4-nt RNA and a UTP ("Old" crystal soaked with UTP, ddCTP, and dinucleotide ApG for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

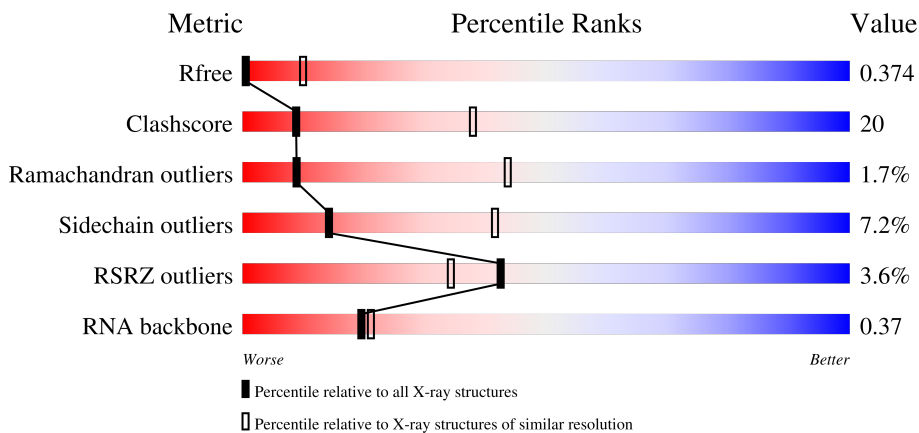
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)
RNA backbone	3102	1049 (5.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 3% 58% 33% 5%
1	BBB	242	 5% 59% 32% 6%
2	CCC	1342	 3% 63% 33% 1%

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Mol	Chain	Length	Quality of chain
3	DDD	1407	
4	EEE	90	
5	FFF	336	
6	111	50	
7	222	50	
8	333	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ZN	DDD	1502	-	-	X	-
8	DOC	333	101	-	-	X	-
9	UTP	CCC	1401	-	-	X	-

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 29026 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP 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
			Total	C	N	O	S			
2	CCC	1341	Total 10577	C 6636	N 1842	O 2056	S 43	0	0	0

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

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

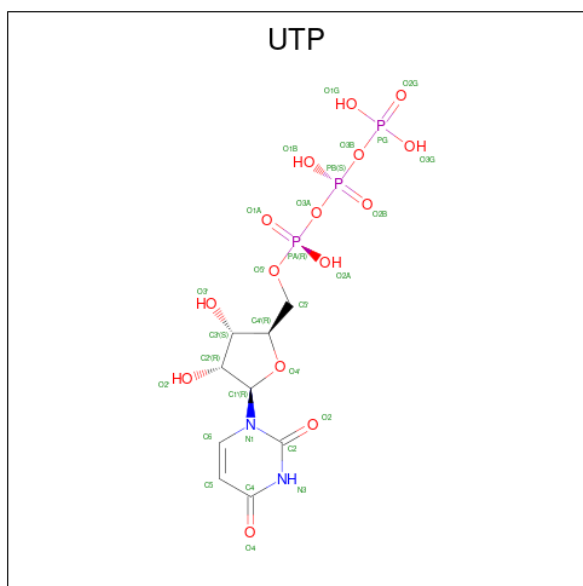
- Molecule 7 is a DNA chain called Synthetic DNA 50-mer (promoter template strand).

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

- Molecule 8 is a RNA chain called RNA 4-mer (dinucleotide ApG primed synthesis).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	333	4	80	38	15	24	3	0	0	0

- Molecule 9 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	CCC	1	29	9	2	15	3	0	0

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

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

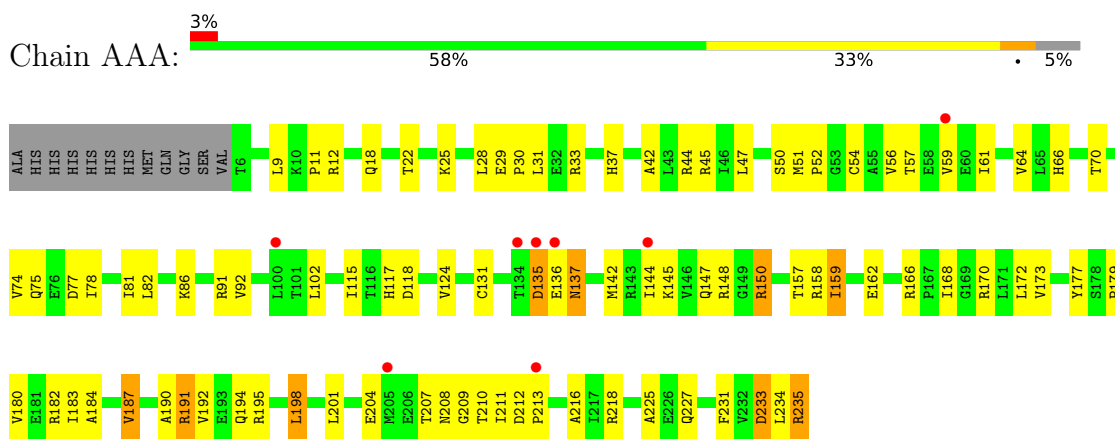
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

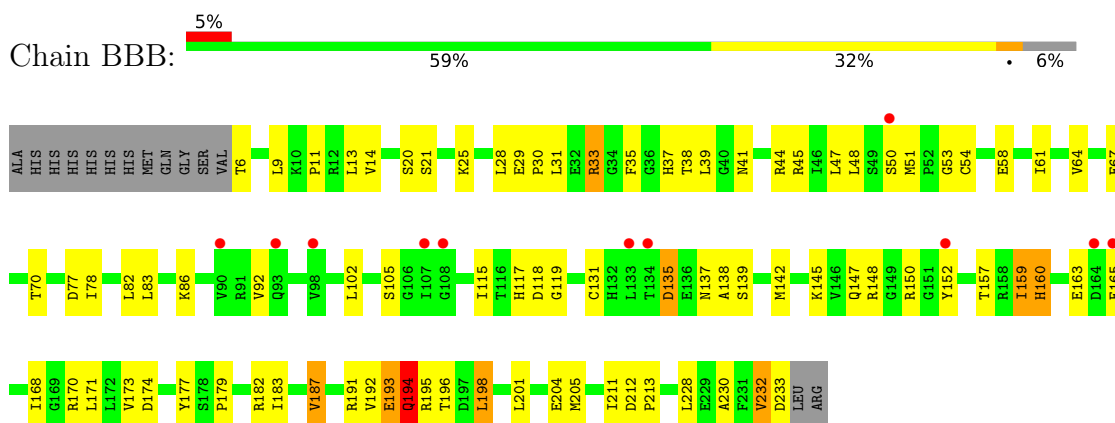
3 Residue-property plots [i](#)

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

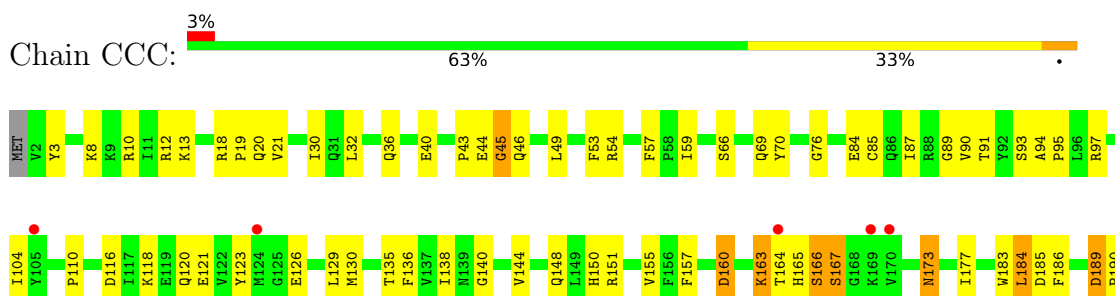
- Molecule 1: DNA-directed RNA polymerase subunit alpha

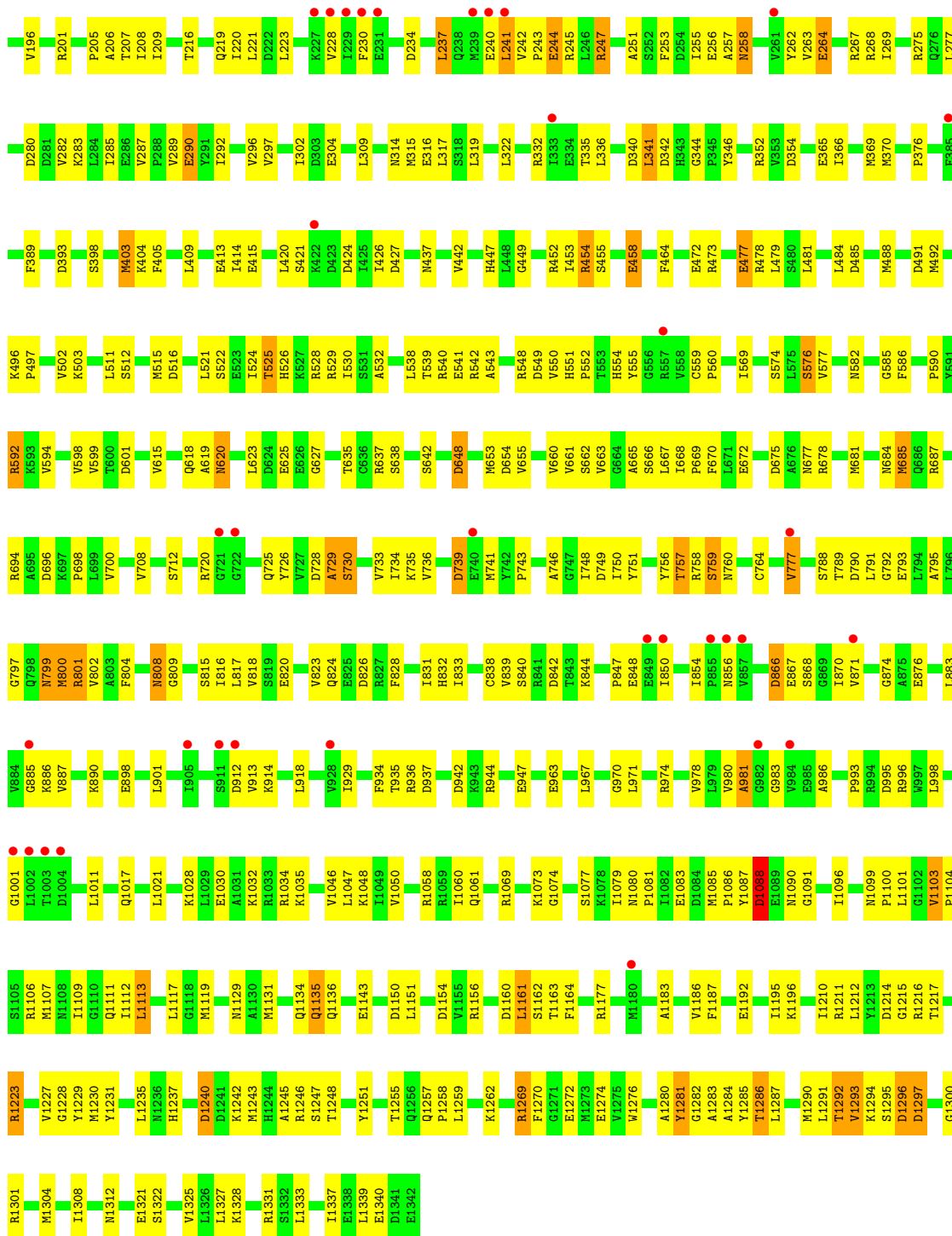


- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta





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

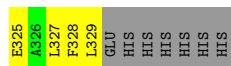
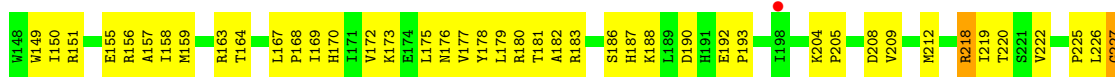
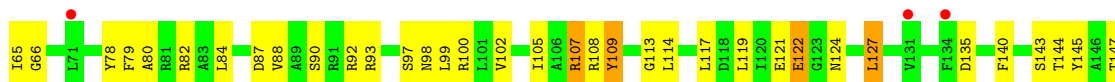
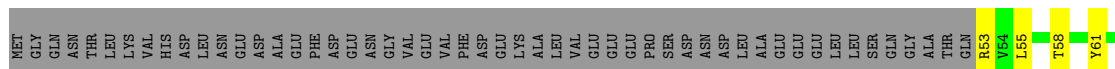


E1343	V1163	G1063	S977	V808	R731	L614	V518	N209	V97
L1344	S1164	S1064	T980	V809	G732	T617	M519	S210	R98
R1345	F1165	A1065	E981	T910	G733	V618	A520	E211	R99
K1348	G1166	E1066	K982	E911	S733	I619	E523	E212	R101
E1349	K1167	R1067	L983	D812	Q736	L620	F620	K213	K108
N1350	E1168	R1068	L984	T816	Q739	A621	G524	R214	A108
V1351	T1169	D1073	L985	H817	L739	D622	M525	R220	S109
I1352	K1170	L1078	D986	E818	Q739	Q623	V526	L221	P110
I1357	R1173	L1079	R987	G820	A741	I624	I527	K222	T111
D1368	R1174	I1080	A896	I820	A744	M625	T528	K345	A112
R1369	L1175	V1081	H897	M821	G744	T626	G529	L223	H113
R1370	V1176	D1082	C898	M822	G745	T627	P530	L224	I114
R1372	A1083	A1083	K911	V825	L746	E443	E532	F227	M115
R1373	Q1084	Q1084	Y995	V825	M747	A637	G444	M237	K118
G1376	D1087	D1087	Y996	G829	K749	S638	K445	L245	S119
ALA	V1088	V1088	G997	D830	P750	G640	L536	L246	L120
ALA	L1089	L1089	I918	D831	D751	I641	Y537	P246	P121
PRO	I1090	I1090	E833	E833	I754	D642	R538	P247	S122
GLN	P1091	P1091	P834	P834	I754	D643	S543	D248	R123
ALA	A1097	A1097	R835	R835	P758	M644	A459	L249	L127
PRO	F1100	F1100	R836	R836	I759	V645	D460	D256	M130
GLN	G1103	G1103	D837	D837	F763	V661	F461	A261	D134
VAL	K1104	K1104	G924	G924	R764	T664	Q465	T262	I135
THR	A1105	A1105	E925	E925	V769	G665	M466	P288	E136
ALA	I1106	I1106	P926	P926	L770	G667	A467	I290	L139
GLU	E1110	E1110	I923	I923	L776	G668	M468	E295	Q157
ASP	D1111	D1111	G934	G934	T776	G669	M468	Q300	Q158
LEU	G1112	G1112	F935	F935	A779	S670	A577	L385	I169
LEU	V1113	V1113	H936	H936	R780	V673	I578	E386	L160
ALA	I1118	I1118	I937	I937	K781	G678	L579	L387	T161
LEU	G1121	G1121	A941	A941	G782	R678	M581	V303	G173
LEU	L1122	L1122	S942	S942	L783	V679	I582	D304	E175
ASN	S1128	S1128	R943	R943	A784	M680	V583	A305	F176
ASN	G1129	G1129	S949	S949	T786	I685	K584	R311	D167
ALA	G1129	G1129	I950	I950	L786	V686	P584	R312	G173
GLY	D1133	D1133	V952	V952	T790	A791	G586	K395	D174
GLY	I1134	I1134	S957	S957	M792	M697	I591	I316	E175
SER	T1135	T1135	K958	K958	S793	M698	V592	S319	F176
ASP	L1138	L1138	T862	T862	Y795	Q702	A595	N320	A162
ASN	E1146	E1146	L864	L864	T797	E704	K599	K321	A162
ASN	K1151	K1151	V877	V877	R798	T705	M604	R322	I185
GLY	L1156	L1156	L872	L872	R799	V706	V506	P323	I185
ASP	A1157	A1157	E873	E873	L800	T707	I500	K332	E197
GLU	E1158	E1158	V878	V878	V801	M708	V501	R332	C198
GLU	G1161	G1161	D879	D879	M802	R709	P502	P323	E197
GLU	I1162	I1162	A879	A879	M804	D710	S503	K332	C198
GLU	V1255	V1255	V880	V880	Q805	R715	V506	G333	L205
I1256	I1256	I1256	V882	V882	D806	Q716	I506	K334	L205
I1256	I1256	I1256	V882	V882	L807	V717	Q613	K335	L205

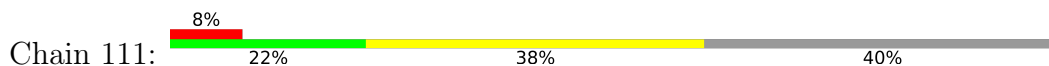
• Molecule 4: DNA-directed RNA polymerase subunit omega



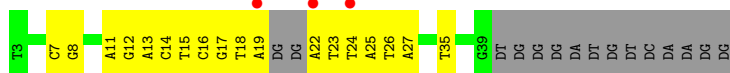
• Molecule 5: RNA polymerase sigma factor RpoS



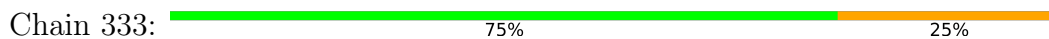
• Molecule 6: Synthetic DNA 50-mer (promoter non-template strand)



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



• Molecule 8: RNA 4-mer (dinucleotide ApG primed synthesis)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.40Å 154.10Å 232.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 4.20 49.08 – 4.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.08-4.20) 99.0 (49.08-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 4.14Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.343 , 0.389 0.330 , 0.374	Depositor DCC
R_{free} test set	1678 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	165.5	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 183.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29026	wwPDB-VP
Average B, all atoms (Å ²)	272.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UTP, ZN, DOC, 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	0.62	0/1809	0.76	0/2450
1	BBB	0.62	0/1789	0.74	0/2425
2	CCC	0.62	0/10746	0.82	3/14499 (0.0%)
3	DDD	0.62	0/10729	0.79	0/14487
4	EEE	0.62	0/629	0.81	0/847
5	FFF	0.64	0/2282	0.66	0/3076
6	111	0.27	0/691	0.63	0/1063
7	222	0.32	0/802	0.66	0/1234
8	333	0.16	0/69	0.52	0/106
All	All	0.61	0/29546	0.78	3/40187 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CCC	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	1088	ASP	CB-CA-C	-6.16	98.08	110.40
2	CCC	1048	LYS	CB-CA-C	-5.83	98.74	110.40
2	CCC	454	ARG	CB-CA-C	-5.04	100.33	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	CCC	1282	GLY	Peptide
2	CCC	376	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1787	0	1813	85	0
1	BBB	1767	0	1789	100	1
2	CCC	10577	0	10591	459	0
3	DDD	10568	0	10782	508	2
4	EEE	627	0	634	16	0
5	FFF	2253	0	2298	157	0
6	111	618	0	341	44	1
7	222	716	0	397	42	0
8	333	80	0	45	7	0
9	CCC	29	0	11	14	0
10	DDD	2	0	0	2	0
11	DDD	2	0	0	0	0
All	All	29026	0	28701	1173	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1173) 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:936:ARG:CG	2:CCC:937:ASP:H	1.31	1.35
6:111:54:DA:H2''	6:111:55:DC:C5	1.61	1.33
2:CCC:1106:ARG:NH1	9:CCC:1401:UTP:O3G	1.69	1.22
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	1.37	1.22
1:BBB:83:LEU:HG	3:DDD:526:VAL:CG1	1.69	1.20
5:FFF:227:GLY:HA2	7:222:17:DG:H22	1.04	1.16
3:DDD:750:PRO:HA	3:DDD:781:LYS:HG2	1.15	1.13
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:NH1	1.62	1.12
2:CCC:868:SER:OG	2:CCC:944:ARG:N	1.80	1.12
6:111:54:DA:H2''	6:111:55:DC:C6	1.86	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:868:SER:CB	2:CCC:944:ARG:HB3	1.82	1.09
3:DDD:836:ARG:HD3	3:DDD:873:GLU:OE2	1.52	1.08
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:HH12	1.10	1.08
9:CCC:1401:UTP:H4'	3:DDD:425:ARG:HH22	1.11	1.05
1:BBB:83:LEU:HG	3:DDD:526:VAL:HG11	1.06	1.04
3:DDD:888:CYS:SG	10:DDD:1502:ZN:ZN	1.46	1.04
2:CCC:936:ARG:HG2	2:CCC:937:ASP:N	1.43	1.04
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.40	1.02
3:DDD:392:THR:CG2	5:FFF:320:GLN:O	2.09	1.01
1:AAA:52:PRO:O	1:AAA:211:ILE:HD11	1.59	1.00
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.43	0.99
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.40	0.99
2:CCC:748:ILE:HD11	2:CCC:970:GLY:HA3	1.45	0.99
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	1.80	0.99
3:DDD:836:ARG:CD	3:DDD:873:GLU:OE2	2.10	0.99
1:BBB:48:LEU:HD22	3:DDD:535:ARG:HG3	1.42	0.98
2:CCC:868:SER:OG	2:CCC:944:ARG:CB	2.13	0.96
6:111:54:DA:C2'	6:111:55:DC:C5	2.47	0.96
2:CCC:32:LEU:HA	2:CCC:130:MET:HE1	1.46	0.96
1:BBB:83:LEU:CG	3:DDD:526:VAL:CG1	2.43	0.95
3:DDD:388:ARG:NH2	3:DDD:414:GLU:OE1	1.98	0.95
2:CCC:868:SER:HB2	2:CCC:944:ARG:HB3	1.48	0.94
9:CCC:1401:UTP:C4'	3:DDD:425:ARG:HH22	1.79	0.94
5:FFF:263:LEU:HD13	5:FFF:281:LEU:HD11	1.49	0.94
5:FFF:227:GLY:HA2	7:222:17:DG:N2	1.84	0.93
5:FFF:144:THR:HG22	6:111:39:DA:H8	1.32	0.93
2:CCC:936:ARG:HG2	2:CCC:937:ASP:H	0.77	0.92
1:BBB:179:PRO:HG3	1:BBB:211:ILE:HD12	1.51	0.92
2:CCC:251:ALA:CB	2:CCC:263:VAL:HG11	1.99	0.92
9:CCC:1401:UTP:H4'	3:DDD:425:ARG:NH2	1.83	0.92
3:DDD:750:PRO:CA	3:DDD:781:LYS:HG2	2.00	0.91
3:DDD:750:PRO:HA	3:DDD:781:LYS:CG	2.01	0.91
3:DDD:836:ARG:HD2	3:DDD:873:GLU:CD	1.91	0.90
3:DDD:895:CYS:HG	10:DDD:1502:ZN:ZN	0.67	0.90
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HD13	1.52	0.89
7:222:17:DG:C2'	7:222:18:DT:O4'	2.20	0.89
2:CCC:866:ASP:OD2	2:CCC:944:ARG:HD3	1.72	0.88
5:FFF:273:VAL:HG13	5:FFF:291:VAL:HG11	1.54	0.88
2:CCC:503:LYS:NZ	7:222:23:DT:OP1	2.07	0.86
3:DDD:1330:ARG:NH2	7:222:7:DC:O3'	2.09	0.86
2:CCC:936:ARG:CG	2:CCC:937:ASP:N	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:83:LEU:CG	3:DDD:526:VAL:HG11	1.99	0.85
2:CCC:496:LYS:HB3	7:222:24:DT:OP1	1.76	0.85
3:DDD:822:MET:SD	3:DDD:838:ARG:O	2.34	0.85
1:BBB:25:LYS:HG2	1:BBB:204:GLU:HG2	1.57	0.85
2:CCC:1295:SER:OG	3:DDD:346:ARG:O	1.92	0.85
3:DDD:816:THR:HG22	3:DDD:818:GLU:H	1.41	0.85
3:DDD:793:SER:OG	3:DDD:928:THR:OG1	1.93	0.85
2:CCC:681:MET:O	2:CCC:685:MET:HG2	1.76	0.84
5:FFF:144:THR:HG22	6:111:39:DA:C8	2.11	0.84
1:AAA:11:PRO:O	1:BBB:230:ALA:HB2	1.76	0.84
2:CCC:868:SER:CB	2:CCC:944:ARG:CB	2.56	0.83
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.60	0.83
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:HA	1.60	0.83
2:CCC:726:TYR:HB3	2:CCC:733:VAL:CG2	2.07	0.83
3:DDD:843:VAL:HG21	3:DDD:897:HIS:O	1.78	0.83
3:DDD:673:VAL:CG1	3:DDD:678:ARG:HB2	2.09	0.82
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.14	0.82
5:FFF:163:ARG:HD3	5:FFF:167:LEU:HD12	1.61	0.82
2:CCC:1077:SER:HA	3:DDD:356:THR:CG2	2.10	0.82
2:CCC:555:TYR:CD1	2:CCC:637:ARG:NH2	2.47	0.82
2:CCC:804:PHE:O	3:DDD:638:SER:HB2	1.80	0.82
5:FFF:164:THR:HB	5:FFF:219:ILE:HD12	1.61	0.82
2:CCC:898:GLU:HG3	5:FFF:259:ILE:CD1	2.08	0.81
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.62	0.81
3:DDD:644:MET:O	3:DDD:764:ARG:NH1	2.12	0.81
3:DDD:22:ILE:HD11	3:DDD:1319:PHE:CE1	2.15	0.81
3:DDD:121:PRO:O	3:DDD:122:SER:HB3	1.81	0.81
5:FFF:119:LEU:HD21	5:FFF:158:ILE:HD11	1.63	0.81
1:BBB:83:LEU:CD1	3:DDD:526:VAL:HG12	2.10	0.80
3:DDD:843:VAL:CG2	3:DDD:897:HIS:O	2.30	0.80
3:DDD:26:SER:OG	3:DDD:28:ASP:OD1	1.98	0.80
5:FFF:156:ARG:NH2	6:111:33:DT:OP2	2.14	0.80
2:CCC:936:ARG:HG3	2:CCC:937:ASP:H	1.42	0.80
5:FFF:263:LEU:HD13	5:FFF:281:LEU:CD1	2.11	0.80
2:CCC:167:SER:O	3:DDD:1065:ALA:HA	1.82	0.79
2:CCC:255:ILE:HD12	2:CCC:263:VAL:HG21	1.64	0.79
2:CCC:186:PHE:CE1	2:CCC:196:VAL:HG22	2.16	0.79
1:BBB:83:LEU:CD2	3:DDD:526:VAL:HB	2.10	0.79
1:BBB:83:LEU:HD11	3:DDD:526:VAL:HB	1.63	0.79
2:CCC:166:SER:OG	3:DDD:1151:LYS:NZ	2.15	0.79
9:CCC:1401:UTP:H5'1	8:333:101:DOC:H3'2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:83:LEU:HD11	3:DDD:526:VAL:CB	2.13	0.79
2:CCC:1340:GLU:O	3:DDD:17:PHE:HB2	1.84	0.78
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HG3	1.66	0.78
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD11	1.64	0.78
2:CCC:165:HIS:CE1	2:CCC:190:PRO:HG3	2.18	0.78
2:CCC:1333:LEU:O	3:DDD:113:HIS:CE1	2.38	0.77
1:BBB:44:ARG:NH1	3:DDD:538:ARG:HD2	1.98	0.77
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CB	2.13	0.77
2:CCC:95:PRO:HB3	5:FFF:190:ASP:HB2	1.66	0.77
3:DDD:1133:ASP:OD2	3:DDD:1134:ILE:N	2.18	0.77
2:CCC:790:ASP:O	2:CCC:792:GLY:N	2.18	0.77
3:DDD:836:ARG:CD	3:DDD:873:GLU:CD	2.53	0.77
3:DDD:458:ASN:OD1	3:DDD:933:ARG:NH2	2.17	0.77
5:FFF:182:ALA:HB1	5:FFF:193:PRO:HG3	1.66	0.77
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.15	0.76
2:CCC:95:PRO:CB	5:FFF:190:ASP:HB2	2.15	0.76
3:DDD:392:THR:HG21	5:FFF:320:GLN:C	2.05	0.76
2:CCC:748:ILE:CD1	2:CCC:970:GLY:HA3	2.15	0.76
2:CCC:1269:ARG:HB2	7:222:14:DC:OP1	1.86	0.76
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.68	0.76
3:DDD:825:VAL:CG1	3:DDD:1242:ARG:HH12	1.95	0.76
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.66	0.76
1:BBB:83:LEU:CD1	3:DDD:526:VAL:CG1	2.63	0.76
2:CCC:1269:ARG:HB2	7:222:14:DC:P	2.26	0.76
5:FFF:170:HIS:NE2	6:111:31:DT:C6	2.54	0.76
3:DDD:1156:LEU:HD22	3:DDD:1224:ARG:HH21	1.51	0.75
7:222:17:DG:H2'	7:222:18:DT:O4'	1.86	0.75
2:CCC:555:TYR:CE1	2:CCC:637:ARG:NH2	2.54	0.75
3:DDD:1029:THR:HG23	3:DDD:1121:LEU:HG	1.68	0.75
1:AAA:57:THR:HG23	1:AAA:158:ARG:NH2	2.01	0.75
2:CCC:237:LEU:HD12	2:CCC:289:VAL:HA	1.67	0.75
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:HD11	1.66	0.75
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:HD2	1.52	0.75
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.68	0.74
2:CCC:230:PHE:CD1	2:CCC:292:ILE:HD11	2.22	0.74
3:DDD:134:ASP:CG	3:DDD:159:ILE:HD11	2.07	0.74
1:AAA:9:LEU:HD21	1:AAA:198:LEU:HD11	1.69	0.74
2:CCC:868:SER:HB2	2:CCC:944:ARG:CB	2.17	0.74
3:DDD:288:PRO:HG3	5:FFF:92:ARG:HG2	1.70	0.74
5:FFF:135:ASP:HB3	6:111:37:DA:N1	2.04	0.73
1:BBB:44:ARG:HH12	3:DDD:538:ARG:CD	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.16	0.73
2:CCC:3:TYR:O	2:CCC:8:LYS:HE3	1.86	0.73
3:DDD:698:MET:O	3:DDD:702:GLN:HB3	1.87	0.73
3:DDD:475:GLU:O	3:DDD:479:GLU:HG2	1.87	0.73
1:AAA:150:ARG:HH12	1:BBB:6:THR:HG23	1.54	0.73
1:BBB:193:GLU:O	1:BBB:194:GLN:HB2	1.88	0.73
2:CCC:868:SER:OG	2:CCC:944:ARG:CA	2.35	0.72
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	1.70	0.72
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.71	0.72
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.20	0.72
3:DDD:703:THR:OG1	3:DDD:704:GLU:N	2.22	0.72
5:FFF:176:ASN:OD1	7:222:26:DT:H72	1.89	0.72
2:CCC:18:ARG:NH2	2:CCC:620:ASN:O	2.23	0.72
5:FFF:226:LEU:O	5:FFF:228:GLY:N	2.22	0.72
3:DDD:931:THR:O	3:DDD:935:PHE:CD2	2.43	0.72
2:CCC:10:ARG:NH2	2:CCC:790:ASP:OD1	2.22	0.72
2:CCC:868:SER:OG	2:CCC:944:ARG:HB3	1.81	0.71
2:CCC:1077:SER:HA	3:DDD:356:THR:HG21	1.71	0.71
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:CE	2.20	0.71
2:CCC:549:ASP:CG	3:DDD:750:PRO:HG3	2.11	0.71
2:CCC:201:ARG:HB2	2:CCC:369:MET:CE	2.21	0.71
2:CCC:898:GLU:OE2	5:FFF:259:ILE:HD13	1.90	0.71
3:DDD:859:PRO:HG2	3:DDD:862:THR:HG21	1.70	0.71
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	1.72	0.71
5:FFF:105:ILE:HG21	5:FFF:150:ILE:HG22	1.72	0.71
2:CCC:251:ALA:HB2	2:CCC:263:VAL:HG11	1.71	0.70
3:DDD:528:THR:O	3:DDD:528:THR:OG1	2.02	0.70
3:DDD:312:ARG:HG2	3:DDD:312:ARG:O	1.91	0.70
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:H	1.55	0.70
3:DDD:958:ILE:HG23	3:DDD:982:LEU:CD1	2.22	0.70
2:CCC:1269:ARG:HD3	7:222:13:DA:H5'	1.73	0.70
2:CCC:1333:LEU:O	3:DDD:113:HIS:HE1	1.74	0.70
1:AAA:56:VAL:HG13	1:AAA:144:ILE:CG2	2.22	0.70
2:CCC:183:TRP:CZ3	6:111:51:DC:H2'	2.26	0.70
2:CCC:870:ILE:HG13	2:CCC:944:ARG:HG2	1.74	0.70
3:DDD:895:CYS:SG	3:DDD:898:CYS:HB2	2.30	0.70
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HB3	1.57	0.69
1:BBB:152:TYR:CE2	3:DDD:536:LEU:HD21	2.27	0.69
2:CCC:257:ALA:HB3	2:CCC:262:TYR:CE2	2.27	0.69
5:FFF:183:ARG:NH2	7:222:26:DT:OP2	2.26	0.69
5:FFF:144:THR:HA	6:111:40:DA:N7	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:231:GLU:OE2	7:222:16:DC:N4	2.25	0.69
1:AAA:227:GLN:OE1	1:BBB:11:PRO:HD3	1.92	0.69
2:CCC:163:LYS:HG2	2:CCC:164:THR:N	2.07	0.69
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.75	0.69
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:NZ	2.08	0.69
3:DDD:750:PRO:HB3	3:DDD:781:LYS:HB2	1.75	0.69
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	1.75	0.68
1:BBB:9:LEU:HD21	1:BBB:198:LEU:HD11	1.74	0.68
2:CCC:93:SER:OG	2:CCC:126:GLU:OE1	2.11	0.68
2:CCC:342:ASP:O	2:CCC:437:ASN:CG	2.31	0.68
2:CCC:244:GLU:HG2	2:CCC:245:ARG:N	2.08	0.68
1:AAA:37:HIS:NE2	1:AAA:187:VAL:HG21	2.09	0.68
3:DDD:519:ASN:OD1	3:DDD:520:ALA:N	2.22	0.68
3:DDD:1343:GLU:OE1	3:DDD:1345:ARG:NH2	2.19	0.68
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.26	0.68
3:DDD:943:ARG:NH1	3:DDD:1128:SER:O	2.27	0.68
1:BBB:30:PRO:HB2	1:BBB:198:LEU:HD12	1.76	0.68
2:CCC:648:ASP:OD1	2:CCC:648:ASP:N	2.25	0.68
5:FFF:192:GLU:HG3	5:FFF:193:PRO:HD2	1.76	0.68
1:BBB:37:HIS:NE2	1:BBB:187:VAL:HG21	2.09	0.67
1:BBB:83:LEU:HD11	3:DDD:526:VAL:C	2.15	0.67
1:BBB:44:ARG:NH1	3:DDD:538:ARG:CD	2.57	0.67
3:DDD:343:LEU:HD11	3:DDD:1324:SER:HB2	1.75	0.67
3:DDD:510:LEU:HD11	3:DDD:624:ILE:HG23	1.74	0.67
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:CD1	2.24	0.67
3:DDD:895:CYS:SG	3:DDD:898:CYS:CB	2.83	0.67
2:CCC:184:LEU:HG	2:CCC:389:PHE:CE2	2.30	0.67
2:CCC:746:ALA:HB2	2:CCC:971:LEU:HD13	1.77	0.67
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	1.95	0.67
2:CCC:870:ILE:CG1	2:CCC:944:ARG:HG2	2.24	0.66
2:CCC:123:TYR:HB3	5:FFF:187:HIS:HA	1.76	0.66
1:AAA:12:ARG:HA	1:BBB:230:ALA:HB1	1.76	0.66
2:CCC:223:LEU:HD13	2:CCC:426:ILE:HD13	1.77	0.66
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	1.78	0.66
3:DDD:707:ILE:HD12	3:DDD:716:GLN:HE21	1.61	0.66
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:CE	2.26	0.66
3:DDD:1275:LEU:HG	3:DDD:1276:GLU:H	1.61	0.66
5:FFF:170:HIS:CG	6:111:31:DT:H73	2.30	0.66
1:AAA:75:GLN:O	2:CCC:729:ALA:HB2	1.96	0.66
2:CCC:1077:SER:HA	3:DDD:356:THR:HG23	1.77	0.66
9:CCC:1401:UTP:O4'	8:333:101:DOC:C2'	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:59:VAL:HG22	1:AAA:144:ILE:HG23	1.78	0.66
1:AAA:179:PRO:HG3	1:AAA:211:ILE:CD1	2.26	0.66
1:BBB:196:THR:HG21	3:DDD:370:LYS:NZ	2.09	0.66
2:CCC:12:ARG:NH2	2:CCC:793:GLU:OE1	2.28	0.65
9:CCC:1401:UTP:O3'	3:DDD:458:ASN:ND2	2.29	0.65
3:DDD:1157:ALA:O	3:DDD:1207:GLY:N	2.28	0.65
5:FFF:98:ASN:HA	6:111:41:DT:O2	1.97	0.65
3:DDD:839:VAL:HG12	3:DDD:864:LEU:CD1	2.26	0.65
2:CCC:1129:ASN:HA	2:CCC:1177:ARG:HG3	1.78	0.65
1:BBB:83:LEU:CD1	3:DDD:526:VAL:HB	2.27	0.65
3:DDD:792:ASN:N	3:DDD:792:ASN:OD1	2.27	0.65
3:DDD:320:ASN:O	3:DDD:321:LYS:HB2	1.97	0.65
3:DDD:835:LEU:HD13	3:DDD:878:ASP:O	1.96	0.65
6:111:31:DT:H1'	6:111:32:DA:H5'	1.76	0.65
2:CCC:856:ASN:OD1	5:FFF:329:LEU:O	2.15	0.65
6:111:50:DT:H2''	6:111:51:DC:H5''	1.79	0.65
2:CCC:663:VAL:O	2:CCC:666:SER:OG	2.14	0.64
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.79	0.64
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.29	0.64
1:BBB:47:LEU:HD13	1:BBB:205:MET:HE2	1.79	0.64
2:CCC:19:PRO:HA	2:CCC:1156:ARG:HD2	1.79	0.64
2:CCC:1339:LEU:HD23	3:DDD:20:ILE:HG23	1.80	0.64
3:DDD:1134:ILE:HG23	3:DDD:1138:LEU:HG	1.78	0.64
1:BBB:163:GLU:O	1:BBB:163:GLU:HG3	1.95	0.64
3:DDD:886:VAL:HG21	3:DDD:1230:THR:HG21	1.78	0.64
3:DDD:807:LEU:CD2	3:DDD:1255:VAL:HG13	2.27	0.64
3:DDD:839:VAL:CG1	3:DDD:864:LEU:CD1	2.76	0.64
3:DDD:320:ASN:O	3:DDD:321:LYS:CB	2.46	0.64
2:CCC:43:PRO:O	2:CCC:54:ARG:NH1	2.31	0.64
2:CCC:748:ILE:HD11	2:CCC:970:GLY:CA	2.25	0.64
2:CCC:736:VAL:O	2:CCC:741:MET:HE3	1.98	0.64
2:CCC:1269:ARG:NE	7:222:13:DA:OP1	2.30	0.64
5:FFF:170:HIS:CD2	6:111:31:DT:H73	2.32	0.63
3:DDD:1003:LEU:HD23	3:DDD:1018:ALA:HB2	1.79	0.63
3:DDD:1134:ILE:HD11	3:DDD:1244:GLN:HG3	1.80	0.63
1:AAA:211:ILE:CG2	1:AAA:216:ALA:HB2	2.28	0.63
1:BBB:159:ILE:HG12	1:BBB:159:ILE:O	1.98	0.63
2:CCC:452:ARG:NH1	2:CCC:458:GLU:OE2	2.28	0.63
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.13	0.63
3:DDD:975:ILE:HD12	3:DDD:997:VAL:HG11	1.80	0.63
2:CCC:241:LEU:HD13	2:CCC:285:ILE:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:519:ASN:HA	3:DDD:523:GLU:CD	2.19	0.63
1:BBB:50:SER:HA	1:BBB:150:ARG:HD2	1.78	0.63
2:CCC:32:LEU:HD23	2:CCC:130:MET:CE	2.29	0.63
2:CCC:292:ILE:CG2	2:CCC:322:LEU:HD11	2.29	0.63
2:CCC:1245:ALA:HB2	3:DDD:372:MET:HG3	1.79	0.63
3:DDD:362:ARG:N	3:DDD:365:GLN:OE1	2.23	0.63
3:DDD:1023:HIS:O	3:DDD:1024:THR:HB	1.97	0.63
5:FFF:143:SER:HB3	6:111:41:DT:H73	1.80	0.63
5:FFF:227:GLY:O	5:FFF:229:ASP:N	2.32	0.63
7:222:17:DG:H2'	7:222:18:DT:C6	2.33	0.63
3:DDD:97:VAL:HG12	3:DDD:101:ARG:HG3	1.81	0.63
2:CCC:263:VAL:HG13	2:CCC:269:ILE:HD11	1.81	0.63
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:CG2	2.29	0.63
2:CCC:157:PHE:O	2:CCC:442:VAL:HG13	1.98	0.62
2:CCC:302:ILE:HG22	2:CCC:309:LEU:HD23	1.80	0.62
2:CCC:548:ARG:HD3	2:CCC:569:ILE:O	1.99	0.62
2:CCC:524:ILE:O	2:CCC:528:ARG:HG2	1.99	0.62
2:CCC:1196:LYS:NZ	3:DDD:642:ASP:OD2	2.33	0.62
2:CCC:734:ILE:CG2	2:CCC:749:ASP:HB2	2.29	0.62
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.29	0.62
1:AAA:30:PRO:HB2	1:AAA:198:LEU:HD12	1.81	0.62
2:CCC:414:ILE:HG13	2:CCC:415:GLU:N	2.14	0.62
3:DDD:395:LYS:HE2	5:FFF:329:LEU:HD13	1.82	0.62
1:BBB:83:LEU:CG	3:DDD:526:VAL:HB	2.29	0.62
2:CCC:672:GLU:HG2	2:CCC:1187:PHE:HA	1.82	0.62
3:DDD:1134:ILE:CD1	3:DDD:1244:GLN:HG3	2.29	0.62
2:CCC:1304:MET:CE	3:DDD:472:LEU:HD13	2.29	0.62
1:BBB:83:LEU:CG	3:DDD:526:VAL:CB	2.78	0.62
2:CCC:297:VAL:HG13	2:CCC:317:LEU:HG	1.82	0.62
2:CCC:541:GLU:HG3	2:CCC:542:ARG:N	2.15	0.62
4:EEE:8:ASP:N	4:EEE:8:ASP:OD1	2.31	0.62
2:CCC:49:LEU:CD2	2:CCC:464:PHE:CE2	2.83	0.62
3:DDD:1282:TYR:CE1	3:DDD:1286:LYS:HD2	2.35	0.62
1:BBB:58:GLU:OE1	1:BBB:170:ARG:NE	2.31	0.61
9:CCC:1401:UTP:O4'	8:333:101:DOC:C3'	2.48	0.61
1:BBB:157:THR:HG22	1:BBB:157:THR:O	1.99	0.61
2:CCC:389:PHE:HB3	2:CCC:420:LEU:HD12	1.82	0.61
1:BBB:193:GLU:O	1:BBB:194:GLN:CB	2.48	0.61
3:DDD:114:ILE:HG12	3:DDD:311:ARG:HD2	1.81	0.61
2:CCC:1337:ILE:O	2:CCC:1337:ILE:HG23	2.01	0.61
3:DDD:58:CYS:SG	3:DDD:60:ARG:HB3	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:CD1	2.29	0.61
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.30	0.61
1:AAA:218:ARG:HD3	1:BBB:232:VAL:HG21	1.82	0.61
2:CCC:577:VAL:HG23	2:CCC:661:VAL:O	1.99	0.61
1:BBB:135:ASP:OD1	1:BBB:138:ALA:HB2	2.01	0.61
2:CCC:263:VAL:CG1	2:CCC:269:ILE:HD11	2.31	0.61
3:DDD:1338:ALA:HB3	3:DDD:1340:LYS:HG3	1.82	0.61
2:CCC:559:CYS:HB2	2:CCC:662:SER:HB3	1.83	0.61
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.83	0.61
5:FFF:144:THR:CG2	6:111:39:DA:H8	2.08	0.61
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE2	1.81	0.61
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.83	0.61
5:FFF:66:GLY:HA3	6:111:42:DG:C5	2.36	0.61
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HD12	1.82	0.61
2:CCC:1281:TYR:OH	3:DDD:431:ARG:O	2.19	0.61
3:DDD:707:ILE:HD12	3:DDD:716:GLN:NE2	2.16	0.61
3:DDD:1156:LEU:HD22	3:DDD:1224:ARG:NH2	2.16	0.61
3:DDD:1156:LEU:HD21	3:DDD:1209:VAL:HG22	1.82	0.61
5:FFF:61:TYR:CZ	5:FFF:65:ILE:HD11	2.36	0.61
3:DDD:609:TYR:HA	3:DDD:617:THR:HG21	1.83	0.60
2:CCC:244:GLU:HG2	2:CCC:245:ARG:H	1.66	0.60
2:CCC:516:ASP:O	2:CCC:522:SER:OG	2.17	0.60
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:H	2.04	0.60
2:CCC:1340:GLU:OE1	3:DDD:1341:ARG:NE	2.34	0.60
3:DDD:245:LEU:HD12	3:DDD:246:PRO:HD2	1.83	0.60
3:DDD:1000:GLY:HA2	3:DDD:1028:ILE:HD12	1.82	0.60
2:CCC:262:TYR:OH	2:CCC:280:ASP:OD2	2.18	0.60
3:DDD:97:VAL:HG11	3:DDD:101:ARG:HE	1.66	0.60
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HG	2.31	0.60
5:FFF:234:LEU:HD13	7:222:19:DA:H61	1.66	0.60
3:DDD:16:GLU:OE2	3:DDD:1369:ARG:NH2	2.35	0.60
3:DDD:514:THR:OG1	3:DDD:595:ALA:HA	2.01	0.60
3:DDD:839:VAL:CG1	3:DDD:864:LEU:HD12	2.31	0.60
2:CCC:3:TYR:O	2:CCC:8:LYS:CE	2.49	0.60
5:FFF:244:ASN:N	5:FFF:244:ASN:OD1	2.34	0.60
3:DDD:139:LEU:HD22	3:DDD:300:GLN:HE22	1.66	0.60
2:CCC:340:ASP:HB3	2:CCC:341:LEU:HG	1.83	0.60
3:DDD:803:VAL:CG2	3:DDD:1313:SER:OG	2.50	0.60
4:EEE:53:GLU:HB3	4:EEE:59:ILE:HG12	1.84	0.59
1:BBB:83:LEU:CD1	3:DDD:526:VAL:CB	2.81	0.59
2:CCC:183:TRP:CZ3	6:111:51:DC:C2'	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:929:GLN:O	3:DDD:933:ARG:HB2	2.02	0.59
3:DDD:709:ARG:CG	3:DDD:709:ARG:O	2.50	0.59
2:CCC:736:VAL:HB	2:CCC:741:MET:HE2	1.84	0.59
2:CCC:1257:GLN:NE2	3:DDD:341:ASN:O	2.35	0.59
2:CCC:1272:GLU:OE1	3:DDD:339:ARG:HD3	2.02	0.59
3:DDD:609:TYR:HA	3:DDD:617:THR:CG2	2.32	0.59
3:DDD:1158:GLU:OE2	3:DDD:1223:LEU:HD21	2.03	0.59
2:CCC:582:ASN:OD1	2:CCC:586:PHE:N	2.34	0.59
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD21	1.85	0.59
2:CCC:1214:ASP:OD2	2:CCC:1217:THR:HG23	2.03	0.59
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CD2	2.38	0.59
3:DDD:816:THR:HG22	3:DDD:818:GLU:N	2.15	0.59
2:CCC:183:TRP:CH2	6:111:51:DC:H2'	2.37	0.59
2:CCC:734:ILE:HD11	2:CCC:777:VAL:HG23	1.85	0.59
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	1.85	0.59
4:EEE:30:MET:HG2	4:EEE:35:LYS:O	2.02	0.59
5:FFF:82:ARG:HG2	5:FFF:87:ASP:HB2	1.84	0.59
9:CCC:1401:UTP:C4'	3:DDD:425:ARG:NH2	2.53	0.59
4:EEE:29:GLN:HE22	4:EEE:64:LEU:HD22	1.68	0.59
1:AAA:66:HIS:CE1	2:CCC:929:ILE:HG13	2.38	0.58
5:FFF:61:TYR:CE2	5:FFF:65:ILE:HD11	2.38	0.58
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.33	0.58
2:CCC:150:HIS:CE1	2:CCC:454:ARG:HG3	2.38	0.58
5:FFF:122:GLU:HG2	5:FFF:157:ALA:HB2	1.84	0.58
5:FFF:218:ARG:HB2	7:222:23:DT:H72	1.84	0.58
1:AAA:145:LYS:HD3	1:AAA:147:GLN:HE21	1.67	0.58
1:AAA:211:ILE:HG21	1:AAA:216:ALA:HB2	1.85	0.58
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.86	0.58
3:DDD:121:PRO:O	3:DDD:122:SER:CB	2.52	0.58
3:DDD:334:LYS:O	3:DDD:339:ARG:HB2	2.04	0.58
1:AAA:22:THR:OG1	1:AAA:207:THR:O	2.17	0.58
1:AAA:66:HIS:CD2	2:CCC:874:GLY:HA2	2.39	0.58
1:BBB:47:LEU:HD13	1:BBB:205:MET:CE	2.33	0.58
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE1	1.85	0.58
5:FFF:170:HIS:CE1	6:111:31:DT:C5	2.91	0.58
2:CCC:1291:LEU:HA	3:DDD:345:LYS:HD2	1.85	0.58
3:DDD:22:ILE:CD1	3:DDD:1319:PHE:CE1	2.85	0.58
5:FFF:168:PRO:HG3	6:111:31:DT:OP2	2.04	0.58
2:CCC:1270:PHE:CE1	2:CCC:1290:MET:CE	2.87	0.58
3:DDD:334:LYS:NZ	7:222:12:DG:OP2	2.21	0.58
3:DDD:974:VAL:HG11	3:DDD:1028:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:227:GLY:CA	7:222:17:DG:H22	1.97	0.58
5:FFF:267:ASN:HB2	5:FFF:270:GLN:HB2	1.86	0.58
1:AAA:66:HIS:HD2	2:CCC:874:GLY:HA2	1.68	0.58
2:CCC:1286:THR:HG23	3:DDD:476:ALA:HB1	1.85	0.58
3:DDD:68:TYR:CD2	3:DDD:78:LEU:HD23	2.39	0.58
3:DDD:797:THR:O	3:DDD:801:VAL:HG23	2.04	0.58
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	1.85	0.58
2:CCC:36:GLN:O	2:CCC:40:GLU:HB2	2.04	0.58
2:CCC:1304:MET:HE1	3:DDD:472:LEU:HD13	1.85	0.58
3:DDD:673:VAL:HG11	3:DDD:678:ARG:HB2	1.83	0.58
2:CCC:144:VAL:HB	2:CCC:526:HIS:CE1	2.39	0.57
2:CCC:342:ASP:O	2:CCC:437:ASN:ND2	2.37	0.57
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	2.04	0.57
3:DDD:1161:GLY:HA3	3:DDD:1179:PRO:HA	1.85	0.57
2:CCC:292:ILE:HB	2:CCC:322:LEU:HD11	1.86	0.57
2:CCC:528:ARG:HD2	2:CCC:663:VAL:HG21	1.86	0.57
2:CCC:901:LEU:CD1	5:FFF:310:LEU:HD21	2.34	0.57
5:FFF:58:THR:OG1	5:FFF:117:LEU:HG	2.03	0.57
1:AAA:135:ASP:OD1	1:AAA:136:GLU:N	2.37	0.57
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.38	0.57
3:DDD:525:MET:H	3:DDD:548:VAL:HG22	1.69	0.57
3:DDD:43:THR:OG1	3:DDD:44:ILE:N	2.37	0.57
2:CCC:369:MET:HG3	2:CCC:370:MET:N	2.19	0.57
3:DDD:1110:GLU:O	3:DDD:1113:VAL:HG23	2.04	0.57
5:FFF:107:ARG:HD2	6:111:43:DT:H3'	1.84	0.57
5:FFF:168:PRO:CB	6:111:31:DT:OP2	2.53	0.57
2:CCC:1101:LEU:HD22	3:DDD:731:ARG:HB2	1.85	0.57
3:DDD:385:LEU:CD2	3:DDD:411:ILE:HD13	2.34	0.57
2:CCC:447:HIS:CD2	2:CCC:449:GLY:H	2.23	0.57
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG23	1.85	0.57
1:AAA:47:LEU:O	1:AAA:180:VAL:HG21	2.05	0.57
2:CCC:1243:MET:SD	3:DDD:445:LYS:HG2	2.45	0.57
3:DDD:176:PHE:O	3:DDD:176:PHE:CD2	2.58	0.57
2:CCC:743:PRO:HA	2:CCC:974:ARG:NH2	2.20	0.57
3:DDD:620:PHE:O	3:DDD:624:ILE:HG13	2.05	0.57
3:DDD:812:ASP:OD1	3:DDD:812:ASP:N	2.37	0.57
3:DDD:923:ILE:HD12	3:DDD:1256:ILE:HD12	1.87	0.57
3:DDD:709:ARG:O	3:DDD:710:ASP:C	2.43	0.57
3:DDD:1309:ILE:HG22	3:DDD:1310:THR:N	2.20	0.57
3:DDD:367:GLY:HA3	3:DDD:448:GLN:HB2	1.85	0.56
5:FFF:298:THR:HG21	5:FFF:301:ARG:HD3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.87	0.56
2:CCC:582:ASN:ND2	2:CCC:586:PHE:HB2	2.20	0.56
3:DDD:279:LEU:HD13	3:DDD:295:GLU:HB3	1.86	0.56
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.35	0.56
5:FFF:119:LEU:CD2	5:FFF:158:ILE:HD11	2.34	0.56
2:CCC:118:LYS:HD3	2:CCC:488:MET:HG2	1.86	0.56
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CD2	2.40	0.56
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:CD	2.35	0.56
1:AAA:82:LEU:HD22	1:AAA:173:VAL:CG2	2.35	0.56
1:BBB:83:LEU:HD11	3:DDD:526:VAL:CG1	2.34	0.56
2:CCC:666:SER:HA	2:CCC:1186:VAL:HG21	1.88	0.56
2:CCC:289:VAL:HG12	2:CCC:319:LEU:HD23	1.87	0.56
3:DDD:935:PHE:HZ	3:DDD:1135:THR:HG1	1.52	0.56
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG22	1.86	0.56
2:CCC:302:ILE:CG2	2:CCC:309:LEU:HD23	2.35	0.56
2:CCC:739:ASP:OD1	2:CCC:739:ASP:N	2.39	0.56
3:DDD:68:TYR:C	3:DDD:92:VAL:HG13	2.27	0.56
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.88	0.56
2:CCC:677:ASN:OD1	3:DDD:779:ALA:HB1	2.05	0.56
3:DDD:686:TRP:CD2	3:DDD:758:PRO:HG3	2.40	0.56
2:CCC:1296:ASP:OD2	2:CCC:1322:SER:OG	2.18	0.56
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.05	0.56
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:HE3	1.88	0.56
5:FFF:259:ILE:CG2	5:FFF:280:LEU:HD21	2.36	0.56
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CZ	2.41	0.55
2:CCC:277:LEU:HD12	2:CCC:282:VAL:HG21	1.89	0.55
2:CCC:870:ILE:CG2	2:CCC:944:ARG:HE	2.19	0.55
2:CCC:1312:ASN:OD1	2:CCC:1312:ASN:O	2.23	0.55
3:DDD:385:LEU:HD23	3:DDD:411:ILE:HD13	1.86	0.55
3:DDD:800:LEU:CD2	3:DDD:1309:ILE:HD11	2.36	0.55
3:DDD:1163:VAL:HG13	3:DDD:1176:VAL:O	2.05	0.55
2:CCC:599:VAL:HG21	2:CCC:623:LEU:HD21	1.88	0.55
5:FFF:93:ARG:O	5:FFF:97:SER:OG	2.17	0.55
5:FFF:271:ARG:O	5:FFF:271:ARG:HG2	2.04	0.55
1:AAA:47:LEU:HA	1:AAA:51:MET:HG2	1.88	0.55
2:CCC:870:ILE:HG21	2:CCC:944:ARG:HE	1.71	0.55
1:AAA:225:ALA:HB2	1:BBB:228:LEU:HD13	1.87	0.55
2:CCC:369:MET:CG	2:CCC:370:MET:N	2.69	0.55
2:CCC:1276:TRP:CH2	3:DDD:798:ARG:HG3	2.42	0.55
5:FFF:102:VAL:HG11	5:FFF:124:ASN:OD1	2.07	0.55
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:843:VAL:HG23	3:DDD:897:HIS:O	2.06	0.55
5:FFF:277:ARG:CD	5:FFF:306:GLN:HE21	2.20	0.55
2:CCC:240:GLU:HA	2:CCC:283:LYS:O	2.07	0.55
2:CCC:253:PHE:CE1	2:CCC:287:VAL:HG12	2.42	0.55
3:DDD:530:PRO:HD3	3:DDD:552:ILE:HD13	1.88	0.55
3:DDD:886:VAL:HG21	3:DDD:1230:THR:CG2	2.37	0.55
5:FFF:182:ALA:CB	5:FFF:193:PRO:HG3	2.36	0.55
2:CCC:549:ASP:OD2	3:DDD:750:PRO:CG	2.55	0.55
3:DDD:335:GLN:O	3:DDD:336:GLY:O	2.24	0.55
3:DDD:622:ASP:HB3	3:DDD:626:TYR:HE2	1.71	0.55
3:DDD:1330:ARG:NH2	7:222:8:DG:P	2.79	0.55
3:DDD:97:VAL:HG11	3:DDD:101:ARG:NE	2.22	0.55
5:FFF:163:ARG:NH2	7:222:26:DT:O4	2.31	0.55
7:222:17:DG:H2''	7:222:18:DT:O4'	2.05	0.55
1:BBB:44:ARG:HH12	3:DDD:538:ARG:CB	2.20	0.54
2:CCC:685:MET:HE2	2:CCC:1235:LEU:HD11	1.88	0.54
2:CCC:1107:MET:HE3	3:DDD:739:GLN:HB2	1.87	0.54
1:BBB:145:LYS:HD3	1:BBB:147:GLN:HE21	1.73	0.54
2:CCC:720:ARG:HD2	2:CCC:736:VAL:HG21	1.89	0.54
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:N	2.61	0.54
1:AAA:209:GLY:O	1:AAA:210:THR:C	2.45	0.54
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD11	1.89	0.54
2:CCC:521:LEU:HD13	2:CCC:667:LEU:HD11	1.88	0.54
3:DDD:965:SER:CB	3:DDD:975:ILE:HA	2.37	0.54
5:FFF:80:ALA:O	5:FFF:84:LEU:HG	2.07	0.54
2:CCC:993:PRO:HG2	2:CCC:996:ARG:CZ	2.37	0.54
3:DDD:609:TYR:CA	3:DDD:617:THR:HG21	2.36	0.54
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.89	0.54
3:DDD:795:TYR:CZ	3:DDD:799:ARG:HD3	2.42	0.54
2:CCC:13:LYS:NZ	2:CCC:1151:LEU:HB3	2.23	0.54
2:CCC:369:MET:HG2	2:CCC:370:MET:HG2	1.90	0.54
2:CCC:808:ASN:HD22	2:CCC:808:ASN:N	2.04	0.54
3:DDD:295:GLU:OE1	5:FFF:121:GLU:HG2	2.08	0.54
3:DDD:807:LEU:HD23	3:DDD:1255:VAL:HG13	1.90	0.54
3:DDD:974:VAL:CG1	3:DDD:1028:ILE:HD13	2.37	0.54
3:DDD:1042:ASP:OD1	3:DDD:1043:GLY:N	2.40	0.54
5:FFF:158:ILE:HG22	7:222:26:DT:O2	2.08	0.54
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG21	1.89	0.54
2:CCC:642:SER:CB	3:DDD:770:LEU:HD21	2.38	0.54
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.37	0.54
5:FFF:135:ASP:CB	6:111:37:DA:N1	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:CD1	2.37	0.54
3:DDD:111:THR:HG21	3:DDD:303:VAL:HG11	1.88	0.54
1:BBB:30:PRO:HB2	1:BBB:198:LEU:CD1	2.38	0.53
3:DDD:803:VAL:HG23	3:DDD:1313:SER:OG	2.08	0.53
5:FFF:122:GLU:HG2	5:FFF:157:ALA:CB	2.38	0.53
2:CCC:1001:GLY:HA2	2:CCC:1011:LEU:CD2	2.38	0.53
3:DDD:395:LYS:CE	5:FFF:329:LEU:HD13	2.38	0.53
3:DDD:791:ALA:HA	7:222:11:DA:C8	2.43	0.53
3:DDD:950:ILE:HD13	3:DDD:995:TYR:HB3	1.90	0.53
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	2.07	0.53
1:BBB:212:ASP:OD1	1:BBB:213:PRO:HD2	2.08	0.53
3:DDD:1314:LEU:HD11	3:DDD:1327:GLU:CD	2.28	0.53
1:AAA:135:ASP:OD1	1:AAA:137:ASN:N	2.39	0.53
3:DDD:151:MET:SD	3:DDD:151:MET:N	2.81	0.53
5:FFF:53:ARG:O	5:FFF:55:LEU:HG	2.07	0.53
2:CCC:1186:VAL:HG12	2:CCC:1187:PHE:CD2	2.43	0.53
2:CCC:1251:TYR:HE2	5:FFF:246:PRO:CD	2.22	0.53
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HG3	2.39	0.53
3:DDD:1064:SER:HA	3:DDD:1067:ARG:HB3	1.91	0.53
4:EEE:18:ASP:O	4:EEE:22:VAL:HG23	2.09	0.53
1:AAA:235:ARG:HB3	1:BBB:13:LEU:HD23	1.90	0.53
2:CCC:734:ILE:HD11	2:CCC:777:VAL:CG2	2.39	0.53
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD13	1.90	0.53
3:DDD:888:CYS:CB	3:DDD:898:CYS:SG	2.97	0.53
3:DDD:1157:ALA:HB3	3:DDD:1208:ASP:H	1.74	0.53
5:FFF:163:ARG:NH2	7:222:25:DA:N6	2.57	0.53
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.89	0.53
3:DDD:464:ASP:OD1	3:DDD:464:ASP:N	2.42	0.53
1:AAA:50:SER:O	1:AAA:150:ARG:HD2	2.08	0.53
3:DDD:476:ALA:HA	3:DDD:479:GLU:HG3	1.90	0.53
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.91	0.53
3:DDD:936:HIS:CE1	3:DDD:937:ILE:HG13	2.44	0.53
3:DDD:1146:GLU:OE2	3:DDD:1309:ILE:CG2	2.57	0.53
3:DDD:63:GLY:O	3:DDD:98:ARG:HD2	2.09	0.53
5:FFF:169:ILE:O	5:FFF:173:LYS:HG2	2.09	0.53
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.91	0.52
1:BBB:83:LEU:CD2	3:DDD:526:VAL:CB	2.81	0.52
2:CCC:89:GLY:HA2	2:CCC:140:GLY:HA3	1.92	0.52
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.90	0.52
2:CCC:1160:ASP:O	2:CCC:1161:LEU:C	2.47	0.52
5:FFF:78:TYR:OH	5:FFF:82:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:218:ARG:NE	7:222:24:DT:O4	2.42	0.52
1:AAA:102:LEU:HB2	1:AAA:115:ILE:HG12	1.91	0.52
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CE2	2.44	0.52
2:CCC:549:ASP:OD2	3:DDD:750:PRO:HG3	2.09	0.52
9:CCC:1401:UTP:C1'	8:333:101:DOC:H2'	2.39	0.52
2:CCC:477:GLU:HG3	2:CCC:478:ARG:N	2.24	0.52
2:CCC:898:GLU:OE2	5:FFF:280:LEU:CD1	2.57	0.52
2:CCC:1257:GLN:HE22	3:DDD:341:ASN:CA	2.21	0.52
3:DDD:209:ASN:HB2	3:DDD:214:ARG:HG3	1.91	0.52
3:DDD:518:VAL:HG23	3:DDD:716:GLN:OE1	2.09	0.52
3:DDD:709:ARG:O	3:DDD:709:ARG:HG3	2.10	0.52
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CG2	2.39	0.52
2:CCC:183:TRP:CH2	6:111:52:DT:H72	2.45	0.52
2:CCC:700:VAL:HG13	2:CCC:1117:LEU:HD23	1.91	0.52
2:CCC:847:PRO:HB3	2:CCC:1047:LEU:HD11	1.90	0.52
3:DDD:395:LYS:HE2	5:FFF:329:LEU:HD22	1.91	0.52
1:AAA:31:LEU:CD1	1:AAA:201:LEU:HB2	2.39	0.52
2:CCC:521:LEU:HD13	2:CCC:667:LEU:CD1	2.40	0.52
2:CCC:1223:ARG:HD3	3:DDD:637:ALA:HA	1.90	0.52
3:DDD:97:VAL:CG1	3:DDD:101:ARG:NE	2.73	0.52
1:BBB:47:LEU:HA	1:BBB:51:MET:HG2	1.91	0.52
3:DDD:574:VAL:O	3:DDD:578:ILE:HG13	2.10	0.52
3:DDD:750:PRO:O	3:DDD:781:LYS:HE3	2.10	0.52
3:DDD:1249:ASN:OD1	3:DDD:1250:ASP:N	2.42	0.52
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD11	1.90	0.52
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.92	0.52
2:CCC:555:TYR:CE1	2:CCC:637:ARG:CZ	2.93	0.52
2:CCC:804:PHE:O	3:DDD:638:SER:CB	2.55	0.52
2:CCC:820:GLU:O	2:CCC:824:GLN:HG3	2.10	0.52
2:CCC:1099:ASN:OD1	2:CCC:1100:PRO:HD2	2.10	0.52
2:CCC:1251:TYR:HE2	5:FFF:246:PRO:HD3	1.75	0.52
3:DDD:427:PRO:HG2	3:DDD:429:LEU:HD21	1.92	0.52
3:DDD:1163:VAL:HG11	3:DDD:1175:LEU:HD11	1.91	0.52
1:AAA:74:VAL:O	2:CCC:729:ALA:CB	2.58	0.51
1:BBB:41:ASN:ND2	2:CCC:1217:THR:HA	2.25	0.51
3:DDD:101:ARG:O	3:DDD:246:PRO:HG3	2.09	0.51
2:CCC:1161:LEU:O	2:CCC:1163:THR:N	2.43	0.51
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HE	2.23	0.51
3:DDD:278:ARG:HB3	3:DDD:295:GLU:OE2	2.10	0.51
3:DDD:1079:LYS:HE3	3:DDD:1087:ASP:OD1	2.09	0.51
5:FFF:159:MET:HG2	7:222:26:DT:N3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.75	0.51
2:CCC:797:GLY:O	2:CCC:1231:TYR:OH	2.29	0.51
3:DDD:519:ASN:HA	3:DDD:523:GLU:OE2	2.10	0.51
3:DDD:1330:ARG:NH2	7:222:8:DG:OP1	2.44	0.51
5:FFF:180:ARG:HH22	7:222:27:DA:H5''	1.74	0.51
1:BBB:64:VAL:HG13	1:BBB:78:ILE:HD13	1.92	0.51
1:BBB:102:LEU:HB2	1:BBB:115:ILE:HG12	1.92	0.51
2:CCC:1291:LEU:HD22	3:DDD:345:LYS:HE3	1.93	0.51
3:DDD:614:LEU:HG	4:EEE:5:THR:HG21	1.91	0.51
3:DDD:1324:SER:OG	3:DDD:1348:LYS:HD3	2.11	0.51
5:FFF:180:ARG:NH2	7:222:27:DA:H5''	2.25	0.51
2:CCC:297:VAL:HG22	2:CCC:315:MET:O	2.11	0.51
2:CCC:661:VAL:HG13	2:CCC:665:ALA:HB3	1.91	0.51
9:CCC:1401:UTP:C5'	8:333:101:DOC:H3'2	2.37	0.51
3:DDD:1292:LEU:O	3:DDD:1296:GLY:N	2.37	0.51
1:AAA:25:LYS:HG2	1:AAA:204:GLU:HG2	1.92	0.51
1:BBB:192:VAL:O	1:BBB:194:GLN:N	2.44	0.51
2:CCC:799:ASN:C	2:CCC:800:MET:HG2	2.30	0.51
3:DDD:112:ALA:H	3:DDD:300:GLN:HE21	1.59	0.51
3:DDD:836:ARG:NH1	3:DDD:873:GLU:OE1	2.43	0.51
3:DDD:1270:GLY:HA2	3:DDD:1298:VAL:O	2.11	0.51
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HG13	1.92	0.51
1:BBB:83:LEU:HD11	3:DDD:526:VAL:HG12	1.91	0.51
2:CCC:66:SER:HB2	2:CCC:479:LEU:HD22	1.93	0.51
2:CCC:1274:GLU:HG2	3:DDD:424:ASN:ND2	2.26	0.51
3:DDD:1308:GLY:O	3:DDD:1310:THR:N	2.44	0.51
5:FFF:168:PRO:CG	6:111:31:DT:OP2	2.59	0.51
2:CCC:551:HIS:H	2:CCC:554:HIS:CE1	2.28	0.50
2:CCC:868:SER:OG	2:CCC:944:ARG:HB2	2.06	0.50
3:DDD:421:VAL:CG1	3:DDD:468:VAL:HG13	2.41	0.50
2:CCC:263:VAL:HG22	2:CCC:269:ILE:HD12	1.91	0.50
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD13	1.92	0.50
3:DDD:1368:ASP:O	3:DDD:1371:ARG:HG2	2.11	0.50
1:BBB:152:TYR:CZ	3:DDD:536:LEU:HD21	2.47	0.50
2:CCC:49:LEU:HD22	2:CCC:464:PHE:CE2	2.46	0.50
3:DDD:279:LEU:O	3:DDD:283:LEU:HG	2.10	0.50
7:222:22:DA:OP1	7:222:22:DA:H3'	2.11	0.50
1:BBB:48:LEU:CD2	3:DDD:535:ARG:HG3	2.30	0.50
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG21	1.94	0.50
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.45	0.50
2:CCC:290:GLU:O	2:CCC:290:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:757:THR:O	2:CCC:833:ILE:HD12	2.11	0.50
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	1.93	0.50
2:CCC:1312:ASN:OD1	2:CCC:1312:ASN:C	2.50	0.50
3:DDD:1238:GLN:O	3:DDD:1242:ARG:HB2	2.11	0.50
5:FFF:109:TYR:CD2	5:FFF:109:TYR:N	2.77	0.50
1:BBB:179:PRO:HG3	1:BBB:211:ILE:CD1	2.32	0.50
2:CCC:409:LEU:HD13	2:CCC:427:ASP:HB3	1.93	0.50
4:EEE:60:ASN:HB3	4:EEE:63:ILE:HD12	1.93	0.50
1:AAA:212:ASP:OD1	1:AAA:213:PRO:HD2	2.11	0.50
2:CCC:155:VAL:CG2	2:CCC:405:PHE:CD2	2.94	0.50
2:CCC:661:VAL:HG12	2:CCC:662:SER:O	2.10	0.50
2:CCC:532:ALA:HB1	2:CCC:538:LEU:HD12	1.94	0.50
2:CCC:870:ILE:HD12	2:CCC:1050:VAL:HG11	1.93	0.50
2:CCC:1283:ALA:HB1	2:CCC:1286:THR:OG1	2.12	0.50
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HD11	2.41	0.50
3:DDD:1082:ASP:OD1	3:DDD:1084:GLN:N	2.45	0.50
3:DDD:1146:GLU:OE2	3:DDD:1309:ILE:HG22	2.11	0.50
1:AAA:231:PHE:CZ	1:BBB:39:LEU:HD13	2.47	0.50
1:BBB:54:CYS:SG	1:BBB:148:ARG:HB2	2.52	0.50
2:CCC:1291:LEU:CD1	3:DDD:1351:VAL:HG13	2.42	0.50
5:FFF:192:GLU:CG	5:FFF:193:PRO:HD2	2.40	0.50
1:AAA:30:PRO:HB2	1:AAA:198:LEU:CD1	2.42	0.49
3:DDD:885:VAL:O	3:DDD:1258:ARG:HD2	2.11	0.49
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CD2	2.47	0.49
2:CCC:87:ILE:HG22	2:CCC:934:PHE:HZ	1.77	0.49
2:CCC:453:ILE:HD11	2:CCC:530:ILE:HD13	1.94	0.49
2:CCC:1117:LEU:HD13	2:CCC:1195:ILE:HG12	1.94	0.49
3:DDD:1041:ILE:CG2	3:DDD:1044:GLN:HG3	2.42	0.49
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	1.94	0.49
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.45	0.49
2:CCC:598:VAL:HG13	2:CCC:627:GLY:HA2	1.95	0.49
2:CCC:1214:ASP:OD1	2:CCC:1214:ASP:C	2.51	0.49
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.41	0.49
3:DDD:115:TRP:CZ2	3:DDD:1329:THR:HG22	2.47	0.49
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.95	0.49
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD21	1.94	0.49
1:BBB:53:GLY:HA3	1:BBB:177:TYR:O	2.12	0.49
2:CCC:871:VAL:CG2	2:CCC:883:LEU:HA	2.42	0.49
3:DDD:333:GLY:O	3:DDD:336:GLY:N	2.37	0.49
3:DDD:555:TYR:O	3:DDD:586:GLY:CA	2.60	0.49
7:222:17:DG:H2'	7:222:18:DT:C1'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.93	0.49
2:CCC:165:HIS:HB3	2:CCC:167:SER:HB3	1.95	0.49
2:CCC:1276:TRP:HH2	3:DDD:798:ARG:HG3	1.77	0.49
3:DDD:1111:ASP:OD1	3:DDD:1112:GLY:N	2.45	0.49
1:AAA:64:VAL:CG1	1:AAA:78:ILE:HD13	2.43	0.49
2:CCC:555:TYR:CD1	2:CCC:637:ARG:CZ	2.96	0.49
2:CCC:1131:MET:HG2	2:CCC:1136:GLN:OE1	2.12	0.49
5:FFF:178:TYR:CE1	5:FFF:209:VAL:HG22	2.48	0.49
5:FFF:327:LEU:C	5:FFF:329:LEU:N	2.66	0.49
2:CCC:277:LEU:CD1	2:CCC:282:VAL:HG21	2.43	0.49
2:CCC:1107:MET:CE	3:DDD:739:GLN:HB2	2.42	0.49
3:DDD:1168:GLU:OE2	3:DDD:1173:ARG:NH1	2.46	0.49
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.27	0.49
1:BBB:33:ARG:NH1	2:CCC:1081:PRO:HB3	2.27	0.49
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	2.13	0.49
2:CCC:478:ARG:NH1	2:CCC:491:ASP:O	2.46	0.49
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	1.94	0.49
3:DDD:622:ASP:HB3	3:DDD:626:TYR:CE2	2.47	0.49
2:CCC:216:THR:HG23	2:CCC:219:GLN:OE1	2.12	0.49
2:CCC:257:ALA:O	2:CCC:258:ASN:HB3	2.13	0.49
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.94	0.49
3:DDD:114:ILE:HG23	3:DDD:115:TRP:N	2.27	0.49
1:AAA:45:ARG:NH1	2:CCC:1216:ARG:HA	2.28	0.49
2:CCC:1280:ALA:HB1	3:DDD:918:ILE:HG12	1.94	0.49
5:FFF:105:ILE:HG21	5:FFF:150:ILE:CG2	2.41	0.49
5:FFF:107:ARG:HD2	6:111:44:DG:OP2	2.12	0.49
2:CCC:839:VAL:HG13	2:CCC:1046:VAL:HG13	1.95	0.48
5:FFF:170:HIS:NE2	6:111:31:DT:C5	2.81	0.48
1:AAA:195:ARG:HD2	1:AAA:198:LEU:HD23	1.94	0.48
2:CCC:866:ASP:CG	2:CCC:944:ARG:HD3	2.31	0.48
3:DDD:108:ALA:HB3	3:DDD:279:LEU:HD23	1.95	0.48
2:CCC:661:VAL:CG1	2:CCC:665:ALA:HB3	2.43	0.48
2:CCC:1083:GLU:H	2:CCC:1083:GLU:CD	2.16	0.48
3:DDD:44:ILE:HG22	3:DDD:51:PRO:HA	1.94	0.48
3:DDD:68:TYR:CE1	3:DDD:93:THR:HA	2.49	0.48
3:DDD:492:SER:HB2	3:DDD:499:ILE:CD1	2.43	0.48
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CG	2.90	0.48
2:CCC:263:VAL:HG12	2:CCC:264:GLU:O	2.13	0.48
3:DDD:500:ILE:HG22	3:DDD:500:ILE:O	2.13	0.48
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:HA	1.95	0.48
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EEE:41:GLU:O	4:EEE:44:ASP:HB2	2.13	0.48
1:AAA:179:PRO:HG3	1:AAA:211:ILE:CG1	2.43	0.48
1:AAA:227:GLN:OE1	1:BBB:11:PRO:CD	2.60	0.48
1:AAA:50:SER:HG	1:BBB:35:PHE:HZ	1.62	0.48
1:BBB:64:VAL:CG1	1:BBB:78:ILE:HD13	2.44	0.48
2:CCC:898:GLU:OE2	5:FFF:280:LEU:HD11	2.14	0.48
2:CCC:1270:PHE:N	3:DDD:345:LYS:O	2.40	0.48
2:CCC:263:VAL:HG22	2:CCC:269:ILE:CD1	2.44	0.48
2:CCC:292:ILE:CB	2:CCC:322:LEU:HD11	2.44	0.48
2:CCC:297:VAL:HG13	2:CCC:317:LEU:CG	2.44	0.48
2:CCC:524:ILE:HD12	2:CCC:708:VAL:HG13	1.95	0.48
2:CCC:1111:GLN:HB2	2:CCC:1230:MET:HE1	1.95	0.48
3:DDD:579:LEU:HB3	3:DDD:592:VAL:HG21	1.96	0.48
1:AAA:190:ALA:O	1:AAA:192:VAL:N	2.47	0.48
2:CCC:660:VAL:HG21	3:DDD:769:VAL:HG12	1.96	0.48
3:DDD:511:TYR:CZ	3:DDD:515:ARG:HD2	2.49	0.48
2:CCC:660:VAL:HG21	3:DDD:769:VAL:CG1	2.44	0.47
2:CCC:800:MET:SD	2:CCC:828:PHE:HE2	2.36	0.47
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.32	0.47
3:DDD:517:CYS:SG	3:DDD:518:VAL:N	2.87	0.47
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HD2	1.61	0.47
1:BBB:182:ARG:HD3	3:DDD:581:MET:HE3	1.96	0.47
2:CCC:84:GLU:OE1	2:CCC:1035:LYS:NZ	2.39	0.47
2:CCC:228:VAL:HG22	2:CCC:245:ARG:NH1	2.29	0.47
2:CCC:1292:THR:CG2	2:CCC:1293:VAL:N	2.76	0.47
3:DDD:1052:GLU:HG2	3:DDD:1053:LEU:H	1.78	0.47
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.29	0.47
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.78	0.47
3:DDD:665:GLN:O	3:DDD:668:PHE:HB3	2.14	0.47
3:DDD:1037:PHE:CZ	3:DDD:1059:LEU:CD1	2.98	0.47
1:AAA:124:VAL:HG21	1:AAA:210:THR:H	1.79	0.47
2:CCC:123:TYR:CD2	5:FFF:186:SER:O	2.67	0.47
3:DDD:377:PHE:O	3:DDD:381:ILE:HG13	2.14	0.47
3:DDD:608:CYS:SG	3:DDD:612:LEU:HD12	2.54	0.47
3:DDD:161:THR:N	3:DDD:164:GLN:HB2	2.30	0.47
3:DDD:822:MET:CE	3:DDD:882:VAL:HG21	2.44	0.47
3:DDD:844:THR:CG2	3:DDD:864:LEU:HD21	2.45	0.47
2:CCC:20:GLN:O	2:CCC:20:GLN:HG3	2.15	0.47
2:CCC:473:ARG:O	2:CCC:477:GLU:HB3	2.14	0.47
2:CCC:734:ILE:HG22	2:CCC:749:ASP:HB2	1.97	0.47
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:115:TRP:O	3:DDD:119:SER:HB3	2.14	0.47
3:DDD:395:LYS:CD	5:FFF:329:LEU:HD13	2.44	0.47
3:DDD:614:LEU:HD23	4:EEE:7:GLN:HB2	1.97	0.47
3:DDD:645:VAL:HG23	3:DDD:645:VAL:O	2.15	0.47
5:FFF:208:ASP:O	5:FFF:212:MET:HG2	2.13	0.47
1:BBB:31:LEU:CD1	1:BBB:201:LEU:HB2	2.45	0.47
1:BBB:41:ASN:HD22	2:CCC:1217:THR:HA	1.79	0.47
1:BBB:83:LEU:HD12	3:DDD:526:VAL:HG12	1.94	0.47
2:CCC:160:ASP:HB3	2:CCC:163:LYS:HD3	1.97	0.47
3:DDD:118:LYS:NZ	3:DDD:136:GLU:OE2	2.47	0.47
3:DDD:334:LYS:HB2	3:DDD:339:ARG:NH1	2.30	0.47
3:DDD:931:THR:O	3:DDD:935:PHE:HD2	1.96	0.47
3:DDD:965:SER:HB2	3:DDD:975:ILE:HA	1.97	0.47
3:DDD:1100:PHE:CD2	3:DDD:1193:TRP:HA	2.50	0.47
4:EEE:8:ASP:HB2	4:EEE:55:GLU:CG	2.45	0.47
2:CCC:550:VAL:HG21	3:DDD:776:THR:CG2	2.45	0.47
3:DDD:197:GLU:OE1	3:DDD:220:ARG:NH2	2.47	0.47
3:DDD:380:PHE:HB3	3:DDD:415:VAL:HG11	1.96	0.47
3:DDD:398:LYS:NZ	5:FFF:251:GLN:HB2	2.30	0.47
3:DDD:584:PRO:HD3	3:DDD:620:PHE:CD1	2.50	0.47
3:DDD:795:TYR:CE2	3:DDD:799:ARG:NE	2.83	0.47
4:EEE:13:ILE:HD12	4:EEE:19:LEU:HA	1.96	0.47
3:DDD:703:THR:O	3:DDD:704:GLU:C	2.53	0.47
3:DDD:925:GLU:HB3	3:DDD:926:PRO:CD	2.45	0.47
5:FFF:175:LEU:O	5:FFF:179:LEU:HG	2.14	0.47
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.45	0.47
1:AAA:135:ASP:OD1	1:AAA:135:ASP:C	2.54	0.47
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG12	1.96	0.47
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.14	0.47
5:FFF:140:PHE:CD1	6:111:38:DT:H5''	2.50	0.47
1:AAA:91:ARG:HG3	1:AAA:210:THR:HA	1.97	0.46
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.96	0.46
1:AAA:211:ILE:HG22	1:AAA:216:ALA:HB2	1.97	0.46
3:DDD:733:SER:H	3:DDD:736:GLN:HG3	1.80	0.46
3:DDD:1186:TYR:CZ	3:DDD:1188:GLU:OE2	2.68	0.46
7:222:25:DA:H2''	7:222:26:DT:H5''	1.97	0.46
2:CCC:155:VAL:HG23	2:CCC:405:PHE:CD2	2.50	0.46
2:CCC:898:GLU:CG	5:FFF:259:ILE:CD1	2.90	0.46
3:DDD:123:ARG:NH2	3:DDD:1334:GLU:HG2	2.30	0.46
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.15	0.46
7:222:15:DT:H2'	7:222:16:DC:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:157:THR:O	1:BBB:157:THR:CG2	2.63	0.46
2:CCC:173:ASN:C	2:CCC:173:ASN:OD1	2.53	0.46
3:DDD:45:ASN:HB2	3:DDD:52:GLU:OE1	2.16	0.46
3:DDD:487:THR:O	3:DDD:490:ILE:HG13	2.16	0.46
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.49	0.46
3:DDD:795:TYR:CE2	3:DDD:799:ARG:CZ	2.98	0.46
2:CCC:53:PHE:HB3	2:CCC:70:TYR:CD2	2.50	0.46
2:CCC:150:HIS:CE1	2:CCC:452:ARG:HD3	2.51	0.46
2:CCC:244:GLU:O	2:CCC:245:ARG:C	2.53	0.46
2:CCC:594:VAL:HG22	2:CCC:599:VAL:HG22	1.96	0.46
2:CCC:838:CYS:SG	2:CCC:886:LYS:HE2	2.56	0.46
3:DDD:305:ALA:CB	3:DDD:316:ILE:HD12	2.45	0.46
3:DDD:805:GLN:HG2	3:DDD:806:ASP:N	2.29	0.46
1:AAA:150:ARG:NH1	1:BBB:6:THR:HG23	2.27	0.46
2:CCC:201:ARG:CB	2:CCC:369:MET:HE2	2.46	0.46
2:CCC:670:PHE:CD2	2:CCC:1113:LEU:HB3	2.50	0.46
3:DDD:198:CYS:SG	3:DDD:224:LEU:HB3	2.56	0.46
4:EEE:17:PHE:O	4:EEE:21:LEU:HG	2.15	0.46
2:CCC:403:MET:HE2	2:CCC:403:MET:HB3	1.85	0.46
2:CCC:512:SER:O	2:CCC:512:SER:OG	2.34	0.46
3:DDD:290:ILE:H	3:DDD:290:ILE:HD12	1.79	0.46
2:CCC:206:ALA:O	2:CCC:209:ILE:HG22	2.16	0.46
2:CCC:1112:ILE:HG22	3:DDD:641:ILE:HG12	1.98	0.46
3:DDD:347:VAL:HG12	3:DDD:348:ASP:O	2.16	0.46
3:DDD:395:LYS:HE2	5:FFF:329:LEU:CD1	2.45	0.46
2:CCC:32:LEU:HD23	2:CCC:130:MET:HE1	1.98	0.46
2:CCC:668:ILE:HG12	2:CCC:1069:ARG:O	2.16	0.46
3:DDD:599:LYS:H	3:DDD:599:LYS:HG3	1.51	0.46
3:DDD:803:VAL:HG22	3:DDD:1313:SER:OG	2.16	0.46
5:FFF:117:LEU:HD23	5:FFF:117:LEU:HA	1.82	0.46
5:FFF:204:LYS:HB3	5:FFF:205:PRO:HD2	1.98	0.46
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:N	2.26	0.46
3:DDD:174:ASP:N	3:DDD:174:ASP:OD1	2.49	0.46
3:DDD:809:VAL:HG22	3:DDD:915:ILE:CD1	2.46	0.46
3:DDD:846:GLU:HG3	3:DDD:881:LYS:HD3	1.98	0.46
2:CCC:150:HIS:HE1	2:CCC:452:ARG:HH11	1.64	0.45
2:CCC:871:VAL:HG23	2:CCC:883:LEU:O	2.16	0.45
2:CCC:1129:ASN:CA	2:CCC:1177:ARG:HG3	2.46	0.45
3:DDD:423:LEU:HB3	3:DDD:466:MET:CE	2.46	0.45
3:DDD:530:PRO:HD3	3:DDD:552:ILE:CD1	2.45	0.45
7:222:17:DG:C2'	7:222:18:DT:C1'	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:189:ASP:OD1	2:CCC:190:PRO:N	2.50	0.45
2:CCC:569:ILE:O	2:CCC:569:ILE:HG23	2.15	0.45
2:CCC:842:ASP:HB3	2:CCC:1047:LEU:HD21	1.99	0.45
2:CCC:866:ASP:OD2	2:CCC:944:ARG:CD	2.54	0.45
3:DDD:622:ASP:O	3:DDD:626:TYR:CD2	2.69	0.45
3:DDD:697:MET:SD	3:DDD:741:ALA:HB3	2.57	0.45
3:DDD:750:PRO:HB2	3:DDD:781:LYS:HE3	1.98	0.45
3:DDD:1314:LEU:CD1	3:DDD:1327:GLU:CD	2.85	0.45
2:CCC:237:LEU:HD11	2:CCC:292:ILE:HD12	1.98	0.45
2:CCC:750:ILE:HG23	2:CCC:750:ILE:O	2.16	0.45
3:DDD:161:THR:H	3:DDD:164:GLN:HB2	1.81	0.45
3:DDD:747:MET:SD	3:DDD:759:ILE:HD12	2.56	0.45
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:CD1	2.45	0.45
3:DDD:1156:LEU:CD2	3:DDD:1224:ARG:NH2	2.80	0.45
1:AAA:159:ILE:O	1:AAA:159:ILE:HG23	2.14	0.45
2:CCC:720:ARG:HB2	2:CCC:749:ASP:OD2	2.17	0.45
3:DDD:58:CYS:SG	3:DDD:61:ILE:HG13	2.57	0.45
3:DDD:205:LEU:HD22	3:DDD:214:ARG:HG2	1.97	0.45
3:DDD:843:VAL:HG21	3:DDD:897:HIS:C	2.37	0.45
3:DDD:872:LEU:CD2	3:DDD:877:VAL:HG21	2.46	0.45
3:DDD:925:GLU:OE1	3:DDD:926:PRO:N	2.49	0.45
1:BBB:160:HIS:CD2	1:BBB:160:HIS:C	2.89	0.45
2:CCC:135:THR:HG21	2:CCC:515:MET:CE	2.46	0.45
2:CCC:720:ARG:HB3	2:CCC:736:VAL:HG13	1.97	0.45
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.46	0.45
2:CCC:1269:ARG:N	7:222:14:DC:OP1	2.43	0.45
3:DDD:809:VAL:CG2	3:DDD:915:ILE:CD1	2.95	0.45
3:DDD:1041:ILE:HG21	3:DDD:1044:GLN:HG3	1.98	0.45
5:FFF:277:ARG:HD3	5:FFF:306:GLN:HE21	1.81	0.45
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.47	0.45
2:CCC:242:VAL:HA	2:CCC:243:PRO:HD2	1.82	0.45
2:CCC:720:ARG:HD3	2:CCC:736:VAL:HG11	1.99	0.45
2:CCC:1285:TYR:HB2	3:DDD:479:GLU:OE2	2.16	0.45
2:CCC:1296:ASP:CB	2:CCC:1321:GLU:H	2.29	0.45
3:DDD:295:GLU:CD	5:FFF:121:GLU:HG2	2.37	0.45
5:FFF:182:ALA:HB1	5:FFF:193:PRO:CG	2.43	0.45
2:CCC:296:VAL:HG13	2:CCC:352:ARG:NH2	2.31	0.45
2:CCC:479:LEU:HD21	2:CCC:492:MET:HE1	1.99	0.45
2:CCC:840:SER:HB3	2:CCC:850:ILE:HD11	1.99	0.45
2:CCC:1192:GLU:OE2	3:DDD:641:ILE:HG22	2.17	0.45
3:DDD:577:ALA:O	3:DDD:580:TRP:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:56:VAL:HG13	1:AAA:144:ILE:HG22	1.95	0.45
2:CCC:944:ARG:O	2:CCC:947:GLU:HG2	2.17	0.45
2:CCC:1028:LYS:O	2:CCC:1032:LYS:HG2	2.16	0.45
2:CCC:1242:LYS:HD3	3:DDD:465:GLN:NE2	2.31	0.45
5:FFF:105:ILE:HG23	5:FFF:109:TYR:CE1	2.52	0.45
5:FFF:225:PRO:HB2	5:FFF:230:SER:HA	1.98	0.45
2:CCC:104:ILE:HD13	2:CCC:484:LEU:HB3	1.99	0.45
2:CCC:1017:GLN:NE2	2:CCC:1021:LEU:HG	2.31	0.45
3:DDD:58:CYS:SG	3:DDD:61:ILE:N	2.90	0.45
3:DDD:127:LEU:HD23	3:DDD:127:LEU:HA	1.84	0.45
3:DDD:1263:LYS:CG	3:DDD:1307:LEU:HD11	2.47	0.45
1:AAA:177:TYR:O	1:AAA:179:PRO:HD3	2.16	0.45
1:AAA:231:PHE:O	1:AAA:235:ARG:OXT	2.35	0.45
1:BBB:196:THR:HG21	3:DDD:370:LYS:HZ3	1.78	0.45
2:CCC:207:THR:CG2	2:CCC:354:ASP:HB2	2.46	0.45
3:DDD:490:ILE:HG12	3:DDD:500:ILE:HD12	1.99	0.45
3:DDD:889:ASP:OD1	3:DDD:1290:ARG:NH2	2.50	0.45
5:FFF:119:LEU:HD21	5:FFF:158:ILE:CD1	2.40	0.45
2:CCC:21:VAL:HG21	2:CCC:592:ARG:CZ	2.47	0.44
2:CCC:453:ILE:CD1	2:CCC:530:ILE:HD13	2.47	0.44
2:CCC:818:VAL:HG12	2:CCC:1096:ILE:HG12	1.98	0.44
2:CCC:848:GLU:OE1	2:CCC:886:LYS:HD3	2.17	0.44
2:CCC:871:VAL:HG23	2:CCC:883:LEU:HA	1.99	0.44
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:OE2	2.17	0.44
9:CCC:1401:UTP:O4'	8:333:101:DOC:H2'	2.17	0.44
3:DDD:71:LEU:HB2	3:DDD:90:VAL:HG21	1.98	0.44
3:DDD:332:LYS:O	3:DDD:333:GLY:O	2.36	0.44
3:DDD:555:TYR:O	3:DDD:586:GLY:HA2	2.18	0.44
1:AAA:145:LYS:O	1:AAA:145:LYS:HG2	2.17	0.44
1:AAA:218:ARG:HD3	1:BBB:232:VAL:CG2	2.48	0.44
2:CCC:97:ARG:NH2	5:FFF:188:LYS:O	2.51	0.44
2:CCC:184:LEU:HD23	2:CCC:184:LEU:HA	1.82	0.44
2:CCC:421:SER:OG	2:CCC:424:ASP:OD2	2.34	0.44
2:CCC:854:ILE:HD11	2:CCC:885:GLY:HA3	1.99	0.44
3:DDD:248:ASP:N	3:DDD:248:ASP:OD1	2.49	0.44
3:DDD:360:TYR:OH	3:DDD:448:GLN:OE1	2.28	0.44
3:DDD:387:LEU:HD12	3:DDD:387:LEU:HA	1.90	0.44
3:DDD:572:THR:HG21	3:DDD:589:TYR:OH	2.17	0.44
3:DDD:1106:ILE:HG22	3:DDD:1106:ILE:O	2.16	0.44
1:AAA:29:GLU:CB	1:AAA:30:PRO:HA	2.45	0.44
1:AAA:56:VAL:CG1	1:AAA:144:ILE:CG2	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:57:PHE:CE1	2:CCC:59:ILE:HD12	2.52	0.44
2:CCC:90:VAL:HG12	2:CCC:91:THR:N	2.32	0.44
2:CCC:818:VAL:HG23	2:CCC:1079:ILE:HG12	1.98	0.44
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	1.99	0.44
3:DDD:818:GLU:HB3	3:DDD:887:SER:HB2	1.99	0.44
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CD1	2.96	0.44
3:DDD:1212:ASP:OD1	3:DDD:1212:ASP:N	2.45	0.44
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	1.99	0.44
2:CCC:32:LEU:CD2	2:CCC:130:MET:CE	2.94	0.44
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.80	0.44
3:DDD:1082:ASP:OD1	3:DDD:1082:ASP:C	2.56	0.44
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.33	0.44
1:BBB:61:ILE:HG12	1:BBB:142:MET:HB3	1.99	0.44
2:CCC:978:VAL:O	2:CCC:981:ALA:HB3	2.17	0.44
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.82	0.44
2:CCC:1328:LYS:HA	2:CCC:1328:LYS:HD3	1.88	0.44
3:DDD:119:SER:O	3:DDD:122:SER:N	2.50	0.44
3:DDD:262:THR:O	5:FFF:222:VAL:HG12	2.17	0.44
3:DDD:1196:LEU:HD22	3:DDD:1210:ILE:HG22	1.99	0.44
5:FFF:270:GLN:OE1	5:FFF:312:ARG:HD2	2.17	0.44
1:AAA:61:ILE:HG12	1:AAA:142:MET:HB3	1.99	0.44
2:CCC:685:MET:HE2	2:CCC:1235:LEU:CD1	2.47	0.44
2:CCC:1081:PRO:CB	2:CCC:1083:GLU:OE2	2.65	0.44
2:CCC:1109:ILE:HG22	2:CCC:1113:LEU:HD12	2.00	0.44
3:DDD:750:PRO:CA	3:DDD:781:LYS:CG	2.80	0.44
5:FFF:135:ASP:HB2	6:111:37:DA:H61	1.82	0.44
5:FFF:170:HIS:CE1	6:111:31:DT:C7	3.00	0.44
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CE2	2.51	0.44
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD21	2.00	0.44
2:CCC:1214:ASP:OD1	2:CCC:1215:GLY:N	2.50	0.44
3:DDD:382:TYR:OH	3:DDD:398:LYS:HG2	2.18	0.44
5:FFF:107:ARG:HD3	6:111:43:DT:H5''	2.00	0.44
1:AAA:210:THR:HB	1:AAA:211:ILE:H	1.47	0.44
3:DDD:528:THR:HG23	3:DDD:532:GLU:OE1	2.18	0.44
3:DDD:1156:LEU:CD2	3:DDD:1209:VAL:HG22	2.47	0.44
5:FFF:108:ARG:HD3	5:FFF:108:ARG:HA	1.84	0.44
5:FFF:183:ARG:O	5:FFF:187:HIS:ND1	2.50	0.44
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CE1	2.53	0.44
3:DDD:750:PRO:HB3	3:DDD:781:LYS:HD3	1.99	0.44
2:CCC:366:ILE:O	2:CCC:369:MET:HG2	2.17	0.43
2:CCC:751:TYR:CD2	2:CCC:751:TYR:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1327:LEU:O	2:CCC:1331:ARG:HG3	2.18	0.43
3:DDD:886:VAL:CG1	3:DDD:1226:VAL:CG1	2.96	0.43
3:DDD:1158:GLU:HA	3:DDD:1223:LEU:HD22	1.99	0.43
2:CCC:93:SER:OG	2:CCC:126:GLU:HB3	2.18	0.43
2:CCC:95:PRO:HG3	5:FFF:190:ASP:CG	2.38	0.43
2:CCC:816:ILE:HD11	2:CCC:1074:GLY:HA3	1.99	0.43
2:CCC:868:SER:HG	2:CCC:944:ARG:H	1.53	0.43
3:DDD:110:PRO:O	3:DDD:182:ALA:HB3	2.18	0.43
3:DDD:1174:ARG:O	3:DDD:1176:VAL:HG23	2.19	0.43
5:FFF:100:ARG:NH1	6:111:42:DG:H8	2.17	0.43
1:AAA:45:ARG:NH2	1:BBB:37:HIS:HB2	2.33	0.43
2:CCC:123:TYR:CE1	5:FFF:190:ASP:O	2.71	0.43
2:CCC:267:ARG:HD3	2:CCC:268:ARG:H	1.83	0.43
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CE2	2.53	0.43
1:BBB:195:ARG:HD2	1:BBB:198:LEU:HD23	1.99	0.43
2:CCC:44:GLU:HG3	2:CCC:45:GLY:H	1.84	0.43
2:CCC:901:LEU:CD1	5:FFF:278:PHE:CE2	2.96	0.43
2:CCC:1017:GLN:HE21	2:CCC:1021:LEU:HG	1.83	0.43
2:CCC:1247:SER:HB3	3:DDD:375:GLU:O	2.18	0.43
3:DDD:667:GLN:O	3:DDD:670:SER:OG	2.22	0.43
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD13	2.00	0.43
7:222:17:DG:O3'	7:222:18:DT:C4'	2.66	0.43
2:CCC:576:SER:OG	2:CCC:577:VAL:N	2.51	0.43
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	2.01	0.43
2:CCC:1161:LEU:HD12	2:CCC:1161:LEU:HA	1.92	0.43
2:CCC:1212:LEU:HD23	2:CCC:1212:LEU:HA	1.86	0.43
3:DDD:703:THR:O	3:DDD:705:THR:N	2.52	0.43
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:CD2	2.43	0.43
5:FFF:87:ASP:OD1	5:FFF:88:VAL:N	2.51	0.43
2:CCC:764:CYS:SG	2:CCC:833:ILE:HD11	2.59	0.43
3:DDD:783:LEU:HD12	3:DDD:783:LEU:HA	1.81	0.43
5:FFF:114:LEU:HB2	5:FFF:119:LEU:HG	2.00	0.43
5:FFF:158:ILE:CG2	7:222:26:DT:O2	2.67	0.43
5:FFF:159:MET:SD	5:FFF:172:VAL:HG11	2.58	0.43
5:FFF:225:PRO:HA	5:FFF:233:ALA:HA	2.01	0.43
2:CCC:244:GLU:O	2:CCC:247:ARG:HB2	2.19	0.43
2:CCC:1134:GLN:O	2:CCC:1136:GLN:N	2.52	0.43
2:CCC:1321:GLU:O	2:CCC:1325:VAL:HG23	2.18	0.43
3:DDD:357:VAL:HG22	3:DDD:461:PHE:CE2	2.53	0.43
3:DDD:705:THR:HG23	3:DDD:707:ILE:HG13	2.00	0.43
3:DDD:872:LEU:HD23	3:DDD:877:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CZ	2.53	0.43
3:DDD:261:ALA:HA	5:FFF:220:THR:O	2.19	0.43
3:DDD:421:VAL:HG11	3:DDD:468:VAL:HG13	2.01	0.43
2:CCC:832:HIS:CD2	2:CCC:1058:ARG:HD2	2.54	0.43
2:CCC:850:ILE:HG22	2:CCC:850:ILE:O	2.19	0.43
3:DDD:664:ILE:HG21	3:DDD:681:LYS:HD3	2.01	0.43
3:DDD:849:LEU:HB2	3:DDD:850:LYS:H	1.72	0.43
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.84	0.43
5:FFF:170:HIS:CD2	5:FFF:170:HIS:H	2.37	0.43
2:CCC:118:LYS:NZ	2:CCC:485:ASP:O	2.30	0.42
2:CCC:599:VAL:HG21	2:CCC:623:LEU:CD2	2.49	0.42
3:DDD:805:GLN:HE22	3:DDD:1321:SER:HB2	1.83	0.42
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	2.01	0.42
5:FFF:100:ARG:NH2	6:111:42:DG:N7	2.66	0.42
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.36	0.42
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.99	0.42
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG22	2.00	0.42
2:CCC:560:PRO:CB	3:DDD:776:THR:HG21	2.42	0.42
2:CCC:1293:VAL:HG12	2:CCC:1300:GLY:C	2.40	0.42
3:DDD:664:ILE:HD13	3:DDD:681:LYS:HG2	2.01	0.42
3:DDD:960:LEU:HB3	3:DDD:963:VAL:HG11	2.01	0.42
5:FFF:140:PHE:CE1	6:111:38:DT:H5''	2.54	0.42
2:CCC:543:ALA:HB3	2:CCC:548:ARG:HH21	1.83	0.42
2:CCC:555:TYR:OH	2:CCC:654:ASP:OD2	2.21	0.42
2:CCC:1086:PRO:HB3	2:CCC:1212:LEU:HD13	2.01	0.42
3:DDD:1318:SER:OG	3:DDD:1349:GLU:HG2	2.19	0.42
5:FFF:155:GLU:CD	7:222:26:DT:H2''	2.39	0.42
1:BBB:165:GLU:O	1:BBB:165:GLU:CG	2.68	0.42
2:CCC:1100:PRO:HB3	3:DDD:639:VAL:HG23	2.01	0.42
2:CCC:1112:ILE:CG2	3:DDD:641:ILE:HG12	2.50	0.42
3:DDD:395:LYS:CE	5:FFF:329:LEU:HD22	2.49	0.42
3:DDD:519:ASN:HA	3:DDD:523:GLU:CG	2.50	0.42
3:DDD:1370:MET:O	3:DDD:1373:ARG:HB2	2.19	0.42
1:BBB:83:LEU:HD11	3:DDD:526:VAL:O	2.20	0.42
2:CCC:963:GLU:O	2:CCC:967:LEU:HB2	2.19	0.42
2:CCC:1080:ASN:HB3	2:CCC:1085:MET:SD	2.58	0.42
3:DDD:68:TYR:HD2	3:DDD:78:LEU:HD23	1.83	0.42
7:222:17:DG:C3'	7:222:18:DT:O4'	2.66	0.42
2:CCC:818:VAL:CG2	2:CCC:1079:ILE:HG12	2.49	0.42
2:CCC:898:GLU:OE2	5:FFF:280:LEU:HD13	2.20	0.42
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:244:GLU:CG	2:CCC:245:ARG:N	2.80	0.42
2:CCC:296:VAL:HB	2:CCC:336:LEU:HD12	2.01	0.42
2:CCC:726:TYR:CZ	2:CCC:728:ASP:HB2	2.54	0.42
2:CCC:1304:MET:HE3	3:DDD:472:LEU:HD13	2.02	0.42
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CE1	2.55	0.42
2:CCC:551:HIS:HA	2:CCC:552:PRO:HD2	1.85	0.42
2:CCC:670:PHE:CE2	2:CCC:1113:LEU:HB3	2.54	0.42
3:DDD:130:MET:SD	3:DDD:157:GLN:HB3	2.59	0.42
3:DDD:502:PRO:HB3	3:DDD:506:VAL:CG1	2.50	0.42
3:DDD:783:LEU:O	3:DDD:786:THR:HG23	2.20	0.42
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	2.19	0.42
2:CCC:216:THR:O	2:CCC:220:ILE:HG13	2.20	0.42
2:CCC:1257:GLN:HE22	3:DDD:341:ASN:HA	1.83	0.42
3:DDD:703:THR:C	3:DDD:705:THR:N	2.72	0.42
3:DDD:707:ILE:CD1	3:DDD:716:GLN:HE21	2.30	0.42
3:DDD:810:THR:OG1	3:DDD:893:GLY:HA3	2.19	0.42
3:DDD:964:LYS:H	3:DDD:977:SER:HB3	1.85	0.42
5:FFF:65:ILE:HG12	5:FFF:99:LEU:HD13	2.02	0.42
5:FFF:177:VAL:O	5:FFF:181:THR:OG1	2.29	0.42
1:AAA:11:PRO:O	1:BBB:230:ALA:CB	2.58	0.42
1:AAA:57:THR:OG1	1:AAA:147:GLN:HB2	2.20	0.42
3:DDD:58:CYS:SG	3:DDD:60:ARG:N	2.93	0.42
3:DDD:1038:THR:O	3:DDD:1040:MET:HG3	2.19	0.42
1:BBB:168:ILE:H	1:BBB:168:ILE:HG13	1.64	0.41
2:CCC:160:ASP:OD1	2:CCC:160:ASP:N	2.53	0.41
2:CCC:1270:PHE:HB2	3:DDD:347:VAL:HG21	2.02	0.41
3:DDD:342:LEU:HD22	3:DDD:1352:ILE:O	2.19	0.41
3:DDD:579:LEU:HD23	3:DDD:579:LEU:HA	1.88	0.41
3:DDD:1100:PHE:CZ	3:DDD:1192:LYS:HG2	2.55	0.41
5:FFF:168:PRO:O	5:FFF:172:VAL:HG23	2.20	0.41
1:BBB:86:LYS:HE2	1:BBB:174:ASP:H	1.85	0.41
1:BBB:152:TYR:CD2	3:DDD:536:LEU:HD21	2.54	0.41
2:CCC:619:ALA:HB2	2:CCC:654:ASP:HB2	2.01	0.41
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.20	0.41
2:CCC:809:GLY:O	3:DDD:357:VAL:HG11	2.20	0.41
5:FFF:145:TYR:CZ	5:FFF:149:TRP:NE1	2.87	0.41
2:CCC:32:LEU:CD2	2:CCC:130:MET:HE3	2.50	0.41
2:CCC:592:ARG:NH1	2:CCC:653:MET:HE1	2.35	0.41
2:CCC:898:GLU:OE1	2:CCC:898:GLU:N	2.52	0.41
2:CCC:1293:VAL:O	2:CCC:1301:ARG:HB3	2.21	0.41
3:DDD:99:ARG:HG3	3:DDD:249:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:749:LYS:CB	3:DDD:750:PRO:HD2	2.50	0.41
3:DDD:843:VAL:HG21	3:DDD:897:HIS:CA	2.51	0.41
5:FFF:100:ARG:HB3	6:111:41:DT:O3'	2.20	0.41
6:111:28:DA:H61	7:222:35:DT:H3	1.69	0.41
1:AAA:117:HIS:CD2	1:AAA:118:ASP:O	2.73	0.41
2:CCC:582:ASN:OD1	2:CCC:585:GLY:N	2.51	0.41
2:CCC:1246:ARG:NH2	2:CCC:1258:PRO:HB3	2.35	0.41
3:DDD:395:LYS:HE2	5:FFF:329:LEU:CD2	2.51	0.41
5:FFF:100:ARG:HG2	6:111:42:DG:H5''	2.01	0.41
1:AAA:51:MET:CE	1:AAA:52:PRO:HD2	2.51	0.41
1:AAA:54:CYS:SG	1:AAA:148:ARG:HB2	2.60	0.41
1:BBB:41:ASN:O	1:BBB:45:ARG:HG3	2.20	0.41
2:CCC:524:ILE:CD1	2:CCC:712:SER:HB3	2.51	0.41
3:DDD:435:GLN:HB2	3:DDD:457:TYR:OH	2.20	0.41
3:DDD:490:ILE:HA	3:DDD:500:ILE:HD12	2.01	0.41
2:CCC:230:PHE:CE1	2:CCC:292:ILE:HD11	2.54	0.41
2:CCC:1087:TYR:HD2	2:CCC:1091:GLY:HA2	1.85	0.41
2:CCC:1160:ASP:O	2:CCC:1161:LEU:O	2.38	0.41
3:DDD:424:ASN:OD1	3:DDD:425:ARG:N	2.54	0.41
3:DDD:746:LEU:HD23	3:DDD:758:PRO:HB3	2.03	0.41
3:DDD:786:THR:HB	3:DDD:932:MET:HA	2.02	0.41
1:AAA:74:VAL:O	2:CCC:729:ALA:HB3	2.20	0.41
2:CCC:838:CYS:HB2	2:CCC:918:LEU:HD22	2.02	0.41
2:CCC:1109:ILE:HD13	2:CCC:1109:ILE:HA	1.90	0.41
3:DDD:679:TYR:HE1	3:DDD:754:ILE:O	2.04	0.41
3:DDD:1165:PHE:HZ	3:DDD:1196:LEU:HD12	1.86	0.41
6:111:26:DT:H2''	6:111:27:DC:C5	2.56	0.41
6:111:54:DA:C2'	6:111:55:DC:C6	2.79	0.41
1:AAA:44:ARG:HA	1:AAA:183:ILE:HD13	2.02	0.41
1:AAA:44:ARG:HH21	2:CCC:1215:GLY:HA2	1.85	0.41
2:CCC:183:TRP:CZ3	6:111:51:DC:H2''	2.54	0.41
2:CCC:684:ASN:CG	2:CCC:687:ARG:HH21	2.20	0.41
2:CCC:1255:THR:HG21	3:DDD:341:ASN:CG	2.40	0.41
5:FFF:127:LEU:HD23	5:FFF:127:LEU:HA	1.87	0.41
2:CCC:12:ARG:HD3	2:CCC:1183:ALA:HB2	2.02	0.41
2:CCC:95:PRO:HB2	5:FFF:190:ASP:HB2	1.97	0.41
2:CCC:148:GLN:OE1	2:CCC:454:ARG:HD2	2.21	0.41
2:CCC:479:LEU:HD23	2:CCC:479:LEU:HA	1.93	0.41
2:CCC:675:ASP:HA	3:DDD:763:PHE:CZ	2.56	0.41
2:CCC:1061:GLN:NE2	2:CCC:1240:ASP:OD1	2.54	0.41
2:CCC:1285:TYR:N	3:DDD:479:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CCC:1401:UTP:H2'	3:DDD:932:MET:SD	2.61	0.41
3:DDD:135:ILE:HG23	3:DDD:185:ILE:CD1	2.51	0.41
3:DDD:161:THR:N	3:DDD:164:GLN:OE1	2.47	0.41
3:DDD:458:ASN:HD22	3:DDD:929:GLN:HE22	1.68	0.41
3:DDD:492:SER:HB2	3:DDD:499:ILE:HD11	2.03	0.41
3:DDD:952:VAL:HG11	3:DDD:984:LEU:HD13	2.03	0.41
3:DDD:1061:VAL:O	3:DDD:1104:LYS:N	2.42	0.41
3:DDD:1169:THR:OG1	3:DDD:1174:ARG:NH2	2.54	0.41
5:FFF:266:LEU:HD21	5:FFF:316:ILE:HD12	2.02	0.41
7:222:17:DG:H2'	7:222:18:DT:N1	2.36	0.41
1:AAA:78:ILE:HA	1:AAA:81:ILE:HD12	2.03	0.41
1:AAA:86:LYS:NZ	2:CCC:826:ASP:OD2	2.54	0.41
1:AAA:195:ARG:HD2	1:AAA:198:LEU:CD2	2.50	0.41
2:CCC:540:ARG:HB2	2:CCC:540:ARG:NH1	2.36	0.41
2:CCC:823:VAL:HG22	2:CCC:1060:ILE:CG2	2.51	0.41
2:CCC:890:LYS:HD2	2:CCC:914:LYS:HE2	2.03	0.41
3:DDD:160:LEU:HB3	3:DDD:164:GLN:HB3	2.03	0.41
3:DDD:322:ARG:HA	3:DDD:323:PRO:HD2	1.91	0.41
3:DDD:364:HIS:CD2	4:EEE:4:VAL:HG13	2.56	0.41
3:DDD:661:VAL:HG23	3:DDD:685:ILE:HG21	2.03	0.41
3:DDD:1163:VAL:O	3:DDD:1201:GLY:HA2	2.21	0.41
5:FFF:259:ILE:HG23	5:FFF:280:LEU:HD21	2.02	0.41
1:AAA:57:THR:CG2	1:AAA:158:ARG:CZ	2.96	0.40
1:BBB:20:SER:OG	1:BBB:21:SER:N	2.54	0.40
2:CCC:189:ASP:OD1	2:CCC:189:ASP:C	2.59	0.40
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB3	2.03	0.40
2:CCC:725:GLN:HB2	2:CCC:735:LYS:HG3	2.03	0.40
9:CCC:1401:UTP:O4'	8:333:101:DOC:H3'2	2.22	0.40
3:DDD:222:LYS:CE	3:DDD:1278:GLU:HG2	2.51	0.40
3:DDD:749:LYS:HB3	3:DDD:750:PRO:HD2	2.02	0.40
3:DDD:785:ASP:HB3	3:DDD:935:PHE:CE2	2.56	0.40
3:DDD:805:GLN:CG	3:DDD:806:ASP:N	2.83	0.40
2:CCC:255:ILE:HG23	2:CCC:285:ILE:HD13	2.03	0.40
2:CCC:898:GLU:CG	5:FFF:259:ILE:HD13	2.51	0.40
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.58	0.40
3:DDD:1047:THR:HB	3:DDD:1062:LEU:HD11	2.03	0.40
2:CCC:76:GLY:O	2:CCC:94:ALA:HB1	2.21	0.40
3:DDD:442:ILE:HD13	3:DDD:448:GLN:OE1	2.21	0.40
3:DDD:994:SER:O	3:DDD:995:TYR:CG	2.75	0.40
2:CCC:136:PHE:HB3	2:CCC:138:ILE:HD11	2.03	0.40
2:CCC:759:SER:OG	2:CCC:760:ASN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1030:GLU:HG3	2:CCC:1034:ARG:CZ	2.50	0.40
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:O	2.22	0.40
3:DDD:1031:VAL:HG11	3:DDD:1089:LEU:O	2.21	0.40
3:DDD:1054:THR:OG1	3:DDD:1055:GLY:N	2.54	0.40
3:DDD:1357:ILE:H	3:DDD:1357:ILE:HG13	1.55	0.40
5:FFF:100:ARG:CG	6:111:42:DG:H5''	2.51	0.40
1:BBB:13:LEU:HD12	1:BBB:14:VAL:N	2.36	0.40
2:CCC:151:ARG:NH1	6:111:52:DT:H73	2.36	0.40
2:CCC:151:ARG:CZ	2:CCC:177:ILE:HD11	2.51	0.40
2:CCC:244:GLU:O	2:CCC:247:ARG:CB	2.69	0.40
2:CCC:980:VAL:O	2:CCC:981:ALA:C	2.59	0.40
3:DDD:113:HIS:CD2	3:DDD:115:TRP:HB2	2.57	0.40
3:DDD:362:ARG:HH21	3:DDD:619:ILE:HG13	1.87	0.40
3:DDD:833:GLU:HG2	3:DDD:838:ARG:HG3	2.04	0.40
3:DDD:1031:VAL:HG21	3:DDD:1097:ALA:CB	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:212:THR:OG1	6:111:27:DC:OP1[3_644]	1.88	0.32
1:BBB:159:ILE:CD1	3:DDD:1054:THR:O[4_445]	2.18	0.02

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%)	209 (92%)	14 (6%)	5 (2%)	6	38
1	BBB	226/242 (93%)	209 (92%)	11 (5%)	6 (3%)	5	34
2	CCC	1339/1342 (100%)	1236 (92%)	78 (6%)	25 (2%)	8	41
3	DDD	1360/1407 (97%)	1251 (92%)	90 (7%)	19 (1%)	11	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	275/336 (82%)	253 (92%)	16 (6%)	6 (2%)	6	38
All	All	3505/3659 (96%)	3231 (92%)	213 (6%)	61 (2%)	9	44

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS
1	BBB	119	GLY
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN
2	CCC	247	ARG
2	CCC	791	LEU
2	CCC	1161	LEU
2	CCC	1162	SER
2	CCC	1281	TYR
3	DDD	53	ARG
3	DDD	519	ASN
5	FFF	227	GLY
1	AAA	234	LEU
2	CCC	258	ASN
2	CCC	625	GLU
2	CCC	730	SER
2	CCC	756	TYR
3	DDD	122	SER
3	DDD	174	ASP
3	DDD	321	LYS
3	DDD	336	GLY
3	DDD	847	ASP
3	DDD	1053	LEU
3	DDD	1309	ILE
5	FFF	228	GLY
5	FFF	282	GLY
1	AAA	233	ASP
2	CCC	45	GLY
2	CCC	455	SER
2	CCC	669	PRO
2	CCC	867	GLU
2	CCC	981	ALA
2	CCC	1103	VAL

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Mol	Chain	Res	Type
2	CCC	1135	GLN
3	DDD	1200	GLU
1	AAA	162	GLU
1	BBB	232	VAL
2	CCC	163	LYS
2	CCC	234	ASP
2	CCC	729	ALA
2	CCC	986	ALA
3	DDD	854	ALA
3	DDD	1024	THR
1	AAA	191	ARG
1	BBB	118	ASP
2	CCC	341	LEU
2	CCC	1297	ASP
3	DDD	986	ASP
3	DDD	1091	PRO
3	DDD	1170	LYS
3	DDD	1297	LYS
5	FFF	328	PHE
3	DDD	825	VAL
5	FFF	113	GLY
1	AAA	168	ILE
3	DDD	829	GLY
2	CCC	983	GLY
3	DDD	1103	GLY
5	FFF	295	ILE
2	CCC	110	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	198/208 (95%)	178 (90%)	20 (10%)	7 28
1	BBB	196/208 (94%)	180 (92%)	16 (8%)	11 37
2	CCC	1156/1157 (100%)	1066 (92%)	90 (8%)	12 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DDD	1135/1168 (97%)	1063 (94%)	72 (6%)	18	45
4	EEE	67/74 (90%)	63 (94%)	4 (6%)	19	47
5	FFF	240/292 (82%)	228 (95%)	12 (5%)	24	51
All	All	2992/3107 (96%)	2778 (93%)	214 (7%)	14	41

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	18	GLN
1	AAA	28	LEU
1	AAA	33	ARG
1	AAA	70	THR
1	AAA	77	ASP
1	AAA	131	CYS
1	AAA	135	ASP
1	AAA	137	ASN
1	AAA	150	ARG
1	AAA	157	THR
1	AAA	159	ILE
1	AAA	166	ARG
1	AAA	170	ARG
1	AAA	187	VAL
1	AAA	191	ARG
1	AAA	194	GLN
1	AAA	198	LEU
1	AAA	208	ASN
1	AAA	233	ASP
1	AAA	235	ARG
1	BBB	28	LEU
1	BBB	33	ARG
1	BBB	70	THR
1	BBB	77	ASP
1	BBB	105	SER
1	BBB	131	CYS
1	BBB	135	ASP
1	BBB	137	ASN
1	BBB	139	SER
1	BBB	159	ILE
1	BBB	160	HIS
1	BBB	187	VAL
1	BBB	191	ARG

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Mol	Chain	Res	Type
1	BBB	194	GLN
1	BBB	198	LEU
1	BBB	233	ASP
2	CCC	30	ILE
2	CCC	69	GLN
2	CCC	85	CYS
2	CCC	116	ASP
2	CCC	120	GLN
2	CCC	121	GLU
2	CCC	160	ASP
2	CCC	166	SER
2	CCC	167	SER
2	CCC	173	ASN
2	CCC	184	LEU
2	CCC	185	ASP
2	CCC	189	ASP
2	CCC	237	LEU
2	CCC	241	LEU
2	CCC	244	GLU
2	CCC	256	GLU
2	CCC	264	GLU
2	CCC	275	ARG
2	CCC	290	GLU
2	CCC	304	GLU
2	CCC	316	GLU
2	CCC	332	ARG
2	CCC	335	THR
2	CCC	393	ASP
2	CCC	398	SER
2	CCC	403	MET
2	CCC	404	LYS
2	CCC	413	GLU
2	CCC	458	GLU
2	CCC	472	GLU
2	CCC	477	GLU
2	CCC	481	LEU
2	CCC	502	VAL
2	CCC	511	LEU
2	CCC	525	THR
2	CCC	529	ARG
2	CCC	539	THR
2	CCC	574	SER

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Mol	Chain	Res	Type
2	CCC	576	SER
2	CCC	592	ARG
2	CCC	601	ASP
2	CCC	618	GLN
2	CCC	620	ASN
2	CCC	635	THR
2	CCC	648	ASP
2	CCC	678	ARG
2	CCC	685	MET
2	CCC	694	ARG
2	CCC	698	PRO
2	CCC	730	SER
2	CCC	739	ASP
2	CCC	757	THR
2	CCC	758	ARG
2	CCC	759	SER
2	CCC	777	VAL
2	CCC	788	SER
2	CCC	789	THR
2	CCC	799	ASN
2	CCC	800	MET
2	CCC	801	ARG
2	CCC	802	VAL
2	CCC	808	ASN
2	CCC	815	SER
2	CCC	817	LEU
2	CCC	831	ILE
2	CCC	844	LYS
2	CCC	866	ASP
2	CCC	876	GLU
2	CCC	912	ASP
2	CCC	935	THR
2	CCC	942	ASP
2	CCC	995	ASP
2	CCC	998	LEU
2	CCC	1073	LYS
2	CCC	1088	ASP
2	CCC	1113	LEU
2	CCC	1135	GLN
2	CCC	1143	GLU
2	CCC	1150	ASP
2	CCC	1154	ASP

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Mol	Chain	Res	Type
2	CCC	1223	ARG
2	CCC	1240	ASP
2	CCC	1248	THR
2	CCC	1262	LYS
2	CCC	1269	ARG
2	CCC	1286	THR
2	CCC	1292	THR
2	CCC	1293	VAL
2	CCC	1296	ASP
3	DDD	34	SER
3	DDD	52	GLU
3	DDD	60	ARG
3	DDD	67	ASP
3	DDD	70	CYS
3	DDD	143	SER
3	DDD	167	ASP
3	DDD	176	PHE
3	DDD	210	SER
3	DDD	223	LEU
3	DDD	237	MET
3	DDD	247	PRO
3	DDD	256	ASP
3	DDD	319	SER
3	DDD	337	ARG
3	DDD	339	ARG
3	DDD	345	LYS
3	DDD	418	GLU
3	DDD	443	GLU
3	DDD	460	ASP
3	DDD	464	ASP
3	DDD	479	GLU
3	DDD	492	SER
3	DDD	503	SER
3	DDD	543	SER
3	DDD	579	LEU
3	DDD	590	SER
3	DDD	591	ILE
3	DDD	599	LYS
3	DDD	604	MET
3	DDD	610	ARG
3	DDD	619	ILE
3	DDD	627	THR

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Mol	Chain	Res	Type
3	DDD	704	GLU
3	DDD	705	THR
3	DDD	715	LYS
3	DDD	717	VAL
3	DDD	731	ARG
3	DDD	736	GLN
3	DDD	747	MET
3	DDD	751	ASP
3	DDD	769	VAL
3	DDD	786	THR
3	DDD	790	THR
3	DDD	792	ASN
3	DDD	812	ASP
3	DDD	830	ASP
3	DDD	835	LEU
3	DDD	840	LEU
3	DDD	849	LEU
3	DDD	860	ARG
3	DDD	861	ASN
3	DDD	862	THR
3	DDD	889	ASP
3	DDD	911	LYS
3	DDD	957	SER
3	DDD	969	SER
3	DDD	970	SER
3	DDD	1021	ASP
3	DDD	1023	HIS
3	DDD	1025	MET
3	DDD	1032	SER
3	DDD	1051	ASP
3	DDD	1064	SER
3	DDD	1073	ASP
3	DDD	1187	GLU
3	DDD	1200	GLU
3	DDD	1283	SER
3	DDD	1303	SER
3	DDD	1309	ILE
3	DDD	1330	ARG
3	DDD	1345	ARG
4	EEE	8	ASP
4	EEE	46	THR
4	EEE	55	GLU

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Mol	Chain	Res	Type
4	EEE	67	ARG
5	FFF	107	ARG
5	FFF	109	TYR
5	FFF	122	GLU
5	FFF	127	LEU
5	FFF	151	ARG
5	FFF	218	ARG
5	FFF	229	ASP
5	FFF	244	ASN
5	FFF	254	ASP
5	FFF	271	ARG
5	FFF	299	ARG
5	FFF	325	GLU

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

5.3.3 RNA [i](#)

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	DOC	333	101	7	16,19,20	0.95	0	20,26,29	1.25	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	DOC	333	101	7	-	2/7/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	333	101	DOC	C2'-C1'-N1	-2.35	107.94	112.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	333	101	DOC	C3'-C4'-C5'-O5'
8	333	101	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	333	101	DOC	7	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	UTP	CCC	1401	11	22,30,30	0.98	1 (4%)	27,47,47	1.01	1 (3%)

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
9	UTP	CCC	1401	11	-	3/20/38/38	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	CCC	1401	UTP	C4-N3	3.21	1.38	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CCC	1401	UTP	C5-C4-N3	-3.87	114.80	123.31

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	CCC	1401	UTP	PB-O3B-PG-O3G
9	CCC	1401	UTP	PA-O3A-PB-O1B
9	CCC	1401	UTP	PA-O3A-PB-O2B

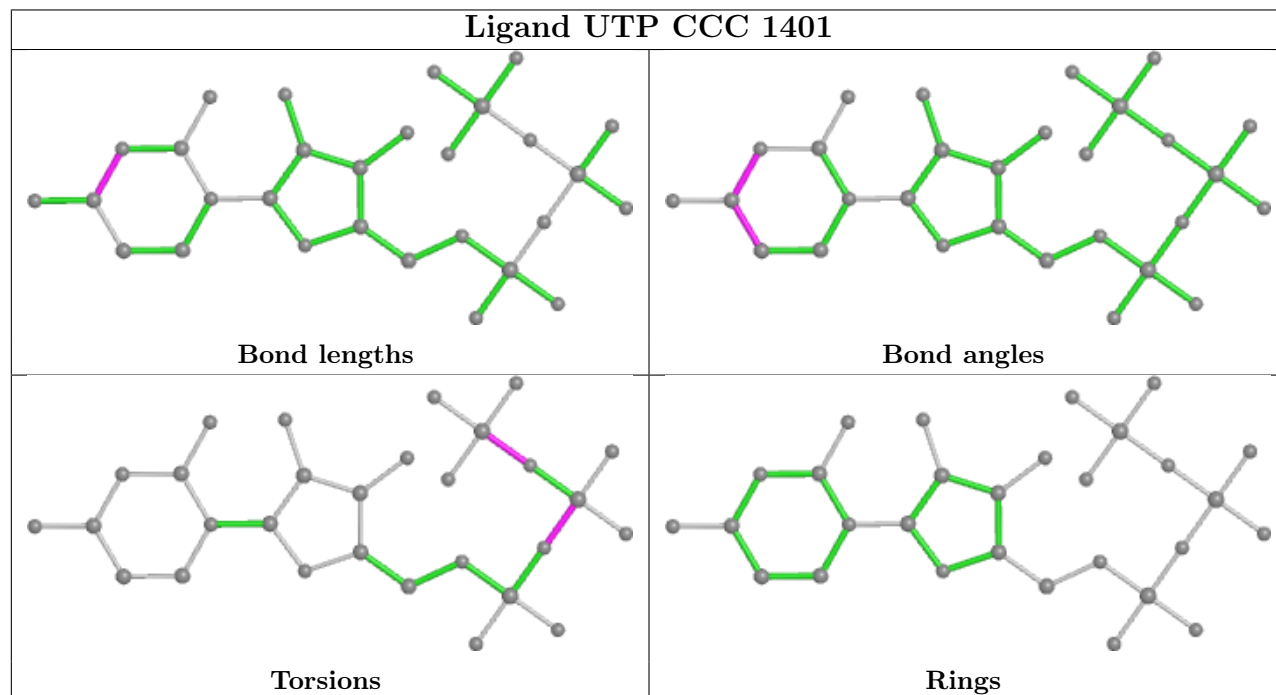
There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	CCC	1401	UTP	14	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	333	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	333	17:U	O3'	101:DOC	P	1.86

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%)	-0.01	8 (3%) 44 35	212, 294, 356, 386	0
1	BBB	228/242 (94%)	0.11	11 (4%) 30 26	215, 288, 363, 434	0
2	CCC	1341/1342 (99%)	-0.14	40 (2%) 50 39	102, 235, 396, 487	0
3	DDD	1362/1407 (96%)	-0.08	51 (3%) 41 33	115, 257, 386, 480	0
4	EEE	79/90 (87%)	-0.05	4 (5%) 28 24	207, 309, 472, 518	0
5	FFF	277/336 (82%)	0.06	7 (2%) 57 47	197, 306, 438, 485	0
6	111	30/50 (60%)	0.07	4 (13%) 3 4	269, 335, 440, 546	0
7	222	35/50 (70%)	0.23	3 (8%) 10 9	267, 350, 509, 513	0
8	333	3/4 (75%)	0.94	0 100 100	351, 351, 399, 414	0
All	All	3585/3763 (95%)	-0.07	128 (3%) 42 34	102, 265, 407, 546	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	111	49	DG	6.0
3	DDD	993	GLU	5.9
3	DDD	854	ALA	5.9
2	CCC	1001	GLY	5.2
3	DDD	943	ARG	5.0
2	CCC	722	GLY	5.0
3	DDD	856	ILE	5.0
4	EEE	78	ALA	4.6
2	CCC	231	GLU	4.5
2	CCC	885	GLY	4.5
2	CCC	230	PHE	4.5
7	222	19	DA	4.3
3	DDD	1118	GLY	4.3
3	DDD	1271	SER	4.3
2	CCC	240	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
2	CCC	169	LYS	4.1
3	DDD	997	VAL	4.1
3	DDD	1129	GLY	4.1
1	AAA	135	ASP	3.9
1	BBB	165	GLU	3.9
3	DDD	1266	ILE	3.8
3	DDD	855	ASP	3.8
3	DDD	992	LYS	3.8
3	DDD	1028	ILE	3.7
3	DDD	879	ALA	3.7
3	DDD	1030	GLU	3.7
1	BBB	164	ASP	3.7
2	CCC	856	ASN	3.7
3	DDD	991	THR	3.7
3	DDD	1029	THR	3.7
3	DDD	748	ALA	3.6
4	EEE	14	GLY	3.6
3	DDD	1066	GLU	3.6
3	DDD	1087	ASP	3.6
1	BBB	50	SER	3.6
3	DDD	880	VAL	3.5
5	FFF	263	LEU	3.5
1	BBB	152	TYR	3.5
1	AAA	136	GLU	3.4
3	DDD	1203	ARG	3.4
3	DDD	942	SER	3.4
2	CCC	984	VAL	3.3
5	FFF	310	LEU	3.3
2	CCC	333	ILE	3.3
2	CCC	721	GLY	3.3
1	BBB	107	ILE	3.2
2	CCC	855	PRO	3.2
3	DDD	995	TYR	3.2
3	DDD	1272	SER	3.2
1	AAA	213	PRO	3.2
2	CCC	1002	LEU	3.1
4	EEE	80	LEU	3.1
3	DDD	976	THR	3.0
3	DDD	1079	LYS	3.0
1	AAA	134	THR	3.0
1	BBB	93	GLN	3.0
3	DDD	750	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	CCC	911	SER	2.9
3	DDD	1097	ALA	2.9
2	CCC	164	THR	2.9
1	AAA	144	ILE	2.9
4	EEE	79	GLU	2.9
1	BBB	133	LEU	2.9
2	CCC	229	ILE	2.8
6	111	50	DT	2.8
1	BBB	108	GLY	2.8
3	DDD	1080	ILE	2.7
2	CCC	912	ASP	2.7
3	DDD	1031	VAL	2.7
2	CCC	124	MET	2.7
3	DDD	853	THR	2.7
3	DDD	1078	LEU	2.7
3	DDD	1121	LEU	2.7
2	CCC	1004	ASP	2.7
2	CCC	557	ARG	2.7
3	DDD	1286	LYS	2.6
2	CCC	1003	THR	2.5
2	CCC	850	ILE	2.5
3	DDD	1110	GLU	2.5
1	AAA	59	VAL	2.5
5	FFF	131	VAL	2.5
1	BBB	90	VAL	2.5
6	111	44	DG	2.5
1	BBB	134	THR	2.5
1	BBB	98	VAL	2.4
2	CCC	385	PHE	2.4
1	AAA	205	MET	2.4
3	DDD	1128	SER	2.4
3	DDD	980	THR	2.4
2	CCC	239	MET	2.4
5	FFF	301	ARG	2.4
5	FFF	198	ILE	2.4
2	CCC	871	VAL	2.4
3	DDD	983	LYS	2.3
2	CCC	105	TYR	2.3
3	DDD	749	LYS	2.3
3	DDD	1000	GLY	2.3
2	CCC	241	LEU	2.3
3	DDD	998	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
5	FFF	134	PHE	2.3
3	DDD	392	THR	2.2
3	DDD	1198	VAL	2.2
7	222	22	DA	2.2
3	DDD	847	ASP	2.2
2	CCC	1180	MET	2.2
2	CCC	740	GLU	2.2
2	CCC	982	GLY	2.1
2	CCC	422	LYS	2.1
5	FFF	71	LEU	2.1
2	CCC	228	VAL	2.1
3	DDD	941	ALA	2.1
3	DDD	1122	ALA	2.1
7	222	24	DT	2.1
3	DDD	965	SER	2.1
2	CCC	849	GLU	2.1
3	DDD	746	LEU	2.1
3	DDD	990	ARG	2.1
2	CCC	857	VAL	2.1
1	AAA	100	LEU	2.1
2	CCC	928	VAL	2.1
3	DDD	1166	GLY	2.1
3	DDD	975	ILE	2.1
2	CCC	227	LYS	2.0
2	CCC	777	VAL	2.0
6	111	43	DT	2.0
2	CCC	170	VAL	2.0
2	CCC	261	VAL	2.0
2	CCC	905	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	DOC	333	101	18/19	0.82	0.36	311,333,341,343	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

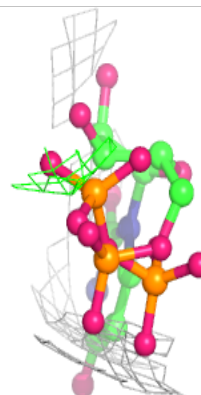
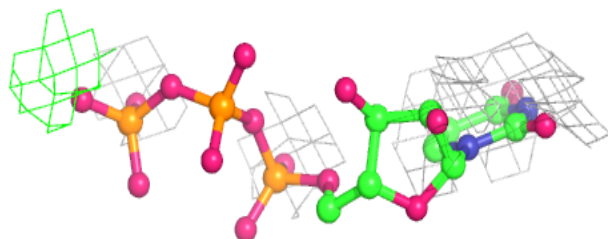
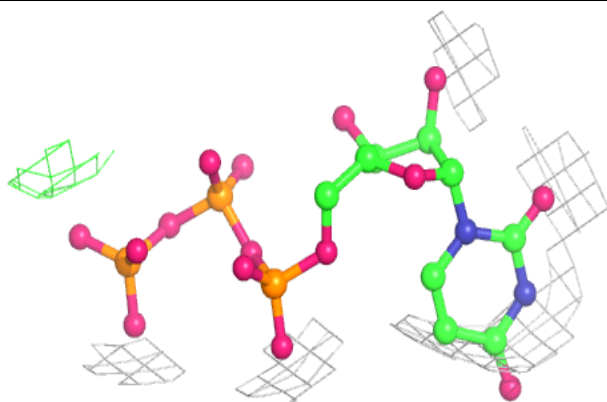
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	ZN	DDD	1501	1/1	0.88	0.02	423,423,423,423	0
11	MG	DDD	1504	1/1	0.89	0.20	148,148,148,148	0
9	UTP	CCC	1401	29/29	0.90	0.37	239,278,320,322	0
11	MG	DDD	1503	1/1	0.95	0.25	170,170,170,170	0
10	ZN	DDD	1502	1/1	0.99	0.12	194,194,194,194	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 CCC 1401:

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.