



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 03:33 AM EST

PDB ID : 6UU8
Title : E. coli mutant sigma-S transcription initiation complex with a 7-nt RNA
("Fresh" mutant crystal soaked with GTP, UTP, and CTP for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
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) : 2.27

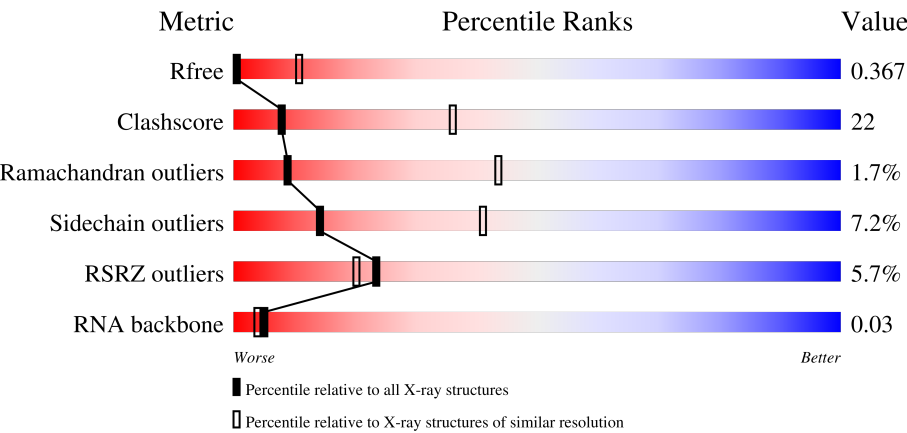
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)
RNA backbone	3102	1058 (5.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div><div>7%</div><div>58%</div><div>33%</div><div>• 5%</div></div>
1	BBB	242	<div><div>4%</div><div>62%</div><div>30%</div><div>• 6%</div></div>
2	CCC	1342	<div><div>3%</div><div>64%</div><div>32%</div><div>•</div></div>
3	DDD	1407	<div><div>6%</div><div>59%</div><div>35%</div><div>• •</div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DPO	DDD	1504	-	-	X	-
9	MG	DDD	1503	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28931 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	268	Total	C	N	O	S	0	0	0
			2186	1370	405	407	4			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP A0A377K1M2
FFF	219	GLY	ILE	engineered mutation	UNP A0A377K1M2
FFF	221	ALA	SER	engineered mutation	UNP A0A377K1M2
FFF	329	LEU	-	expression tag	UNP A0A377K1M2
FFF	330	GLU	-	expression tag	UNP A0A377K1M2
FFF	331	HIS	-	expression tag	UNP A0A377K1M2
FFF	332	HIS	-	expression tag	UNP A0A377K1M2
FFF	333	HIS	-	expression tag	UNP A0A377K1M2
FFF	334	HIS	-	expression tag	UNP A0A377K1M2
FFF	335	HIS	-	expression tag	UNP A0A377K1M2
FFF	336	HIS	-	expression tag	UNP A0A377K1M2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	29	Total	C	N	O	P	0	0	0
			595	283	107	176	29			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	32	Total	C	N	O	P	0	0	0
			652	312	117	192	31			

- Molecule 8 is a RNA chain called RNA 7-mer (de novo synthesized).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	7	Total	C	N	O	P	0	0	0
			160	67	27	57	9			

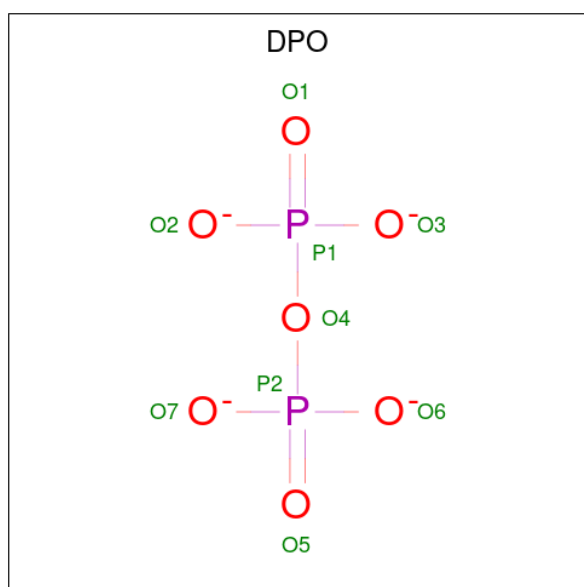
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 11 is DIPHOSPHATE (three-letter code: DPO) (formula: O₇P₂).

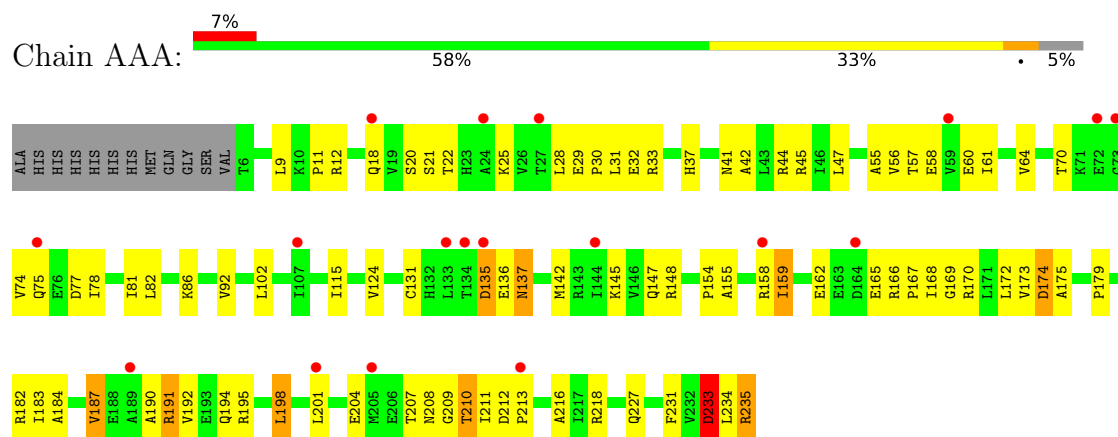


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	DDD	1	Total	O	P	0	0
			9	7	2		

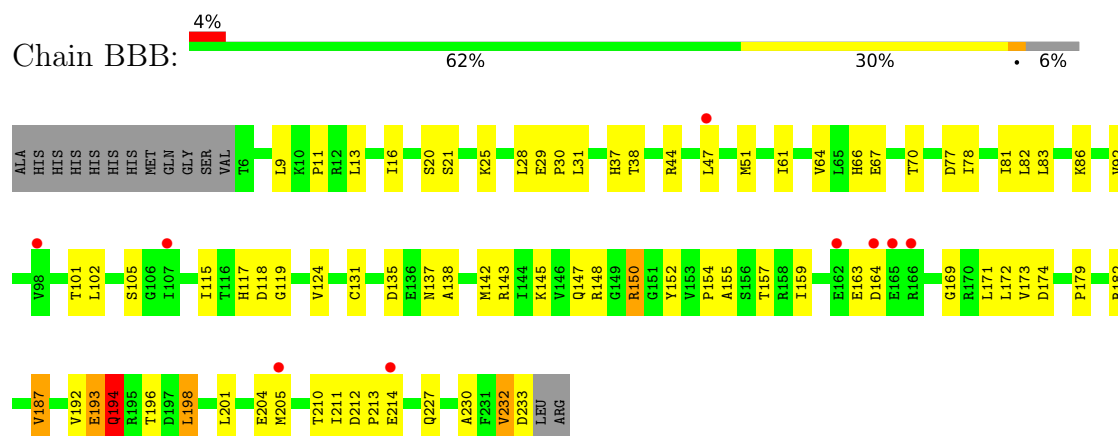
3 Residue-property plots [i](#)

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

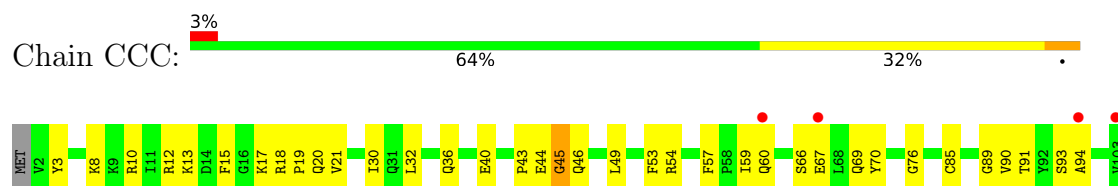
- Molecule 1: DNA-directed RNA polymerase subunit alpha

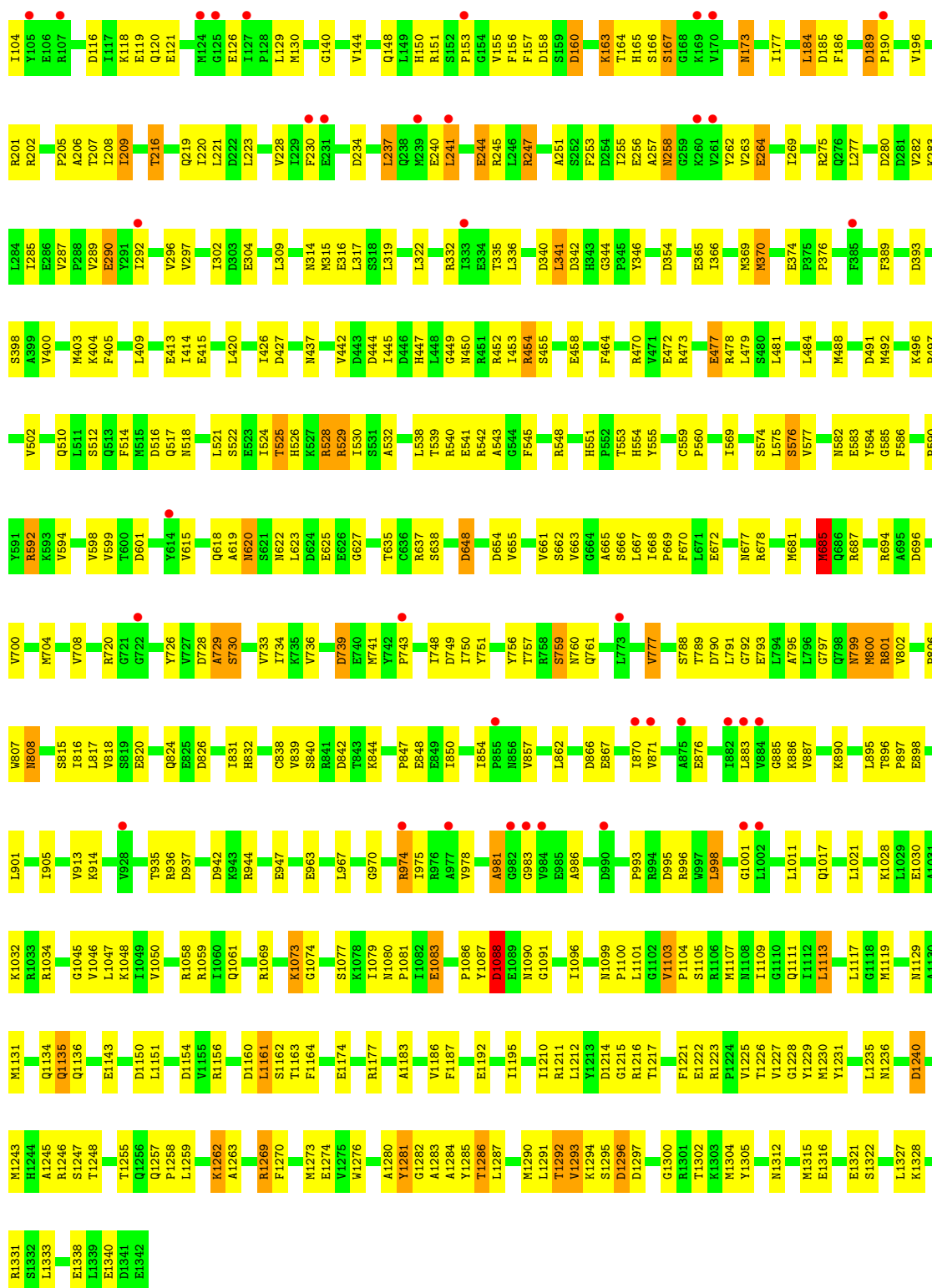


- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

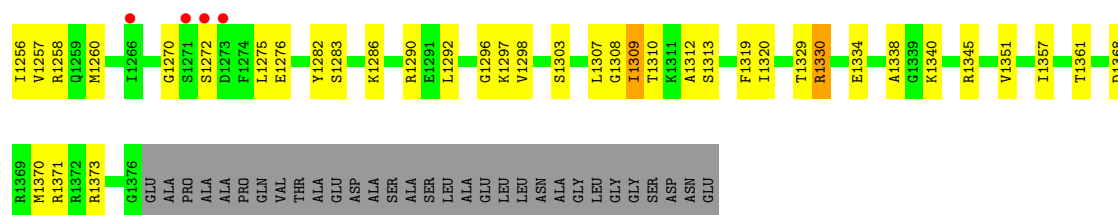




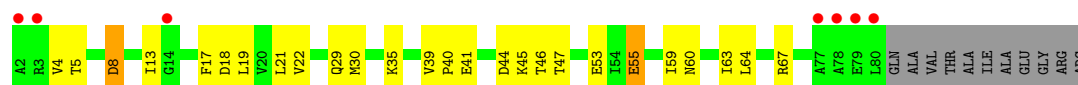
• Molecule 3: DNA-directed RNA polymerase subunit beta'



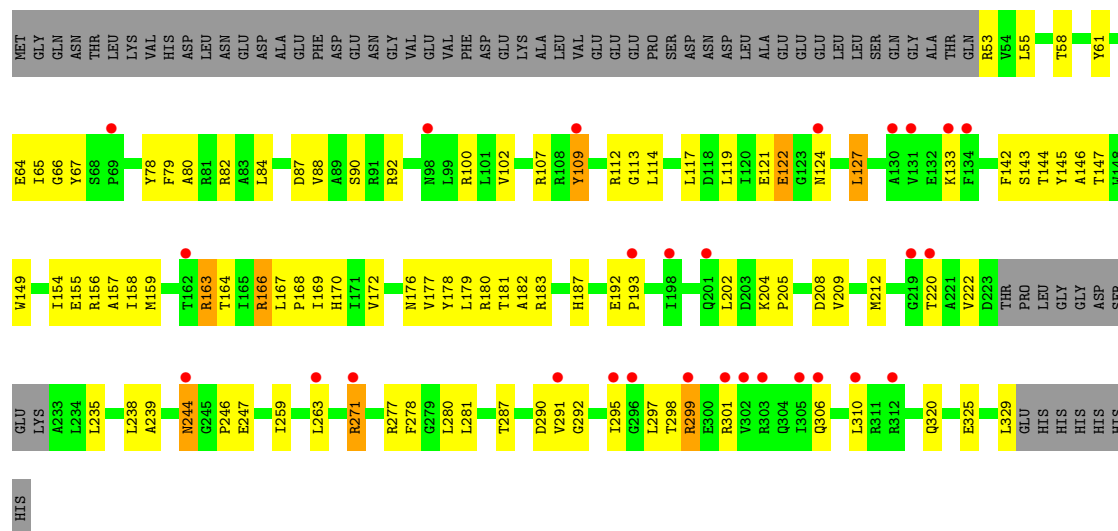
E1158	D1073	E981	A936	V825	I754	G665	S503	E418	G333	T212	V97	MET
I1159	A1077	L982	H897	I826	I755	E666	Q504	E421	K334	K213	R98	LYS
G1160	L1078	D986	C988	E527	P758	G585	D505	V422	Q335	E214	R101	ASP
I1162	K1079	D986	R901	V831	I759	G586	V506	L423	G336	R220	A108	LEU
V1163	I1080	E993	K911	L835	N762	S590	L510	M424	F338	L223	S109	LYS
S1164	S994	S994	I915	R836	F763	I591	Y511	R425	R339	L224	P110	PHE
F1165	R996	Y996	I915	R838	R764	V592	M513	A426	Q340	F227	T111	LEU
E1168	A1083	G996	G916	V839	R764	G671	M513	T428	N341	K232	A112	ALA
T1169	Q1084	V997	V917	V839	L673	L672	T514	L429	R347	K233	H113	GLN
K1170	I1087	G1000	I918	L840	G678	A595	R515	R430	K345	K232	I114	THR
R1173	V1088	L1003	S922	G841	N768	K598	R516	H433	R346	P234	W115	LYS
R1174	L1089	L1003	I923	R842	L770	K599	C517	L432	V347	K233	K118	THR
R1175	P1090	T1016	I923	R842	Q771	S602	N519	I434	V357	M237	S119	E16
V1176	G1092	G1017	G924	T844	I774	A520	A520	I434	V357	M237	S119	F17
P1179	T1093	A1018	E925	A845	I775	E523	E523	E443	G358	L245	P121	K21
Y1186	P1096	N1019	P926	D847	T776	G524	G524	G444	P359	P246	S122	I22
E1187	A1097	D1021	T928	V848	H777	M525	M525	K445	Y360	P247	R123	S26
E1188	Q1098	L830	Q929	K850	G778	L612	V526	Q448	L362	D248	L127	P27
M1189	Y1099	T931	T931	P851	T703	G613	L527	L452	L363	D256	M130	D28
W1193	G1103	T1024	N932	G852	E704	L614	T528	A456	Q365	A261	D134	S34
R1194	K1104	M1025	R933	T853	T705	T617	E532	A456	C366	T262	I136	E42
Q1195	A1105	T1028	F935	A854	T786	V618	A533	A457	G367	E278	E136	T43
L1196	I1106	T1029	H936	D855	I707	I619	E534	M458	L368	L279	L139	I44
N1197	V1107	E1030	I937	L856	L788	F620	R535	F461	P369	K370	L139	N45
F1198	E1110	V1031	V858	L857	K789	A621	L536	D464	K371	L283	S143	T48
F1199	E1111	S1032	P859	R859	A791	D622	Y537	Q465	K372	P288	M151	F49
E1200	D1111	A941	R860	R860	S792	G623	R338	Q466	E375	L290	Q157	K50
R1203	G1112	S942	R861	T862	G794	M625	L541	A467	L376	D289	Q158	P51
V1209	V1113	R1036	L863	T795	G795	Y626	S543	V468	F377	E295	T159	E52
I1210	Q1114	F1037	L864	T796	I722	T627	S543	L472	K378	E295	L160	R53
P1214	I1115	E947	H865	T797	Y723	G628	L544	E475	F379	Q300	T161	F57
L1223	S1116	S948	C869	R798	W724	F629	H545	A476	Y382	V303	Q164	C58
R1224	D1042	D1043	S957	R799	A730	A630	A546	Q477	G383	D304	D167	A69
G1225	Q1044	Q1043	I958	L800	R731	A632	V548	L478	K384	A305	D167	R60
V1226	T1047	L960	L872	L800	G732	R634	V550	E479	L385	R311	G173	I61
T1230	D1051	V963	E873	D802	S733	S635	I552	T487	E386	R312	D174	F62
Q1238	L1052	K964	E879	V808	Q739	S638	D558	M488	R388	L316	E175	D67
R1242	L1054	S965	K881	V808	A741	I641	V564	I490	T392	S319	F176	Y68
Q1243	S1058	V968	R883	V882	G742	D643	K570	S492	K395	R320	A182	F69
G1245	L1059	S969	S884	V885	H743	M644	K570	S492	K395	R320	A182	C70
V1246	V1061	G971	V886	G745	R744	V645	V574	P493	K398	R322	E197	L71
N1249	V974	C988	S887	L746	G745	I646	A577	M495	K399	P323	C198	L78
D1250	H817	D889	V887	T816	G745	I646	A577	P493	K398	R322	E197	V90
V1255	E818	D889	V887	T816	G745	I646	A577	P493	K398	R322	E197	S91
	S1063	I975	C988	H817	G745	I646	A577	P493	K398	R322	E197	T92
	A1065	T976	D889	V887	G745	I646	A577	P493	K398	R322	E197	V93
	E1066	S977	G993	V894	T750	E662	M581	E414	V415	M330	N209	
	R1067	T980	V894	D751	E662	M581	E414	V415	M330	R332	E211	



- Molecule 4: DNA-directed RNA polymerase subunit omega



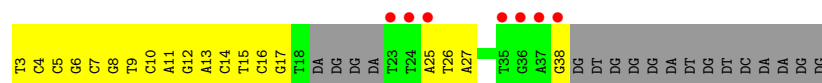
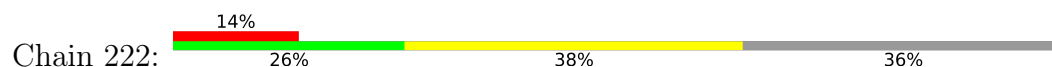
- Molecule 5: RNA polymerase sigma factor RpoS



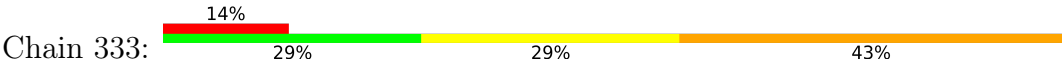
- Molecule 6: Synthetic DNA 50-mer (promoter non-template strand)



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



- Molecule 8: RNA 7-mer (de novo synthesized)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.46Å 154.50Å 235.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 4.40 49.38 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.38-4.40) 99.1 (49.38-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.357 , 0.380 0.344 , 0.367	Depositor DCC
R_{free} test set	1496 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	163.9	Xtriage
Anisotropy	0.949	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 208.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28931	wwPDB-VP
Average B, all atoms (Å ²)	293.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	0.66	0/1809	0.81	0/2450
1	BBB	0.70	0/1789	0.80	0/2425
2	CCC	0.67	0/10745	0.89	12/14499 (0.1%)
3	DDD	0.67	0/10729	0.84	1/14487 (0.0%)
4	EEE	0.69	0/629	0.88	0/847
5	FFF	0.66	0/2213	0.64	0/2981
6	111	0.30	0/665	0.65	0/1022
7	222	0.26	0/729	0.62	0/1121
8	333	0.28	0/142	0.60	0/219
All	All	0.65	0/29450	0.83	13/40051 (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 (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	153	PRO	N-CD-CG	-8.32	90.73	103.20
2	CCC	1088	ASP	CB-CA-C	-6.47	97.46	110.40
2	CCC	1048	LYS	CB-CA-C	-6.11	98.18	110.40
2	CCC	528	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	CCC	1087	TYR	CB-CG-CD1	5.52	124.31	121.00
2	CCC	685	MET	CA-CB-CG	5.47	122.60	113.30
2	CCC	974	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	454	ARG	CB-CA-C	-5.15	100.09	110.40
3	DDD	278	ARG	CG-CD-NE	5.12	122.55	111.80
2	CCC	153	PRO	N-CA-CB	-5.08	97.01	102.60
2	CCC	1087	TYR	CB-CG-CD2	-5.07	117.96	121.00
2	CCC	216	THR	CA-CB-OG1	-5.04	98.42	109.00
2	CCC	685	MET	N-CA-CB	5.01	119.62	110.60

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

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	90	0
1	BBB	1767	0	1789	98	0
2	CCC	10576	0	10591	440	0
3	DDD	10568	0	10781	597	0
4	EEE	627	0	634	21	0
5	FFF	2186	0	2230	122	1
6	111	595	0	327	22	0
7	222	652	0	364	39	0
8	333	160	0	75	16	0
9	CCC	1	0	0	0	0
9	DDD	1	0	0	0	0
10	DDD	2	0	0	1	0
11	DDD	9	0	0	2	0
All	All	28931	0	28604	1235	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:846:GLU:HG3	3:DDD:860:ARG:NH2	1.42	1.35
2:CCC:896:THR:OG1	2:CCC:897:PRO:HD2	1.22	1.34
3:DDD:525:MET:N	3:DDD:548:VAL:HG23	1.42	1.31
2:CCC:157:PHE:O	2:CCC:442:VAL:HG13	1.31	1.28
3:DDD:846:GLU:CG	3:DDD:860:ARG:NH2	1.96	1.28
3:DDD:525:MET:O	3:DDD:548:VAL:HG22	1.26	1.27
3:DDD:646:ILE:HG23	3:DDD:741:ALA:O	1.40	1.17
3:DDD:43:THR:HG21	5:FFF:164:THR:HG22	1.15	1.13
3:DDD:846:GLU:HA	3:DDD:860:ARG:CZ	1.78	1.12
3:DDD:525:MET:N	3:DDD:548:VAL:CG2	2.14	1.10
2:CCC:157:PHE:O	2:CCC:442:VAL:CG1	1.99	1.10
2:CCC:444:ASP:O	2:CCC:450:ASN:ND2	1.84	1.10
3:DDD:847:ASP:OD1	3:DDD:860:ARG:HB2	1.49	1.09
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	1.11	1.08
3:DDD:948:SER:CB	3:DDD:1022:PRO:HG3	1.83	1.08
3:DDD:395:LYS:HE2	5:FFF:329:LEU:HD22	1.35	1.07
2:CCC:510:GLN:HG3	8:333:15:A:O2'	1.54	1.07
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.38	1.06
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	1.90	1.05
2:CCC:1073:LYS:NZ	8:333:20:G:OP1	1.88	1.05
3:DDD:846:GLU:HA	3:DDD:860:ARG:NE	1.71	1.04
1:BBB:67:GLU:CB	1:BBB:171:LEU:HD22	1.87	1.03
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	1.04	1.03
3:DDD:948:SER:HB2	3:DDD:1022:PRO:CG	1.88	1.03
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.40	1.01
5:FFF:263:LEU:HD13	5:FFF:281:LEU:CD1	1.91	1.00
2:CCC:896:THR:OG1	2:CCC:897:PRO:CD	2.08	1.00
3:DDD:839:VAL:CG1	3:DDD:864:LEU:HD12	1.92	0.99
1:AAA:75:GLN:O	2:CCC:729:ALA:HB2	1.63	0.98
7:222:14:DC:O2	8:333:16:G:N1	1.96	0.97
3:DDD:525:MET:O	3:DDD:548:VAL:CG2	2.13	0.97
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.43	0.96
2:CCC:1105:SER:OG	3:DDD:731:ARG:NH1	1.99	0.96
3:DDD:888:CYS:SG	10:DDD:1502:ZN:ZN	1.54	0.96
3:DDD:491:LEU:HD13	3:DDD:610:ARG:NH2	1.81	0.96
1:BBB:25:LYS:HG2	1:BBB:204:GLU:HG2	1.49	0.95
2:CCC:896:THR:HG1	2:CCC:897:PRO:HD2	1.22	0.95
2:CCC:1221:PHE:CE1	3:DDD:633:ALA:O	2.19	0.95
3:DDD:322:ARG:HD3	3:DDD:323:PRO:HD2	1.46	0.94
3:DDD:501:VAL:HG21	3:DDD:602:SER:OG	1.66	0.94
3:DDD:750:PRO:HD3	3:DDD:777:HIS:HB3	1.49	0.94
3:DDD:491:LEU:CD1	3:DDD:610:ARG:HH21	1.78	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:525:MET:H	3:DDD:548:VAL:HG23	1.04	0.94
7:222:14:DC:O2	8:333:16:G:N2	2.02	0.93
1:BBB:67:GLU:HB3	1:BBB:171:LEU:CD2	1.96	0.92
1:AAA:56:VAL:O	1:AAA:175:ALA:HB2	1.68	0.92
1:BBB:83:LEU:HG	3:DDD:526:VAL:CG1	2.00	0.92
3:DDD:388:ARG:NH2	3:DDD:414:GLU:OE1	2.03	0.91
2:CCC:32:LEU:HA	2:CCC:130:MET:HE1	1.49	0.91
3:DDD:846:GLU:H	3:DDD:860:ARG:HE	1.14	0.91
3:DDD:846:GLU:CA	3:DDD:860:ARG:NE	2.32	0.90
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:HA	1.53	0.90
5:FFF:109:TYR:OH	5:FFF:155:GLU:HG3	1.70	0.90
1:BBB:193:GLU:O	1:BBB:194:GLN:HB2	1.71	0.90
2:CCC:251:ALA:CB	2:CCC:263:VAL:HG11	2.02	0.89
3:DDD:846:GLU:HG3	3:DDD:860:ARG:HH21	1.14	0.89
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	1.88	0.89
5:FFF:109:TYR:OH	5:FFF:155:GLU:CG	2.20	0.89
3:DDD:646:ILE:CG2	3:DDD:741:ALA:O	2.21	0.89
3:DDD:948:SER:HB2	3:DDD:1022:PRO:HG3	0.91	0.89
5:FFF:163:ARG:HD3	5:FFF:167:LEU:HD12	1.55	0.89
1:BBB:78:ILE:HG21	1:BBB:171:LEU:HD11	1.55	0.88
5:FFF:263:LEU:HD13	5:FFF:281:LEU:HD11	1.54	0.88
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CD2	2.08	0.88
3:DDD:525:MET:C	3:DDD:548:VAL:HG22	1.94	0.88
1:BBB:83:LEU:HD11	3:DDD:526:VAL:O	1.74	0.87
3:DDD:846:GLU:N	3:DDD:860:ARG:HE	1.72	0.87
2:CCC:158:ASP:OD2	2:CCC:445:ILE:HD11	1.74	0.86
1:BBB:179:PRO:HG3	1:BBB:211:ILE:HD12	1.56	0.86
3:DDD:865:HIS:CE1	3:DDD:901:ARG:HH22	1.93	0.86
2:CCC:726:TYR:HB3	2:CCC:733:VAL:CG2	2.04	0.86
3:DDD:491:LEU:CD1	3:DDD:610:ARG:NH2	2.36	0.85
7:222:14:DC:O2	8:333:16:G:C2	2.28	0.85
3:DDD:846:GLU:HG2	3:DDD:860:ARG:NH2	1.91	0.85
3:DDD:491:LEU:HD11	3:DDD:610:ARG:HH21	1.40	0.85
3:DDD:525:MET:H	3:DDD:548:VAL:CG2	1.81	0.85
3:DDD:525:MET:HB2	3:DDD:548:VAL:HG21	1.56	0.85
3:DDD:793:SER:OG	3:DDD:928:THR:OG1	1.92	0.85
3:DDD:673:VAL:CG1	3:DDD:678:ARG:HB2	2.07	0.85
3:DDD:359:PRO:O	3:DDD:625:MET:HE1	1.76	0.84
3:DDD:525:MET:CA	3:DDD:548:VAL:CG2	2.54	0.84
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.60	0.84
1:BBB:86:LYS:HE2	1:BBB:174:ASP:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HD13	1.56	0.84
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:NH1	1.93	0.84
1:BBB:78:ILE:HG21	1:BBB:171:LEU:CD1	2.08	0.83
2:CCC:1295:SER:OG	3:DDD:346:ARG:O	1.95	0.83
2:CCC:898:GLU:HG3	5:FFF:259:ILE:CD1	2.08	0.83
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HG3	1.60	0.83
1:BBB:212:ASP:OD1	1:BBB:213:PRO:HD2	1.76	0.83
2:CCC:555:TYR:CD1	2:CCC:637:ARG:NH2	2.47	0.83
3:DDD:839:VAL:HG12	3:DDD:864:LEU:CD1	2.03	0.83
2:CCC:1221:PHE:HE1	3:DDD:633:ALA:O	1.56	0.83
3:DDD:525:MET:C	3:DDD:548:VAL:CG2	2.47	0.83
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.61	0.83
3:DDD:395:LYS:HG2	5:FFF:329:LEU:HD13	1.59	0.83
3:DDD:846:GLU:H	3:DDD:860:ARG:NE	1.77	0.82
3:DDD:528:THR:O	3:DDD:528:THR:OG1	1.94	0.82
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	1.80	0.82
3:DDD:846:GLU:HG3	3:DDD:860:ARG:HH22	1.44	0.82
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD11	1.62	0.81
2:CCC:681:MET:O	2:CCC:685:MET:HG2	1.80	0.81
3:DDD:643:ASP:HB3	3:DDD:722:ILE:CD1	2.09	0.81
2:CCC:1333:LEU:O	3:DDD:113:HIS:CE1	2.34	0.81
2:CCC:790:ASP:O	2:CCC:792:GLY:N	2.14	0.81
3:DDD:121:PRO:O	3:DDD:122:SER:HB3	1.82	0.80
3:DDD:475:GLU:O	3:DDD:479:GLU:HG2	1.81	0.80
3:DDD:759:ILE:HG12	3:DDD:771:GLN:HG2	1.62	0.80
3:DDD:614:LEU:HG	4:EEE:5:THR:HG21	1.62	0.80
2:CCC:165:HIS:CE1	2:CCC:190:PRO:HG3	2.16	0.80
1:AAA:9:LEU:HD21	1:AAA:198:LEU:HD11	1.63	0.79
3:DDD:506:VAL:HG22	3:DDD:629:PHE:CZ	2.18	0.79
3:DDD:22:ILE:HD11	3:DDD:1319:PHE:CE1	2.17	0.79
2:CCC:186:PHE:CE1	2:CCC:196:VAL:HG22	2.16	0.79
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:HE3	1.65	0.79
1:BBB:86:LYS:HE2	1:BBB:174:ASP:N	1.98	0.79
3:DDD:513:MET:HE1	3:DDD:631:TYR:CE2	2.18	0.78
2:CCC:255:ILE:HD12	2:CCC:263:VAL:HG21	1.65	0.78
2:CCC:898:GLU:CG	5:FFF:259:ILE:CD1	2.60	0.78
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	1.84	0.78
3:DDD:846:GLU:CG	3:DDD:860:ARG:HH21	1.79	0.78
3:DDD:1156:LEU:HD21	3:DDD:1209:VAL:HG22	1.66	0.78
3:DDD:26:SER:OG	3:DDD:28:ASP:OD1	1.99	0.78
1:BBB:67:GLU:N	1:BBB:171:LEU:HD21	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.65	0.77
2:CCC:901:LEU:CD1	5:FFF:278:PHE:CE2	2.67	0.77
3:DDD:846:GLU:N	3:DDD:860:ARG:NE	2.31	0.77
1:AAA:174:ASP:OD2	2:CCC:1059:ARG:NH2	2.17	0.77
1:BBB:179:PRO:HG3	1:BBB:211:ILE:CD1	2.15	0.77
3:DDD:846:GLU:N	3:DDD:860:ARG:HG3	1.99	0.77
5:FFF:156:ARG:NH2	6:111:33:DT:OP2	2.18	0.77
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.65	0.77
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.66	0.77
2:CCC:237:LEU:HD12	2:CCC:289:VAL:HA	1.66	0.76
3:DDD:432:LEU:HD12	3:DDD:499:ILE:HD13	1.67	0.76
3:DDD:43:THR:CG2	5:FFF:164:THR:HG22	2.08	0.76
2:CCC:3:TYR:O	2:CCC:8:LYS:HE3	1.83	0.76
3:DDD:452:LEU:HB3	3:DDD:500:ILE:HG23	1.68	0.76
1:AAA:75:GLN:C	2:CCC:729:ALA:HB2	2.07	0.76
2:CCC:447:HIS:HD2	2:CCC:449:GLY:H	1.34	0.76
1:AAA:227:GLN:OE1	1:BBB:11:PRO:HD3	1.85	0.75
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.14	0.75
3:DDD:1029:THR:HG23	3:DDD:1121:LEU:HG	1.69	0.75
1:AAA:55:ALA:HB1	1:AAA:175:ALA:HB1	1.69	0.74
3:DDD:399:LYS:HE3	5:FFF:329:LEU:HD21	1.67	0.74
5:FFF:107:ARG:HD3	6:111:43:DT:H4'	1.70	0.74
2:CCC:555:TYR:CE1	2:CCC:637:ARG:NH2	2.55	0.74
2:CCC:1333:LEU:O	3:DDD:113:HIS:HE1	1.70	0.74
1:AAA:86:LYS:NZ	2:CCC:826:ASP:OD2	2.20	0.74
1:AAA:11:PRO:O	1:BBB:230:ALA:HB2	1.86	0.74
7:222:12:DG:N2	8:333:18:C:O2	2.19	0.74
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.70	0.74
2:CCC:447:HIS:CD2	2:CCC:449:GLY:H	2.04	0.74
2:CCC:1105:SER:HB3	3:DDD:731:ARG:HD2	1.70	0.74
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:H	1.52	0.73
3:DDD:816:THR:HG22	3:DDD:818:GLU:H	1.52	0.73
1:AAA:60:GLU:HG3	1:AAA:169:GLY:O	1.88	0.73
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG21	1.69	0.73
1:BBB:9:LEU:HD21	1:BBB:198:LEU:HD11	1.70	0.73
5:FFF:182:ALA:HB1	5:FFF:193:PRO:HG3	1.68	0.73
2:CCC:1105:SER:CB	3:DDD:731:ARG:HD2	2.19	0.73
3:DDD:703:THR:OG1	3:DDD:704:GLU:N	2.21	0.73
1:BBB:174:ASP:OD2	3:DDD:525:MET:CE	2.37	0.73
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:CE	2.19	0.73
6:111:25:DC:O2	7:222:38:DG:N2	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:44:ARG:HH12	3:DDD:538:ARG:CD	2.02	0.72
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG12	1.71	0.72
3:DDD:895:CYS:SG	3:DDD:898:CYS:HB2	2.27	0.72
3:DDD:510:LEU:HD11	3:DDD:624:ILE:HG23	1.71	0.72
3:DDD:1156:LEU:HD21	3:DDD:1224:ARG:HH21	1.54	0.72
2:CCC:230:PHE:CD1	2:CCC:292:ILE:HD11	2.25	0.72
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	1.70	0.72
3:DDD:698:MET:O	3:DDD:702:GLN:HB3	1.89	0.72
1:BBB:83:LEU:HG	3:DDD:526:VAL:HG11	1.70	0.72
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.72	0.71
2:CCC:244:GLU:HG2	2:CCC:245:ARG:N	2.05	0.71
2:CCC:808:ASN:HA	3:DDD:629:PHE:HB3	1.70	0.71
1:AAA:158:ARG:HD2	1:AAA:172:LEU:CD2	2.19	0.71
2:CCC:18:ARG:NH2	2:CCC:620:ASN:O	2.23	0.71
1:AAA:227:GLN:OE1	1:BBB:11:PRO:CD	2.39	0.71
1:AAA:58:GLU:HG2	1:AAA:172:LEU:HD12	1.72	0.71
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.24	0.71
3:DDD:518:VAL:HG23	3:DDD:716:GLN:OE1	1.91	0.71
2:CCC:890:LYS:HG3	2:CCC:914:LYS:HE3	1.72	0.71
3:DDD:895:CYS:SG	3:DDD:898:CYS:CB	2.79	0.71
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD13	1.72	0.70
2:CCC:1281:TYR:OH	3:DDD:431:ARG:O	2.09	0.70
3:DDD:43:THR:HG21	5:FFF:164:THR:CG2	2.09	0.70
2:CCC:1304:MET:HE1	3:DDD:472:LEU:HD13	1.71	0.70
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	1.73	0.70
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:HH12	1.54	0.70
2:CCC:93:SER:OG	2:CCC:126:GLU:OE1	2.08	0.70
1:BBB:124:VAL:HG21	1:BBB:210:THR:HG22	1.73	0.70
3:DDD:501:VAL:CG2	3:DDD:602:SER:OG	2.39	0.70
3:DDD:505:ASP:HB2	3:DDD:629:PHE:CD1	2.26	0.70
2:CCC:452:ARG:NH1	2:CCC:458:GLU:OE2	2.19	0.70
3:DDD:359:PRO:O	3:DDD:625:MET:CE	2.38	0.70
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:HD11	1.73	0.70
3:DDD:134:ASP:CG	3:DDD:159:ILE:HD11	2.12	0.70
3:DDD:935:PHE:HZ	3:DDD:1135:THR:HG1	1.38	0.70
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:CG2	2.22	0.70
3:DDD:958:ILE:HG23	3:DDD:982:LEU:CD1	2.22	0.70
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.22	0.69
3:DDD:312:ARG:HG2	3:DDD:312:ARG:O	1.92	0.69
5:FFF:119:LEU:HD21	5:FFF:158:ILE:HD11	1.74	0.69
2:CCC:648:ASP:OD1	2:CCC:648:ASP:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.20	0.69
5:FFF:159:MET:SD	5:FFF:172:VAL:HG11	2.33	0.69
3:DDD:362:ARG:N	3:DDD:365:GLN:OE1	2.21	0.69
3:DDD:1133:ASP:OD2	3:DDD:1134:ILE:N	2.26	0.69
2:CCC:257:ALA:HB3	2:CCC:262:TYR:CE2	2.28	0.69
2:CCC:890:LYS:HE3	2:CCC:914:LYS:HE2	1.75	0.69
3:DDD:519:ASN:OD1	3:DDD:520:ALA:N	2.22	0.69
3:DDD:643:ASP:HB3	3:DDD:722:ILE:HG13	1.75	0.69
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:CA	2.22	0.69
1:BBB:78:ILE:CG2	1:BBB:171:LEU:CD1	2.70	0.69
1:BBB:193:GLU:O	1:BBB:194:GLN:CB	2.41	0.69
2:CCC:514:PHE:HZ	7:222:16:DC:H5'	1.57	0.69
2:CCC:1221:PHE:CD1	3:DDD:633:ALA:O	2.45	0.69
2:CCC:10:ARG:NH2	2:CCC:790:ASP:OD1	2.25	0.69
2:CCC:163:LYS:HG2	2:CCC:164:THR:N	2.06	0.69
1:BBB:67:GLU:CB	1:BBB:171:LEU:CD2	2.65	0.68
3:DDD:643:ASP:HB3	3:DDD:722:ILE:HD12	1.74	0.68
1:AAA:158:ARG:CD	1:AAA:172:LEU:HD21	2.21	0.68
3:DDD:525:MET:CB	3:DDD:548:VAL:HG21	2.22	0.68
1:BBB:155:ALA:O	1:BBB:159:ILE:HG22	1.93	0.68
2:CCC:201:ARG:HB2	2:CCC:369:MET:CE	2.24	0.68
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.26	0.68
2:CCC:251:ALA:HB2	2:CCC:263:VAL:HG11	1.72	0.68
3:DDD:506:VAL:HG13	3:DDD:625:MET:HA	1.76	0.68
2:CCC:1192:GLU:OE2	3:DDD:641:ILE:HG22	1.94	0.68
3:DDD:646:ILE:HG12	3:DDD:741:ALA:O	1.94	0.68
2:CCC:663:VAL:O	2:CCC:666:SER:OG	2.11	0.68
1:BBB:44:ARG:NH1	3:DDD:538:ARG:HD2	2.09	0.68
3:DDD:432:LEU:HD12	3:DDD:499:ILE:CD1	2.24	0.68
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD11	1.76	0.67
7:222:13:DA:H2'	7:222:14:DC:C6	2.29	0.67
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.77	0.67
1:AAA:211:ILE:CG2	1:AAA:216:ALA:HB2	2.24	0.67
3:DDD:792:ASN:N	3:DDD:792:ASN:OD1	2.24	0.67
2:CCC:342:ASP:O	2:CCC:437:ASN:CG	2.32	0.67
3:DDD:392:THR:CG2	5:FFF:320:GLN:O	2.43	0.67
3:DDD:646:ILE:HD11	3:DDD:764:ARG:HB3	1.77	0.67
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.09	0.66
2:CCC:157:PHE:C	2:CCC:442:VAL:HG13	2.12	0.66
3:DDD:643:ASP:HB3	3:DDD:722:ILE:CG1	2.25	0.66
3:DDD:846:GLU:H	3:DDD:860:ARG:HG3	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:143:SER:CB	6:111:41:DT:H72	2.26	0.66
2:CCC:43:PRO:O	2:CCC:54:ARG:NH1	2.28	0.66
2:CCC:1192:GLU:OE2	3:DDD:641:ILE:CG2	2.42	0.66
2:CCC:184:LEU:HG	2:CCC:389:PHE:CE2	2.31	0.66
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE2	1.77	0.66
3:DDD:865:HIS:O	3:DDD:869:CYS:SG	2.51	0.66
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.77	0.66
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.77	0.66
2:CCC:19:PRO:HA	2:CCC:1156:ARG:HD2	1.78	0.65
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	1.96	0.65
3:DDD:320:ASN:O	3:DDD:321:LYS:CB	2.44	0.65
3:DDD:931:THR:O	3:DDD:935:PHE:CD2	2.49	0.65
3:DDD:807:LEU:CD2	3:DDD:1255:VAL:HG13	2.25	0.65
2:CCC:1255:THR:HG23	2:CCC:1322:SER:HB3	1.78	0.65
3:DDD:97:VAL:HG12	3:DDD:101:ARG:HG3	1.78	0.65
3:DDD:320:ASN:O	3:DDD:321:LYS:HB2	1.96	0.65
2:CCC:32:LEU:HD23	2:CCC:130:MET:CE	2.26	0.65
3:DDD:504:GLN:HE22	3:DDD:731:ARG:HH21	1.42	0.65
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.28	0.65
5:FFF:244:ASN:N	5:FFF:244:ASN:OD1	2.30	0.65
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.27	0.65
2:CCC:223:LEU:HD13	2:CCC:426:ILE:HD13	1.78	0.65
1:BBB:44:ARG:NH1	3:DDD:538:ARG:CD	2.60	0.65
3:DDD:937:ILE:HD11	11:DDD:1504:DPO:O4	1.95	0.64
2:CCC:1257:GLN:NE2	3:DDD:341:ASN:O	2.30	0.64
3:DDD:114:ILE:HG12	3:DDD:311:ARG:HD2	1.79	0.64
3:DDD:506:VAL:CG1	3:DDD:625:MET:HA	2.27	0.64
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.26	0.64
2:CCC:3:TYR:O	2:CCC:8:LYS:CE	2.45	0.64
3:DDD:58:CYS:SG	3:DDD:60:ARG:HB3	2.37	0.64
2:CCC:577:VAL:HG23	2:CCC:661:VAL:O	1.97	0.64
2:CCC:1192:GLU:CG	3:DDD:641:ILE:HG21	2.28	0.64
2:CCC:1192:GLU:HG3	3:DDD:641:ILE:HG21	1.77	0.64
2:CCC:1270:PHE:CE1	2:CCC:1290:MET:CE	2.81	0.64
1:BBB:67:GLU:CA	1:BBB:171:LEU:HD21	2.27	0.64
2:CCC:158:ASP:HA	2:CCC:442:VAL:CG1	2.27	0.64
2:CCC:1245:ALA:HB2	3:DDD:372:MET:HG3	1.78	0.64
1:AAA:58:GLU:OE1	1:AAA:170:ARG:HD3	1.98	0.64
3:DDD:1023:HIS:O	3:DDD:1024:THR:HB	1.96	0.64
1:AAA:37:HIS:NE2	1:AAA:187:VAL:HG21	2.13	0.63
3:DDD:836:ARG:HG3	3:DDD:869:CYS:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:886:VAL:HG21	3:DDD:1230:THR:HG21	1.78	0.63
3:DDD:839:VAL:CG1	3:DDD:864:LEU:CD1	2.69	0.63
3:DDD:846:GLU:CB	3:DDD:860:ARG:NH2	2.61	0.63
2:CCC:1270:PHE:CE1	2:CCC:1290:MET:HE1	2.33	0.63
2:CCC:263:VAL:HG13	2:CCC:269:ILE:HD11	1.81	0.63
3:DDD:625:MET:HG2	3:DDD:629:PHE:CE2	2.33	0.63
3:DDD:791:ALA:HB2	7:222:9:DT:C7	2.28	0.63
3:DDD:797:THR:O	3:DDD:801:VAL:HG23	1.99	0.63
1:BBB:78:ILE:CG2	1:BBB:171:LEU:HD13	2.29	0.63
2:CCC:548:ARG:HD3	2:CCC:569:ILE:O	1.98	0.63
3:DDD:491:LEU:HD13	3:DDD:610:ARG:HH22	1.61	0.63
2:CCC:340:ASP:HB3	2:CCC:341:LEU:HG	1.81	0.63
3:DDD:97:VAL:HG11	3:DDD:101:ARG:HE	1.64	0.63
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:CD1	2.29	0.63
2:CCC:510:GLN:CG	8:333:15:A:O2'	2.39	0.63
3:DDD:1156:LEU:CD2	3:DDD:1224:ARG:HH21	2.12	0.62
2:CCC:118:LYS:HD3	2:CCC:488:MET:HG2	1.82	0.62
3:DDD:42:GLU:OE2	5:FFF:166:ARG:HD2	1.98	0.62
3:DDD:525:MET:CA	3:DDD:548:VAL:HG21	2.29	0.62
2:CCC:157:PHE:O	2:CCC:442:VAL:HG12	1.98	0.62
3:DDD:385:LEU:CD2	3:DDD:411:ILE:HD13	2.28	0.62
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.80	0.62
2:CCC:743:PRO:HA	2:CCC:974:ARG:CZ	2.29	0.62
3:DDD:1330:ARG:NH2	7:222:6:DG:OP1	2.32	0.62
3:DDD:1275:LEU:HG	3:DDD:1276:GLU:H	1.65	0.62
3:DDD:1338:ALA:HB3	3:DDD:1340:LYS:HG3	1.82	0.62
2:CCC:263:VAL:CG1	2:CCC:269:ILE:HD11	2.30	0.62
3:DDD:644:MET:HB3	3:DDD:741:ALA:HB2	1.82	0.62
5:FFF:259:ILE:CG2	5:FFF:280:LEU:HD21	2.29	0.62
2:CCC:389:PHE:HB3	2:CCC:420:LEU:HD12	1.82	0.62
2:CCC:292:ILE:CG2	2:CCC:322:LEU:HD11	2.30	0.62
3:DDD:506:VAL:CG2	3:DDD:629:PHE:CZ	2.82	0.62
3:DDD:614:LEU:CG	4:EEE:5:THR:HG21	2.30	0.62
3:DDD:949:SER:HB2	3:DDD:1019:ASN:HD22	1.62	0.62
3:DDD:514:THR:OG1	3:DDD:595:ALA:HA	2.00	0.61
2:CCC:898:GLU:CG	5:FFF:259:ILE:HD13	2.28	0.61
2:CCC:1304:MET:CE	3:DDD:472:LEU:HD13	2.30	0.61
4:EEE:8:ASP:N	4:EEE:8:ASP:OD1	2.33	0.61
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.82	0.61
3:DDD:519:ASN:HA	3:DDD:523:GLU:CD	2.21	0.61
2:CCC:12:ARG:NH2	2:CCC:793:GLU:OE1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:541:GLU:HG3	2:CCC:542:ARG:N	2.16	0.61
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG22	1.80	0.61
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.81	0.61
3:DDD:614:LEU:CD2	4:EEE:5:THR:HG21	2.30	0.61
2:CCC:1129:ASN:HA	2:CCC:1177:ARG:HG3	1.81	0.61
3:DDD:513:MET:CE	3:DDD:631:TYR:CZ	2.83	0.61
3:DDD:552:ILE:HG23	3:DDD:580:TRP:CD1	2.35	0.61
3:DDD:846:GLU:CA	3:DDD:860:ARG:CZ	2.65	0.61
3:DDD:975:ILE:HD12	3:DDD:997:VAL:HG11	1.82	0.61
2:CCC:297:VAL:HG13	2:CCC:317:LEU:HG	1.82	0.61
2:CCC:510:GLN:HG3	8:333:15:A:HO2'	1.64	0.61
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HG	2.30	0.61
5:FFF:259:ILE:HG21	5:FFF:280:LEU:CD1	2.31	0.61
5:FFF:263:LEU:CD1	5:FFF:281:LEU:HG	2.31	0.61
1:AAA:30:PRO:HB2	1:AAA:198:LEU:HD12	1.83	0.61
2:CCC:302:ILE:HG22	2:CCC:309:LEU:HD23	1.82	0.61
3:DDD:609:TYR:HA	3:DDD:617:THR:HG21	1.83	0.61
3:DDD:673:VAL:HG11	3:DDD:678:ARG:HB2	1.81	0.61
3:DDD:1134:ILE:HG23	3:DDD:1138:LEU:HG	1.82	0.61
1:BBB:196:THR:HG21	3:DDD:370:LYS:NZ	2.15	0.61
3:DDD:262:THR:O	5:FFF:222:VAL:HG12	2.01	0.61
1:BBB:86:LYS:HG3	1:BBB:173:VAL:CG1	2.31	0.60
3:DDD:385:LEU:HD23	3:DDD:411:ILE:HD13	1.83	0.60
3:DDD:456:ALA:HB2	3:DDD:499:ILE:HG21	1.82	0.60
3:DDD:929:GLN:O	3:DDD:933:ARG:HB2	2.02	0.60
2:CCC:262:TYR:OH	2:CCC:280:ASP:OD2	2.18	0.60
2:CCC:289:VAL:HG12	2:CCC:319:LEU:HD23	1.82	0.60
2:CCC:743:PRO:HA	2:CCC:974:ARG:NH2	2.16	0.60
3:DDD:1156:LEU:CD2	3:DDD:1209:VAL:HA	2.29	0.60
5:FFF:222:VAL:HG22	5:FFF:235:LEU:HB2	1.83	0.60
2:CCC:49:LEU:CD2	2:CCC:464:PHE:CE2	2.84	0.60
2:CCC:1192:GLU:CD	3:DDD:641:ILE:CG2	2.70	0.60
5:FFF:119:LEU:CD2	5:FFF:158:ILE:HD11	2.31	0.60
1:BBB:30:PRO:HB2	1:BBB:198:LEU:HD12	1.83	0.60
2:CCC:514:PHE:CZ	7:222:16:DC:H5'	2.35	0.60
3:DDD:22:ILE:CD1	3:DDD:1319:PHE:CE1	2.84	0.60
2:CCC:150:HIS:CE1	2:CCC:454:ARG:HG3	2.37	0.60
3:DDD:68:TYR:CD2	3:DDD:78:LEU:HD23	2.37	0.60
3:DDD:759:ILE:HG23	3:DDD:771:GLN:NE2	2.17	0.60
1:BBB:67:GLU:CA	1:BBB:171:LEU:CD2	2.80	0.60
3:DDD:846:GLU:CG	3:DDD:860:ARG:HH22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:135:ASP:OD1	1:BBB:138:ALA:HB2	2.02	0.60
2:CCC:292:ILE:HB	2:CCC:322:LEU:HD11	1.84	0.60
3:DDD:334:LYS:O	3:DDD:339:ARG:HB2	2.02	0.60
3:DDD:609:TYR:HA	3:DDD:617:THR:CG2	2.32	0.60
2:CCC:524:ILE:O	2:CCC:528:ARG:HG2	2.01	0.60
3:DDD:803:VAL:CG2	3:DDD:1313:SER:OG	2.50	0.60
6:111:58:DG:C2	7:222:6:DG:C2	2.90	0.60
2:CCC:1312:ASN:OD1	2:CCC:1312:ASN:O	2.20	0.59
3:DDD:1000:GLY:HA2	3:DDD:1028:ILE:HD12	1.83	0.59
1:BBB:86:LYS:HZ3	1:BBB:174:ASP:HB2	1.67	0.59
1:AAA:155:ALA:CB	1:AAA:174:ASP:OD1	2.50	0.59
2:CCC:36:GLN:O	2:CCC:40:GLU:HB2	2.02	0.59
3:DDD:1110:GLU:O	3:DDD:1113:VAL:HG23	2.02	0.59
3:DDD:1161:GLY:HA3	3:DDD:1179:PRO:HA	1.83	0.59
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	1.85	0.59
3:DDD:139:LEU:HD22	3:DDD:300:GLN:HE22	1.67	0.59
3:DDD:791:ALA:HB2	7:222:9:DT:H71	1.83	0.59
3:DDD:825:VAL:CG1	3:DDD:1242:ARG:HH12	2.14	0.59
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.32	0.59
2:CCC:158:ASP:HA	2:CCC:442:VAL:HG11	1.82	0.59
2:CCC:241:LEU:HD13	2:CCC:285:ILE:HD12	1.84	0.59
3:DDD:43:THR:OG1	3:DDD:44:ILE:N	2.35	0.59
3:DDD:836:ARG:O	3:DDD:840:LEU:HB2	2.02	0.59
3:DDD:843:VAL:HG21	3:DDD:897:HIS:O	2.03	0.59
1:AAA:211:ILE:HG21	1:AAA:216:ALA:HB2	1.83	0.59
3:DDD:399:LYS:CE	5:FFF:329:LEU:HD21	2.33	0.59
3:DDD:513:MET:CE	3:DDD:631:TYR:CE2	2.84	0.59
3:DDD:846:GLU:H	3:DDD:860:ARG:CG	2.15	0.59
1:BBB:37:HIS:NE2	1:BBB:187:VAL:HG21	2.18	0.59
3:DDD:1003:LEU:HD23	3:DDD:1018:ALA:HB2	1.85	0.59
5:FFF:109:TYR:CD2	5:FFF:154:ILE:HG21	2.38	0.59
2:CCC:532:ALA:HB1	2:CCC:538:LEU:HD12	1.85	0.59
3:DDD:245:LEU:HD12	3:DDD:246:PRO:HD2	1.84	0.59
1:BBB:152:TYR:CD2	3:DDD:541:LEU:HD13	2.38	0.59
3:DDD:842:ARG:H	3:DDD:864:LEU:HB2	1.67	0.58
3:DDD:1282:TYR:CE1	3:DDD:1286:LYS:HD2	2.38	0.58
1:BBB:154:PRO:HD2	1:BBB:157:THR:HB	1.84	0.58
2:CCC:414:ILE:HG13	2:CCC:415:GLU:N	2.18	0.58
7:222:14:DC:H6	7:222:14:DC:O5'	1.84	0.58
2:CCC:369:MET:HG3	2:CCC:370:MET:N	2.17	0.58
2:CCC:1285:TYR:HB2	3:DDD:479:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:288:PRO:HG3	5:FFF:92:ARG:HG2	1.86	0.58
2:CCC:1226:THR:H	3:DDD:638:SER:CB	2.16	0.58
3:DDD:646:ILE:HD11	3:DDD:764:ARG:HD3	1.86	0.58
1:AAA:212:ASP:OD1	1:AAA:213:PRO:HD2	2.04	0.58
3:DDD:645:VAL:HG23	3:DDD:645:VAL:O	2.03	0.58
1:BBB:192:VAL:O	1:BBB:194:GLN:N	2.37	0.58
4:EEE:30:MET:HG2	4:EEE:35:LYS:O	2.03	0.58
5:FFF:192:GLU:HG3	5:FFF:193:PRO:HD2	1.86	0.58
2:CCC:510:GLN:NE2	8:333:15:A:O3'	2.37	0.58
2:CCC:559:CYS:HB2	2:CCC:662:SER:HB3	1.86	0.58
3:DDD:518:VAL:HG22	3:DDD:547:ARG:HH22	1.67	0.58
3:DDD:807:LEU:HD23	3:DDD:1255:VAL:HG13	1.86	0.58
3:DDD:842:ARG:HD3	3:DDD:882:VAL:HG21	1.85	0.58
2:CCC:736:VAL:O	2:CCC:741:MET:HE3	2.04	0.57
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD21	1.85	0.57
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.87	0.57
3:DDD:279:LEU:HD13	3:DDD:295:GLU:HB3	1.85	0.57
6:111:56:DG:H1	7:222:7:DC:H42	1.52	0.57
2:CCC:447:HIS:HD2	2:CCC:449:GLY:N	2.03	0.57
3:DDD:707:ILE:HD12	3:DDD:716:GLN:HE21	1.69	0.57
3:DDD:846:GLU:CB	3:DDD:860:ARG:HH21	2.17	0.57
1:BBB:86:LYS:NZ	1:BBB:174:ASP:HB2	2.19	0.57
3:DDD:512:TYR:CD1	3:DDD:635:SER:HB3	2.40	0.57
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD11	1.85	0.57
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:CD	2.34	0.57
5:FFF:133:LYS:NZ	6:111:35:DC:OP2	2.29	0.57
2:CCC:1291:LEU:HA	3:DDD:345:LYS:HD2	1.87	0.57
2:CCC:720:ARG:HD2	2:CCC:736:VAL:HG21	1.86	0.57
4:EEE:29:GLN:HE22	4:EEE:64:LEU:HD22	1.69	0.57
2:CCC:734:ILE:CG2	2:CCC:749:ASP:HB2	2.34	0.57
2:CCC:1186:VAL:HG12	2:CCC:1187:PHE:CD2	2.39	0.57
3:DDD:1134:ILE:CD1	3:DDD:1244:GLN:HG3	2.35	0.57
3:DDD:1156:LEU:HD21	3:DDD:1224:ARG:NH2	2.18	0.57
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.87	0.57
1:AAA:145:LYS:HD3	1:AAA:147:GLN:HE21	1.70	0.57
1:BBB:174:ASP:OD2	3:DDD:525:MET:HE3	2.04	0.57
2:CCC:901:LEU:O	2:CCC:905:ILE:HD12	2.04	0.57
3:DDD:625:MET:HG2	3:DDD:629:PHE:HE2	1.69	0.57
3:DDD:825:VAL:CG1	3:DDD:1242:ARG:NH1	2.67	0.57
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.35	0.57
2:CCC:582:ASN:OD1	2:CCC:586:PHE:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1163:VAL:HG13	3:DDD:1176:VAL:O	2.05	0.56
3:DDD:1309:ILE:HG22	3:DDD:1310:THR:N	2.20	0.56
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG23	1.86	0.56
3:DDD:923:ILE:HD12	3:DDD:1256:ILE:HD12	1.87	0.56
5:FFF:168:PRO:HB2	5:FFF:170:HIS:HD2	1.70	0.56
1:AAA:209:GLY:O	1:AAA:210:THR:C	2.43	0.56
1:AAA:218:ARG:HD3	1:BBB:232:VAL:HG21	1.85	0.56
2:CCC:685:MET:HE2	2:CCC:1235:LEU:HD11	1.87	0.56
1:AAA:45:ARG:NH2	1:BBB:37:HIS:HB2	2.19	0.56
1:BBB:145:LYS:HD3	1:BBB:147:GLN:HE21	1.69	0.56
2:CCC:342:ASP:O	2:CCC:437:ASN:ND2	2.38	0.56
2:CCC:898:GLU:HG2	5:FFF:259:ILE:CD1	2.36	0.56
3:DDD:824:PRO:HD3	3:DDD:878:ASP:O	2.05	0.56
3:DDD:974:VAL:HG11	3:DDD:1028:ILE:HD13	1.88	0.56
5:FFF:61:TYR:CZ	5:FFF:65:ILE:HD11	2.41	0.56
5:FFF:176:ASN:HA	7:222:26:DT:H73	1.88	0.56
2:CCC:599:VAL:HG21	2:CCC:623:LEU:HD21	1.87	0.56
2:CCC:672:GLU:HG2	2:CCC:1187:PHE:HA	1.87	0.56
2:CCC:734:ILE:HD11	2:CCC:777:VAL:HG23	1.88	0.56
2:CCC:993:PRO:HG2	2:CCC:996:ARG:CZ	2.35	0.56
3:DDD:176:PHE:O	3:DDD:176:PHE:CD2	2.58	0.56
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	1.86	0.56
3:DDD:620:PHE:O	3:DDD:624:ILE:HG13	2.05	0.56
5:FFF:298:THR:HG21	5:FFF:301:ARG:HD3	1.87	0.56
3:DDD:118:LYS:NZ	3:DDD:136:GLU:OE2	2.39	0.56
5:FFF:122:GLU:HG2	5:FFF:157:ALA:HB2	1.86	0.56
1:BBB:47:LEU:HA	1:BBB:51:MET:HG2	1.88	0.56
2:CCC:1214:ASP:OD2	2:CCC:1217:THR:HG23	2.06	0.56
3:DDD:97:VAL:HG11	3:DDD:101:ARG:NE	2.20	0.56
3:DDD:458:ASN:OD1	3:DDD:933:ARG:NH2	2.37	0.56
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.36	0.56
4:EEE:53:GLU:HB3	4:EEE:59:ILE:HG12	1.87	0.56
1:AAA:56:VAL:O	1:AAA:175:ALA:CB	2.47	0.56
3:DDD:367:GLY:HA3	3:DDD:448:GLN:HB2	1.86	0.56
3:DDD:513:MET:HE1	3:DDD:631:TYR:CZ	2.40	0.56
3:DDD:709:ARG:O	3:DDD:710:ASP:C	2.43	0.56
1:BBB:182:ARG:HG3	3:DDD:534:GLU:OE2	2.06	0.55
3:DDD:795:TYR:CZ	3:DDD:799:ARG:HD3	2.41	0.55
3:DDD:950:ILE:HD13	3:DDD:995:TYR:HB3	1.88	0.55
2:CCC:244:GLU:HG2	2:CCC:245:ARG:H	1.69	0.55
2:CCC:806:PRO:HB3	3:DDD:505:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:61:TYR:CE2	5:FFF:65:ILE:HD11	2.41	0.55
1:AAA:44:ARG:NH2	2:CCC:1083:GLU:O	2.39	0.55
1:AAA:135:ASP:OD1	1:AAA:136:GLU:N	2.39	0.55
2:CCC:582:ASN:ND2	2:CCC:586:PHE:HB2	2.21	0.55
2:CCC:1105:SER:HB3	3:DDD:731:ARG:HG3	1.87	0.55
3:DDD:686:TRP:CD2	3:DDD:758:PRO:HG3	2.41	0.55
2:CCC:736:VAL:HB	2:CCC:741:MET:HE2	1.88	0.55
3:DDD:888:CYS:CB	3:DDD:898:CYS:SG	2.95	0.55
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CD2	2.42	0.55
2:CCC:739:ASP:OD1	2:CCC:739:ASP:N	2.40	0.55
5:FFF:263:LEU:CD1	5:FFF:281:LEU:CD1	2.78	0.55
2:CCC:89:GLY:HA2	2:CCC:140:GLY:HA3	1.89	0.55
2:CCC:1283:ALA:HB1	2:CCC:1286:THR:OG1	2.07	0.55
3:DDD:843:VAL:CG2	3:DDD:897:HIS:O	2.55	0.55
2:CCC:253:PHE:CE1	2:CCC:287:VAL:HG12	2.42	0.55
5:FFF:82:ARG:HG2	5:FFF:87:ASP:HB2	1.88	0.55
2:CCC:277:LEU:HD12	2:CCC:282:VAL:HG21	1.89	0.55
2:CCC:661:VAL:HG13	2:CCC:665:ALA:HB3	1.87	0.55
2:CCC:666:SER:HA	2:CCC:1186:VAL:HG21	1.89	0.55
2:CCC:1269:ARG:HD3	7:222:11:DA:OP1	2.07	0.55
3:DDD:68:TYR:C	3:DDD:92:VAL:HG13	2.28	0.55
3:DDD:709:ARG:O	3:DDD:709:ARG:CG	2.55	0.55
3:DDD:1042:ASP:OD1	3:DDD:1043:GLY:N	2.40	0.55
2:CCC:1286:THR:HG23	3:DDD:476:ALA:HB1	1.88	0.55
3:DDD:491:LEU:HA	3:DDD:498:PRO:HA	1.89	0.54
3:DDD:1152:GLU:CD	3:DDD:1193:TRP:HH2	2.10	0.54
5:FFF:109:TYR:OH	5:FFF:155:GLU:HG2	2.07	0.54
2:CCC:369:MET:CG	2:CCC:370:MET:N	2.69	0.54
2:CCC:1222:GLU:HB2	3:DDD:512:TYR:OH	2.07	0.54
3:DDD:812:ASP:OD1	3:DDD:812:ASP:N	2.39	0.54
3:DDD:844:THR:HG21	3:DDD:864:LEU:HD21	1.89	0.54
5:FFF:166:ARG:CG	5:FFF:166:ARG:HH11	2.21	0.54
3:DDD:552:ILE:HG13	3:DDD:589:TYR:CE1	2.43	0.54
3:DDD:803:VAL:HG23	3:DDD:1313:SER:OG	2.07	0.54
1:AAA:58:GLU:HG2	1:AAA:172:LEU:CD1	2.37	0.54
2:CCC:240:GLU:HA	2:CCC:283:LYS:O	2.08	0.54
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HG3	2.38	0.54
3:DDD:487:THR:O	3:DDD:490:ILE:HG13	2.08	0.54
2:CCC:1243:MET:SD	3:DDD:445:LYS:HG2	2.48	0.54
3:DDD:707:ILE:HD12	3:DDD:716:GLN:NE2	2.23	0.54
1:AAA:135:ASP:OD1	1:AAA:137:ASN:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:111:THR:HG21	3:DDD:303:VAL:HG11	1.88	0.54
3:DDD:505:ASP:HB2	3:DDD:629:PHE:HD1	1.68	0.54
3:DDD:517:CYS:SG	3:DDD:518:VAL:N	2.81	0.54
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:CD1	2.38	0.54
1:AAA:74:VAL:O	2:CCC:729:ALA:HB3	2.07	0.54
3:DDD:492:SER:O	3:DDD:495:ASN:O	2.25	0.54
5:FFF:102:VAL:HG11	5:FFF:124:ASN:OD1	2.08	0.54
2:CCC:1192:GLU:CD	3:DDD:641:ILE:HG21	2.29	0.54
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:CD1	2.37	0.54
3:DDD:151:MET:SD	3:DDD:151:MET:N	2.80	0.54
1:BBB:83:LEU:HG	3:DDD:526:VAL:HG12	1.88	0.54
2:CCC:936:ARG:CG	2:CCC:937:ASP:N	2.71	0.54
3:DDD:886:VAL:HG21	3:DDD:1230:THR:CG2	2.38	0.54
3:DDD:965:SER:CB	3:DDD:975:ILE:HA	2.37	0.54
1:BBB:155:ALA:HB1	1:BBB:172:LEU:HD23	1.90	0.53
2:CCC:896:THR:CB	2:CCC:897:PRO:HD2	2.31	0.53
2:CCC:1160:ASP:O	2:CCC:1161:LEU:C	2.46	0.53
3:DDD:476:ALA:HA	3:DDD:479:GLU:HG3	1.90	0.53
3:DDD:1134:ILE:HD11	3:DDD:1244:GLN:HG3	1.90	0.53
1:AAA:11:PRO:O	1:BBB:230:ALA:CB	2.53	0.53
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HD3	1.73	0.53
1:BBB:83:LEU:HD11	3:DDD:526:VAL:C	2.27	0.53
1:BBB:83:LEU:CG	3:DDD:526:VAL:HB	2.38	0.53
2:CCC:542:ARG:NH2	6:111:54:DA:C6	2.76	0.53
3:DDD:546:ALA:HB3	3:DDD:574:VAL:CG2	2.38	0.53
3:DDD:609:TYR:CA	3:DDD:617:THR:HG21	2.37	0.53
3:DDD:622:ASP:HB3	3:DDD:626:TYR:HE2	1.73	0.53
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	2.08	0.53
1:BBB:86:LYS:HG3	1:BBB:173:VAL:HG12	1.89	0.53
3:DDD:494:ALA:HB2	3:DDD:922:SER:HB3	1.90	0.53
1:AAA:31:LEU:CD1	1:AAA:201:LEU:HB2	2.38	0.53
3:DDD:846:GLU:CA	3:DDD:860:ARG:HE	2.09	0.53
3:DDD:942:SER:O	3:DDD:942:SER:OG	2.23	0.53
5:FFF:53:ARG:O	5:FFF:55:LEU:HG	2.07	0.53
2:CCC:228:VAL:HG22	2:CCC:245:ARG:NH1	2.24	0.53
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CZ	2.44	0.53
2:CCC:528:ARG:HD2	2:CCC:663:VAL:HG21	1.91	0.53
3:DDD:63:GLY:O	3:DDD:98:ARG:HD2	2.09	0.53
5:FFF:180:ARG:NH2	7:222:27:DA:O5'	2.42	0.53
1:AAA:25:LYS:HG2	1:AAA:204:GLU:HG2	1.90	0.53
3:DDD:395:LYS:HG2	5:FFF:329:LEU:CD1	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:843:VAL:HG21	3:DDD:897:HIS:HA	1.91	0.53
1:BBB:86:LYS:CE	1:BBB:174:ASP:HB2	2.38	0.53
3:DDD:494:ALA:CB	3:DDD:922:SER:HB3	2.39	0.53
3:DDD:846:GLU:HA	3:DDD:860:ARG:NH2	2.23	0.53
2:CCC:677:ASN:OD1	3:DDD:779:ALA:HB1	2.08	0.52
3:DDD:800:LEU:CD2	3:DDD:1309:ILE:HD11	2.37	0.52
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.23	0.52
3:DDD:643:ASP:CB	3:DDD:722:ILE:CD1	2.85	0.52
3:DDD:974:VAL:CG1	3:DDD:1028:ILE:HD13	2.39	0.52
5:FFF:159:MET:CE	5:FFF:169:ILE:HG23	2.39	0.52
3:DDD:335:GLN:O	3:DDD:336:GLY:O	2.26	0.52
5:FFF:178:TYR:CE1	5:FFF:209:VAL:HG22	2.44	0.52
1:AAA:159:ILE:O	1:AAA:159:ILE:HG23	2.09	0.52
2:CCC:808:ASN:HD22	2:CCC:808:ASN:N	2.06	0.52
2:CCC:820:GLU:O	2:CCC:824:GLN:HG3	2.10	0.52
2:CCC:1105:SER:HB3	3:DDD:731:ARG:CD	2.39	0.52
3:DDD:512:TYR:CE1	3:DDD:635:SER:HB3	2.45	0.52
5:FFF:144:THR:HG22	6:111:39:DA:H8	1.74	0.52
3:DDD:1308:GLY:O	3:DDD:1310:THR:N	2.43	0.52
2:CCC:263:VAL:HG22	2:CCC:269:ILE:HD12	1.91	0.52
2:CCC:369:MET:HG2	2:CCC:370:MET:HG2	1.92	0.52
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.90	0.52
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	1.91	0.52
3:DDD:949:SER:CB	3:DDD:1019:ASN:HD22	2.23	0.52
3:DDD:1249:ASN:OD1	3:DDD:1250:ASP:N	2.42	0.52
8:333:16:G:H3'	8:333:17:U:C5	2.44	0.52
2:CCC:700:VAL:HG13	2:CCC:1117:LEU:HD23	1.91	0.52
2:CCC:936:ARG:HG2	2:CCC:937:ASP:N	2.24	0.52
2:CCC:1312:ASN:OD1	2:CCC:1312:ASN:C	2.47	0.52
3:DDD:209:ASN:HB2	3:DDD:214:ARG:HG3	1.91	0.52
3:DDD:1156:LEU:HD21	3:DDD:1209:VAL:CG2	2.38	0.52
5:FFF:183:ARG:NH2	7:222:26:DT:OP2	2.43	0.52
1:BBB:83:LEU:CD2	3:DDD:526:VAL:HB	2.39	0.52
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CE2	2.45	0.52
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.91	0.52
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD21	1.92	0.52
2:CCC:569:ILE:O	2:CCC:569:ILE:HG23	2.09	0.52
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.91	0.52
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	1.91	0.52
4:EEE:18:ASP:O	4:EEE:22:VAL:HG23	2.10	0.52
1:AAA:45:ARG:NH1	2:CCC:1216:ARG:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:167:PRO:HG2	1:AAA:170:ARG:HB2	1.91	0.52
3:DDD:261:ALA:HA	5:FFF:220:THR:O	2.10	0.52
3:DDD:513:MET:HE3	3:DDD:631:TYR:CZ	2.45	0.52
5:FFF:263:LEU:HD13	5:FFF:281:LEU:HD12	1.82	0.52
3:DDD:885:VAL:O	3:DDD:1258:ARG:HD2	2.10	0.51
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:HG21	1.91	0.51
3:DDD:1052:GLU:HG2	3:DDD:1053:LEU:H	1.74	0.51
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.09	0.51
2:CCC:734:ILE:HD11	2:CCC:777:VAL:CG2	2.40	0.51
3:DDD:506:VAL:HG22	3:DDD:629:PHE:CE1	2.45	0.51
3:DDD:847:ASP:OD1	3:DDD:860:ARG:CB	2.38	0.51
5:FFF:277:ARG:CD	5:FFF:306:GLN:HE21	2.23	0.51
1:BBB:86:LYS:CG	1:BBB:173:VAL:HG12	2.40	0.51
2:CCC:302:ILE:CG2	2:CCC:309:LEU:HD23	2.39	0.51
2:CCC:444:ASP:HB3	2:CCC:447:HIS:HB2	1.93	0.51
2:CCC:478:ARG:NH1	2:CCC:491:ASP:O	2.44	0.51
3:DDD:101:ARG:O	3:DDD:246:PRO:HG3	2.10	0.51
6:111:38:DT:H2"	6:111:39:DA:C8	2.45	0.51
7:222:7:DC:H5"	7:222:7:DC:H6	1.74	0.51
1:AAA:155:ALA:HB2	1:AAA:174:ASP:OD1	2.09	0.51
2:CCC:151:ARG:CZ	2:CCC:177:ILE:HD11	2.40	0.51
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD11	1.92	0.51
2:CCC:661:VAL:CG1	2:CCC:665:ALA:HB3	2.41	0.51
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	1.92	0.51
3:DDD:826:ILE:HG23	3:DDD:831:VAL:HG22	1.92	0.51
3:DDD:1169:THR:OG1	3:DDD:1174:ARG:NH2	2.43	0.51
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.93	0.51
1:BBB:212:ASP:OD1	1:BBB:213:PRO:CD	2.55	0.51
3:DDD:97:VAL:CG1	3:DDD:101:ARG:NE	2.73	0.51
5:FFF:143:SER:HB2	6:111:41:DT:H72	1.93	0.51
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.75	0.51
2:CCC:871:VAL:CG2	2:CCC:883:LEU:HA	2.41	0.51
3:DDD:279:LEU:O	3:DDD:283:LEU:HG	2.10	0.51
3:DDD:333:GLY:O	3:DDD:336:GLY:N	2.36	0.51
3:DDD:505:ASP:HB2	3:DDD:629:PHE:CE1	2.45	0.51
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:H	2.13	0.51
5:FFF:122:GLU:HG2	5:FFF:157:ALA:CB	2.41	0.51
5:FFF:259:ILE:HG21	5:FFF:280:LEU:CG	2.40	0.51
3:DDD:1156:LEU:HB2	3:DDD:1223:LEU:CD1	2.41	0.51
2:CCC:366:ILE:O	2:CCC:369:MET:HG2	2.10	0.51
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HE	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:278:ARG:HB3	3:DDD:295:GLU:OE2	2.11	0.51
1:AAA:158:ARG:CD	1:AAA:172:LEU:HD11	2.41	0.51
2:CCC:847:PRO:HB3	2:CCC:1047:LEU:HD11	1.92	0.51
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.40	0.51
3:DDD:427:PRO:HG2	3:DDD:429:LEU:HD21	1.92	0.51
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.92	0.51
3:DDD:1064:SER:HA	3:DDD:1067:ARG:HB3	1.93	0.51
4:EEE:41:GLU:O	4:EEE:44:ASP:HB2	2.11	0.51
2:CCC:1001:GLY:HA2	2:CCC:1011:LEU:CD2	2.41	0.50
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CE2	2.47	0.50
3:DDD:114:ILE:HG23	3:DDD:115:TRP:N	2.25	0.50
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.27	0.50
2:CCC:477:GLU:HG3	2:CCC:478:ARG:N	2.26	0.50
2:CCC:1255:THR:HG21	3:DDD:341:ASN:CG	2.31	0.50
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.75	0.50
3:DDD:1292:LEU:O	3:DDD:1296:GLY:N	2.38	0.50
2:CCC:119:GLU:O	2:CCC:119:GLU:HG3	2.10	0.50
2:CCC:297:VAL:HG22	2:CCC:315:MET:O	2.11	0.50
3:DDD:825:VAL:HG23	3:DDD:838:ARG:HD2	1.94	0.50
3:DDD:1238:GLN:O	3:DDD:1242:ARG:HB2	2.11	0.50
5:FFF:66:GLY:HA2	5:FFF:100:ARG:NH2	2.26	0.50
1:AAA:102:LEU:HB2	1:AAA:115:ILE:HG12	1.94	0.50
5:FFF:78:TYR:OH	5:FFF:82:ARG:NH1	2.44	0.50
5:FFF:144:THR:HG22	6:111:39:DA:C8	2.46	0.50
3:DDD:339:ARG:NH2	7:222:8:DG:OP1	2.33	0.50
3:DDD:1111:ASP:OD1	3:DDD:1112:GLY:N	2.44	0.50
2:CCC:1161:LEU:O	2:CCC:1163:THR:N	2.45	0.50
3:DDD:464:ASP:OD1	3:DDD:464:ASP:N	2.44	0.50
3:DDD:935:PHE:HZ	3:DDD:1135:THR:OG1	1.93	0.50
5:FFF:159:MET:HE1	5:FFF:169:ILE:HG23	1.94	0.50
2:CCC:555:TYR:CE1	2:CCC:637:ARG:CZ	2.95	0.50
2:CCC:1291:LEU:CD1	3:DDD:1351:VAL:HG13	2.41	0.50
3:DDD:518:VAL:HG22	3:DDD:547:ARG:NH2	2.26	0.50
1:BBB:64:VAL:HG13	1:BBB:78:ILE:HD13	1.94	0.50
2:CCC:521:LEU:HD13	2:CCC:667:LEU:HD11	1.93	0.50
3:DDD:377:PHE:O	3:DDD:381:ILE:HG13	2.12	0.50
3:DDD:423:LEU:HB3	3:DDD:466:MET:HE1	1.93	0.50
4:EEE:60:ASN:HB3	4:EEE:63:ILE:HD12	1.94	0.50
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG21	1.94	0.50
2:CCC:66:SER:HB2	2:CCC:479:LEU:HD22	1.94	0.50
2:CCC:898:GLU:CG	5:FFF:259:ILE:HD11	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:491:LEU:HD11	3:DDD:610:ARG:NH2	2.14	0.50
1:BBB:47:LEU:HD13	1:BBB:205:MET:HE2	1.93	0.49
2:CCC:257:ALA:O	2:CCC:258:ASN:HB3	2.12	0.49
2:CCC:1017:GLN:NE2	2:CCC:1021:LEU:HG	2.27	0.49
2:CCC:1338:GLU:OE2	3:DDD:21:LYS:HE2	2.11	0.49
3:DDD:121:PRO:O	3:DDD:122:SER:CB	2.53	0.49
3:DDD:1041:ILE:CG2	3:DDD:1044:GLN:HG3	2.42	0.49
3:DDD:1368:ASP:O	3:DDD:1371:ARG:HG2	2.12	0.49
5:FFF:182:ALA:CB	5:FFF:193:PRO:HG3	2.40	0.49
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.42	0.49
5:FFF:112:ARG:NH2	7:222:25:DA:O3'	2.46	0.49
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.93	0.49
2:CCC:1290:MET:SD	3:DDD:347:VAL:HG11	2.51	0.49
2:CCC:155:VAL:CG2	2:CCC:405:PHE:CD2	2.95	0.49
2:CCC:661:VAL:HG12	2:CCC:662:SER:O	2.11	0.49
2:CCC:797:GLY:O	2:CCC:1231:TYR:OH	2.31	0.49
2:CCC:816:ILE:HD11	2:CCC:1074:GLY:HA3	1.93	0.49
3:DDD:115:TRP:CZ2	3:DDD:1329:THR:HG22	2.47	0.49
5:FFF:166:ARG:HH11	5:FFF:166:ARG:HG3	1.77	0.49
2:CCC:244:GLU:O	2:CCC:245:ARG:C	2.50	0.49
2:CCC:1101:LEU:HD21	3:DDD:730:ALA:HB1	1.94	0.49
3:DDD:395:LYS:CG	5:FFF:329:LEU:HD13	2.37	0.49
2:CCC:447:HIS:CE1	2:CCC:553:THR:HG21	2.48	0.49
2:CCC:555:TYR:CD1	2:CCC:637:ARG:CZ	2.96	0.49
2:CCC:871:VAL:HG23	2:CCC:883:LEU:O	2.13	0.49
3:DDD:584:PRO:HD3	3:DDD:620:PHE:CD1	2.48	0.49
3:DDD:747:MET:SD	3:DDD:759:ILE:HD12	2.53	0.49
3:DDD:1082:ASP:OD1	3:DDD:1084:GLN:N	2.46	0.49
3:DDD:1270:GLY:HA2	3:DDD:1298:VAL:O	2.13	0.49
1:AAA:74:VAL:O	2:CCC:729:ALA:CB	2.60	0.49
3:DDD:68:TYR:CE1	3:DDD:93:THR:HA	2.48	0.49
3:DDD:1307:LEU:HB2	3:DDD:1312:ALA:HB2	1.94	0.49
4:EEE:17:PHE:O	4:EEE:21:LEU:HG	2.13	0.49
2:CCC:524:ILE:HD12	2:CCC:708:VAL:HG13	1.93	0.49
2:CCC:936:ARG:CG	2:CCC:937:ASP:H	2.26	0.49
3:DDD:362:ARG:HH21	3:DDD:619:ILE:HG13	1.77	0.49
2:CCC:594:VAL:HG22	2:CCC:599:VAL:HG22	1.94	0.49
2:CCC:840:SER:HB3	2:CCC:850:ILE:HD11	1.95	0.49
3:DDD:614:LEU:CD2	4:EEE:5:THR:CG2	2.91	0.49
3:DDD:826:ILE:HG12	3:DDD:831:VAL:HG22	1.95	0.49
1:BBB:152:TYR:CZ	3:DDD:536:LEU:HD21	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:799:ASN:C	2:CCC:800:MET:HG2	2.33	0.48
2:CCC:1305:TYR:CZ	5:FFF:247:GLU:HG3	2.48	0.48
2:CCC:13:LYS:NZ	2:CCC:1151:LEU:HB3	2.28	0.48
2:CCC:479:LEU:HD21	2:CCC:492:MET:HE1	1.95	0.48
2:CCC:598:VAL:HG13	2:CCC:627:GLY:HA2	1.94	0.48
3:DDD:795:TYR:CE2	3:DDD:799:ARG:CZ	2.96	0.48
1:AAA:12:ARG:HA	1:BBB:230:ALA:HB1	1.95	0.48
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	1.95	0.48
1:AAA:211:ILE:HG22	1:AAA:216:ALA:HB2	1.94	0.48
2:CCC:49:LEU:HD22	2:CCC:464:PHE:CE2	2.48	0.48
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE1	1.95	0.48
2:CCC:1077:SER:HA	3:DDD:356:THR:CG2	2.43	0.48
1:BBB:83:LEU:HG	3:DDD:526:VAL:CB	2.43	0.48
2:CCC:263:VAL:HG12	2:CCC:264:GLU:O	2.13	0.48
2:CCC:551:HIS:H	2:CCC:554:HIS:CE1	2.31	0.48
3:DDD:1037:PHE:CZ	3:DDD:1059:LEU:CD1	2.97	0.48
3:DDD:1079:LYS:HE3	3:DDD:1087:ASP:OD1	2.11	0.48
3:DDD:1153:PRO:HA	3:DDD:1214:PRO:O	2.13	0.48
5:FFF:144:THR:HG21	6:111:39:DA:OP2	2.14	0.48
1:AAA:124:VAL:HG21	1:AAA:210:THR:H	1.79	0.48
1:BBB:124:VAL:HG21	1:BBB:210:THR:CG2	2.43	0.48
2:CCC:1083:GLU:H	2:CCC:1083:GLU:CD	2.16	0.48
2:CCC:1105:SER:CB	3:DDD:731:ARG:HG3	2.43	0.48
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.96	0.48
5:FFF:263:LEU:CD1	5:FFF:281:LEU:HD11	2.36	0.48
2:CCC:20:GLN:O	2:CCC:20:GLN:HG3	2.14	0.48
2:CCC:1274:GLU:HG2	3:DDD:424:ASN:ND2	2.29	0.48
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.96	0.48
2:CCC:720:ARG:HD3	2:CCC:736:VAL:HG11	1.96	0.48
2:CCC:1099:ASN:OD1	2:CCC:1100:PRO:HD2	2.14	0.48
3:DDD:490:ILE:HA	3:DDD:500:ILE:HD12	1.95	0.48
3:DDD:504:GLN:HE22	3:DDD:731:ARG:NH2	2.10	0.48
5:FFF:183:ARG:O	5:FFF:187:HIS:ND1	2.46	0.48
2:CCC:216:THR:HG23	2:CCC:219:GLN:OE1	2.13	0.48
3:DDD:883:ARG:HG2	3:DDD:898:CYS:HA	1.96	0.48
7:222:14:DC:H2'	7:222:15:DT:C6	2.49	0.48
1:AAA:195:ARG:HD2	1:AAA:198:LEU:HD23	1.95	0.48
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.44	0.48
2:CCC:44:GLU:HG3	2:CCC:45:GLY:H	1.78	0.48
2:CCC:473:ARG:O	2:CCC:477:GLU:HB3	2.13	0.48
3:DDD:295:GLU:OE1	5:FFF:121:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.96	0.48
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CG	2.91	0.48
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:N	2.67	0.48
6:111:58:DG:C2	7:222:6:DG:N2	2.82	0.48
1:BBB:44:ARG:NH1	3:DDD:538:ARG:HD3	2.27	0.48
2:CCC:748:ILE:HD11	2:CCC:970:GLY:HA3	1.96	0.48
2:CCC:818:VAL:HG12	2:CCC:1096:ILE:HG12	1.95	0.48
2:CCC:1304:MET:HE1	3:DDD:472:LEU:CD1	2.41	0.48
3:DDD:421:VAL:CG1	3:DDD:468:VAL:HG13	2.43	0.48
3:DDD:936:HIS:HE1	11:DDD:1504:DPO:O1	1.96	0.48
2:CCC:32:LEU:CD2	2:CCC:130:MET:CE	2.91	0.47
2:CCC:277:LEU:CD1	2:CCC:282:VAL:HG21	2.43	0.47
2:CCC:1111:GLN:HB2	2:CCC:1230:MET:HE1	1.95	0.47
2:CCC:1117:LEU:HD13	2:CCC:1195:ILE:HG12	1.95	0.47
2:CCC:1327:LEU:O	2:CCC:1331:ARG:HG3	2.14	0.47
4:EEE:13:ILE:HD12	4:EEE:19:LEU:HA	1.96	0.47
5:FFF:259:ILE:HG12	5:FFF:280:LEU:HD21	1.96	0.47
2:CCC:1296:ASP:CB	2:CCC:1321:GLU:H	2.26	0.47
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	1.95	0.47
3:DDD:646:ILE:HD13	3:DDD:762:ASN:HD21	1.80	0.47
3:DDD:965:SER:HB2	3:DDD:975:ILE:HA	1.97	0.47
5:FFF:80:ALA:O	5:FFF:84:LEU:HG	2.14	0.47
1:AAA:57:THR:HG23	1:AAA:158:ARG:NH2	2.29	0.47
1:BBB:82:LEU:HB3	1:BBB:173:VAL:HG22	1.95	0.47
2:CCC:263:VAL:HG22	2:CCC:269:ILE:CD1	2.44	0.47
2:CCC:292:ILE:CB	2:CCC:322:LEU:HD11	2.43	0.47
2:CCC:685:MET:HE2	2:CCC:1235:LEU:CD1	2.45	0.47
2:CCC:870:ILE:HD12	2:CCC:1050:VAL:HG11	1.96	0.47
3:DDD:44:ILE:HG22	3:DDD:51:PRO:HA	1.95	0.47
3:DDD:115:TRP:O	3:DDD:119:SER:HB3	2.15	0.47
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:HA	1.96	0.47
1:AAA:86:LYS:HG2	1:AAA:174:ASP:O	2.15	0.47
2:CCC:296:VAL:HB	2:CCC:336:LEU:HD12	1.96	0.47
5:FFF:263:LEU:HD13	5:FFF:281:LEU:CG	2.45	0.47
2:CCC:32:LEU:CD2	2:CCC:130:MET:HE3	2.45	0.47
2:CCC:521:LEU:HD13	2:CCC:667:LEU:CD1	2.45	0.47
3:DDD:519:ASN:HA	3:DDD:523:GLU:OE2	2.15	0.47
3:DDD:644:MET:HG3	3:DDD:722:ILE:CD1	2.43	0.47
3:DDD:1150:PRO:HD2	3:DDD:1153:PRO:HB3	1.97	0.47
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CD2	2.50	0.47
2:CCC:453:ILE:HD11	2:CCC:530:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:108:ALA:HB3	3:DDD:279:LEU:HD23	1.97	0.47
3:DDD:205:LEU:HD22	3:DDD:214:ARG:HG2	1.96	0.47
3:DDD:552:ILE:CG2	3:DDD:580:TRP:CD1	2.97	0.47
4:EEE:8:ASP:HB2	4:EEE:55:GLU:CG	2.45	0.47
1:AAA:32:GLU:OE2	1:BBB:150:ARG:NH2	2.47	0.47
1:AAA:179:PRO:HG3	1:AAA:211:ILE:CD1	2.45	0.47
2:CCC:807:TRP:CH2	2:CCC:1086:PRO:HD3	2.50	0.47
2:CCC:839:VAL:HG13	2:CCC:1046:VAL:HG13	1.97	0.47
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:OE2	2.14	0.47
2:CCC:1281:TYR:CE1	3:DDD:431:ARG:HG3	2.49	0.47
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.33	0.47
3:DDD:382:TYR:OH	3:DDD:398:LYS:HG2	2.15	0.47
3:DDD:502:PRO:HB3	3:DDD:506:VAL:CG1	2.45	0.47
3:DDD:872:LEU:HD23	3:DDD:877:VAL:HG21	1.97	0.47
2:CCC:297:VAL:HG13	2:CCC:317:LEU:CG	2.45	0.47
2:CCC:1340:GLU:O	3:DDD:17:PHE:HB2	2.15	0.47
3:DDD:795:TYR:CE2	3:DDD:799:ARG:NE	2.82	0.47
3:DDD:1156:LEU:HB2	3:DDD:1223:LEU:HD13	1.97	0.47
3:DDD:1163:VAL:HG11	3:DDD:1175:LEU:HD11	1.95	0.47
5:FFF:263:LEU:CD1	5:FFF:281:LEU:CG	2.92	0.47
1:AAA:154:PRO:HA	1:AAA:174:ASP:HB3	1.96	0.47
1:BBB:82:LEU:HD11	1:BBB:171:LEU:HD13	1.97	0.47
2:CCC:165:HIS:HB3	2:CCC:167:SER:HB3	1.97	0.47
2:CCC:1284:ALA:HB3	3:DDD:1361:THR:HB	1.97	0.47
2:CCC:1292:THR:CG2	2:CCC:1293:VAL:N	2.78	0.47
3:DDD:837:ASP:OD1	3:DDD:837:ASP:N	2.48	0.47
2:CCC:148:GLN:OE1	2:CCC:454:ARG:HD2	2.15	0.47
2:CCC:1214:ASP:OD1	2:CCC:1214:ASP:C	2.50	0.47
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.14	0.47
1:BBB:16:ILE:HD13	1:BBB:214:GLU:OE2	2.15	0.46
1:BBB:82:LEU:HD11	1:BBB:171:LEU:HB3	1.97	0.46
2:CCC:750:ILE:HG23	2:CCC:750:ILE:O	2.15	0.46
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:N	2.24	0.46
3:DDD:174:ASP:N	3:DDD:174:ASP:OD1	2.48	0.46
1:AAA:190:ALA:O	1:AAA:192:VAL:N	2.48	0.46
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.48	0.46
3:DDD:198:CYS:SG	3:DDD:224:LEU:HB3	2.56	0.46
3:DDD:321:LYS:HE3	6:111:52:DT:OP1	2.16	0.46
5:FFF:168:PRO:O	5:FFF:172:VAL:HG23	2.15	0.46
1:AAA:58:GLU:OE1	1:AAA:170:ARG:CD	2.62	0.46
2:CCC:206:ALA:O	2:CCC:209:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:290:GLU:O	2:CCC:290:GLU:HG2	2.15	0.46
3:DDD:608:CYS:SG	3:DDD:612:LEU:HD12	2.55	0.46
3:DDD:805:GLN:HG2	3:DDD:806:ASP:N	2.29	0.46
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	1.97	0.46
7:222:14:DC:C2	8:333:16:G:N1	2.66	0.46
2:CCC:670:PHE:CD2	2:CCC:1113:LEU:HB3	2.51	0.46
3:DDD:504:GLN:HB3	3:DDD:505:ASP:H	1.58	0.46
3:DDD:622:ASP:O	3:DDD:626:TYR:CD2	2.69	0.46
3:DDD:849:LEU:HB3	3:DDD:857:LEU:H	1.79	0.46
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.32	0.46
1:AAA:124:VAL:HG11	1:AAA:209:GLY:CA	2.46	0.46
3:DDD:384:LYS:NZ	4:EEE:45:LYS:NZ	2.64	0.46
3:DDD:705:THR:HG23	3:DDD:707:ILE:HG13	1.98	0.46
3:DDD:803:VAL:HG22	3:DDD:1313:SER:OG	2.16	0.46
3:DDD:859:PRO:HG2	3:DDD:862:THR:HG21	1.98	0.46
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HD11	2.45	0.46
5:FFF:58:THR:OG1	5:FFF:117:LEU:HG	2.15	0.46
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HD2	1.71	0.46
1:BBB:179:PRO:CG	1:BBB:211:ILE:HD12	2.35	0.46
2:CCC:850:ILE:HG22	2:CCC:850:ILE:O	2.16	0.46
2:CCC:1276:TRP:CH2	3:DDD:798:ARG:HG3	2.50	0.46
2:CCC:1285:TYR:CD2	3:DDD:1361:THR:HG21	2.51	0.46
3:DDD:262:THR:C	5:FFF:222:VAL:HG12	2.36	0.46
3:DDD:347:VAL:HG12	3:DDD:348:ASP:O	2.16	0.46
3:DDD:558:ASP:HB2	3:DDD:564:VAL:HG23	1.97	0.46
3:DDD:809:VAL:HG22	3:DDD:915:ILE:CD1	2.46	0.46
1:AAA:174:ASP:OD1	1:AAA:174:ASP:N	2.49	0.46
2:CCC:155:VAL:HG23	2:CCC:405:PHE:CD2	2.50	0.46
2:CCC:167:SER:O	3:DDD:1065:ALA:HA	2.16	0.46
2:CCC:1214:ASP:OD1	2:CCC:1215:GLY:N	2.48	0.46
3:DDD:58:CYS:SG	3:DDD:61:ILE:N	2.89	0.46
3:DDD:112:ALA:H	3:DDD:300:GLN:HE21	1.64	0.46
2:CCC:202:ARG:NH2	7:222:3:DT:H5''	2.31	0.46
2:CCC:529:ARG:NH2	8:333:17:U:O3'	2.46	0.46
2:CCC:751:TYR:N	2:CCC:751:TYR:CD2	2.84	0.46
2:CCC:1107:MET:SD	3:DDD:736:GLN:NE2	2.88	0.46
3:DDD:161:THR:H	3:DDD:164:GLN:HB2	1.81	0.46
3:DDD:488:ASN:OD1	4:EEE:5:THR:HG23	2.15	0.46
3:DDD:809:VAL:CG2	3:DDD:915:ILE:CD1	2.94	0.46
6:111:58:DG:N2	7:222:6:DG:C2	2.83	0.46
3:DDD:305:ALA:CB	3:DDD:316:ILE:HD12	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG11	1.97	0.46
3:DDD:130:MET:SD	3:DDD:157:GLN:HB3	2.56	0.45
3:DDD:816:THR:HG22	3:DDD:818:GLU:N	2.28	0.45
3:DDD:925:GLU:OE1	3:DDD:926:PRO:N	2.49	0.45
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.49	0.45
1:BBB:64:VAL:CG1	1:BBB:78:ILE:HD13	2.46	0.45
1:BBB:174:ASP:OD2	3:DDD:525:MET:HE2	2.14	0.45
3:DDD:45:ASN:HB2	3:DDD:52:GLU:OE1	2.16	0.45
3:DDD:759:ILE:HG12	3:DDD:771:GLN:CG	2.40	0.45
1:BBB:67:GLU:N	1:BBB:171:LEU:CD2	2.74	0.45
2:CCC:90:VAL:HG12	2:CCC:91:THR:N	2.30	0.45
2:CCC:189:ASP:OD1	2:CCC:190:PRO:N	2.50	0.45
3:DDD:119:SER:O	3:DDD:122:SER:N	2.49	0.45
3:DDD:665:GLN:O	3:DDD:668:PHE:HB3	2.16	0.45
5:FFF:145:TYR:CZ	5:FFF:149:TRP:NE1	2.83	0.45
2:CCC:104:ILE:HD13	2:CCC:484:LEU:HB3	1.98	0.45
2:CCC:144:VAL:HB	2:CCC:526:HIS:CE1	2.52	0.45
2:CCC:196:VAL:CG2	2:CCC:206:ALA:HA	2.31	0.45
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	1.99	0.45
3:DDD:703:THR:O	3:DDD:704:GLU:C	2.54	0.45
3:DDD:844:THR:CG2	3:DDD:864:LEU:CD2	2.93	0.45
3:DDD:943:ARG:NH1	3:DDD:1128:SER:O	2.49	0.45
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.98	0.45
1:BBB:152:TYR:HD2	3:DDD:541:LEU:HD13	1.81	0.45
2:CCC:576:SER:OG	2:CCC:577:VAL:N	2.49	0.45
3:DDD:517:CYS:N	3:DDD:545:HIS:HB3	2.31	0.45
3:DDD:791:ALA:HB2	7:222:9:DT:C5	2.50	0.45
3:DDD:791:ALA:CB	7:222:9:DT:H71	2.47	0.45
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.79	0.45
2:CCC:871:VAL:HG23	2:CCC:883:LEU:HA	1.99	0.45
2:CCC:400:VAL:HG22	2:CCC:584:TYR:HB3	1.99	0.45
2:CCC:543:ALA:HB3	2:CCC:548:ARG:HH21	1.81	0.45
2:CCC:978:VAL:O	2:CCC:981:ALA:HB3	2.17	0.45
3:DDD:697:MET:SD	3:DDD:741:ALA:HB3	2.57	0.45
3:DDD:1174:ARG:O	3:DDD:1176:VAL:HG23	2.16	0.45
2:CCC:173:ASN:C	2:CCC:173:ASN:OD1	2.54	0.45
2:CCC:1109:ILE:HG22	2:CCC:1113:LEU:HD12	1.99	0.45
3:DDD:614:LEU:HD23	4:EEE:5:THR:CG2	2.47	0.45
3:DDD:930:LEU:CD1	3:DDD:1246:VAL:HG21	2.47	0.45
1:BBB:31:LEU:CD1	1:BBB:201:LEU:HB2	2.47	0.45
2:CCC:967:LEU:HD12	2:CCC:967:LEU:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1081:PRO:CB	2:CCC:1083:GLU:OE2	2.64	0.45
2:CCC:1131:MET:HG2	2:CCC:1136:GLN:OE1	2.17	0.45
3:DDD:558:ASP:OD2	3:DDD:564:VAL:HG21	2.17	0.45
3:DDD:886:VAL:CG1	3:DDD:1226:VAL:CG1	2.95	0.45
3:DDD:1168:GLU:OE2	3:DDD:1173:ARG:NH1	2.50	0.45
2:CCC:720:ARG:HB3	2:CCC:736:VAL:HG13	1.98	0.45
3:DDD:546:ALA:HB3	3:DDD:574:VAL:HG23	1.98	0.45
3:DDD:889:ASP:OD1	3:DDD:1290:ARG:NH2	2.50	0.45
3:DDD:1106:ILE:HG22	3:DDD:1106:ILE:O	2.16	0.45
5:FFF:179:LEU:HD12	7:222:26:DT:C7	2.47	0.45
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HG13	1.99	0.44
2:CCC:516:ASP:O	2:CCC:522:SER:OG	2.30	0.44
2:CCC:518:ASN:OD1	2:CCC:1236:ASN:ND2	2.50	0.44
2:CCC:807:TRP:HZ3	2:CCC:1086:PRO:HG3	1.82	0.44
5:FFF:208:ASP:O	5:FFF:212:MET:HG2	2.17	0.44
7:222:15:DT:O2	8:333:15:A:N1	2.50	0.44
3:DDD:161:THR:N	3:DDD:164:GLN:HB2	2.32	0.44
3:DDD:528:THR:HG23	3:DDD:532:GLU:OE1	2.18	0.44
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HA	1.99	0.44
2:CCC:993:PRO:HG2	2:CCC:996:ARG:NH1	2.33	0.44
3:DDD:248:ASP:N	3:DDD:248:ASP:OD1	2.49	0.44
1:BBB:66:HIS:C	1:BBB:171:LEU:HD21	2.37	0.44
2:CCC:53:PHE:HB3	2:CCC:70:TYR:CD2	2.53	0.44
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB3	2.00	0.44
2:CCC:374:GLU:OE1	6:111:44:DG:N2	2.43	0.44
2:CCC:1028:LYS:O	2:CCC:1032:LYS:HG2	2.17	0.44
2:CCC:1302:THR:HA	5:FFF:246:PRO:HB3	1.98	0.44
3:DDD:290:ILE:HG23	5:FFF:64:GLU:OE1	2.17	0.44
3:DDD:667:GLN:O	3:DDD:670:SER:OG	2.24	0.44
3:DDD:1158:GLU:HA	3:DDD:1223:LEU:HD22	1.98	0.44
3:DDD:1186:TYR:CZ	3:DDD:1188:GLU:OE2	2.71	0.44
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	2.00	0.44
1:AAA:29:GLU:CB	1:AAA:30:PRO:HA	2.46	0.44
2:CCC:808:ASN:CA	3:DDD:629:PHE:HB3	2.43	0.44
3:DDD:703:THR:O	3:DDD:705:THR:N	2.51	0.44
1:AAA:30:PRO:HB2	1:AAA:198:LEU:CD1	2.47	0.44
1:AAA:165:GLU:HG3	1:AAA:165:GLU:O	2.18	0.44
1:BBB:61:ILE:HG12	1:BBB:142:MET:HB3	2.00	0.44
2:CCC:32:LEU:HD23	2:CCC:130:MET:HE1	1.97	0.44
2:CCC:93:SER:OG	2:CCC:126:GLU:HB3	2.16	0.44
2:CCC:720:ARG:HB2	2:CCC:749:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1101:LEU:HD13	3:DDD:504:GLN:HG3	2.00	0.44
3:DDD:505:ASP:N	3:DDD:505:ASP:OD1	2.48	0.44
3:DDD:709:ARG:O	3:DDD:709:ARG:HG3	2.18	0.44
3:DDD:960:LEU:HB3	3:DDD:963:VAL:HG11	2.00	0.44
3:DDD:1031:VAL:HG11	3:DDD:1089:LEU:O	2.18	0.44
5:FFF:87:ASP:OD1	5:FFF:88:VAL:N	2.50	0.44
7:222:9:DT:H2'	7:222:10:DC:C6	2.52	0.44
1:AAA:44:ARG:HA	1:AAA:183:ILE:HD13	2.00	0.44
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD21	2.00	0.44
2:CCC:842:ASP:HB3	2:CCC:1047:LEU:HD21	1.99	0.44
2:CCC:1105:SER:OG	3:DDD:731:ARG:HD2	2.18	0.44
3:DDD:423:LEU:HB3	3:DDD:466:MET:CE	2.47	0.44
3:DDD:503:SER:HA	3:DDD:507:VAL:HG23	2.00	0.44
3:DDD:703:THR:C	3:DDD:705:THR:N	2.70	0.44
6:111:58:DG:N2	7:222:6:DG:N3	2.65	0.44
7:222:8:DG:O5'	7:222:8:DG:H8	2.01	0.44
7:222:16:DC:H2'	7:222:17:DG:C8	2.53	0.44
2:CCC:583:GLU:HG3	2:CCC:584:TYR:CD2	2.53	0.44
2:CCC:599:VAL:HG21	2:CCC:623:LEU:CD2	2.47	0.44
2:CCC:838:CYS:SG	2:CCC:886:LYS:HE2	2.58	0.44
2:CCC:1129:ASN:CA	2:CCC:1177:ARG:HG3	2.48	0.44
3:DDD:1152:GLU:CD	3:DDD:1193:TRP:CH2	2.91	0.44
5:FFF:166:ARG:CG	5:FFF:166:ARG:NH1	2.79	0.44
2:CCC:1101:LEU:CD2	3:DDD:730:ALA:HB1	2.48	0.44
3:DDD:234:PRO:O	3:DDD:237:MET:HG3	2.18	0.44
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:CD1	2.48	0.44
3:DDD:1041:ILE:HG21	3:DDD:1044:GLN:HG3	2.00	0.44
1:AAA:41:ASN:ND2	2:CCC:1216:ARG:O	2.50	0.43
2:CCC:12:ARG:HD3	2:CCC:1183:ALA:HB2	1.99	0.43
3:DDD:646:ILE:H	3:DDD:646:ILE:HG13	1.66	0.43
1:AAA:135:ASP:OD1	1:AAA:135:ASP:C	2.57	0.43
2:CCC:244:GLU:CG	2:CCC:245:ARG:N	2.80	0.43
3:DDD:321:LYS:HE3	6:111:52:DT:P	2.58	0.43
3:DDD:362:ARG:NH2	3:DDD:619:ILE:HG13	2.32	0.43
3:DDD:364:HIS:HB3	3:DDD:487:THR:CG2	2.48	0.43
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.48	0.43
7:222:15:DT:O2	8:333:15:A:C2	2.71	0.43
2:CCC:60:GLN:HG2	2:CCC:67:GLU:CB	2.49	0.43
2:CCC:538:LEU:HD23	2:CCC:542:ARG:NH2	2.32	0.43
3:DDD:622:ASP:HB3	3:DDD:626:TYR:CE2	2.53	0.43
3:DDD:747:MET:HE2	3:DDD:747:MET:HB3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:784:ALA:O	3:DDD:788:LEU:HG	2.18	0.43
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:CZ	2.46	0.43
2:CCC:517:GLN:H	2:CCC:761:GLN:HE22	1.66	0.43
3:DDD:127:LEU:HD23	3:DDD:127:LEU:HA	1.86	0.43
3:DDD:387:LEU:HD12	3:DDD:387:LEU:HA	1.92	0.43
3:DDD:513:MET:SD	3:DDD:631:TYR:CD2	3.11	0.43
6:111:57:DC:H2''	6:111:58:DG:H5'	1.99	0.43
1:BBB:86:LYS:CE	1:BBB:173:VAL:HG12	2.49	0.43
2:CCC:726:TYR:CZ	2:CCC:728:ASP:HB2	2.53	0.43
3:DDD:599:LYS:H	3:DDD:599:LYS:HG3	1.50	0.43
3:DDD:836:ARG:HD3	3:DDD:873:GLU:OE2	2.18	0.43
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	2.19	0.43
2:CCC:1134:GLN:O	2:CCC:1136:GLN:N	2.51	0.43
3:DDD:515:ARG:HH12	3:DDD:724:MET:HG2	1.83	0.43
3:DDD:865:HIS:HE1	3:DDD:901:ARG:HH22	1.60	0.43
1:AAA:64:VAL:CG1	1:AAA:78:ILE:HD13	2.49	0.43
1:AAA:231:PHE:O	1:AAA:235:ARG:OXT	2.36	0.43
2:CCC:216:THR:N	2:CCC:219:GLN:OE1	2.39	0.43
2:CCC:545:PHE:CE1	3:DDD:788:LEU:HD12	2.53	0.43
2:CCC:854:ILE:HD11	2:CCC:885:GLY:HA3	1.99	0.43
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.83	0.43
3:DDD:519:ASN:HA	3:DDD:523:GLU:CG	2.49	0.43
3:DDD:546:ALA:HB3	3:DDD:574:VAL:HG21	2.01	0.43
3:DDD:795:TYR:OH	3:DDD:799:ARG:HD3	2.17	0.43
3:DDD:810:THR:OG1	3:DDD:893:GLY:HA3	2.18	0.43
3:DDD:1047:THR:HB	3:DDD:1062:LEU:HD11	2.01	0.43
2:CCC:150:HIS:CE1	2:CCC:452:ARG:HD3	2.54	0.43
2:CCC:619:ALA:HB2	2:CCC:654:ASP:HB2	2.00	0.43
2:CCC:759:SER:OG	2:CCC:760:ASN:N	2.51	0.43
2:CCC:944:ARG:O	2:CCC:947:GLU:HG2	2.19	0.43
1:AAA:11:PRO:HD3	1:BBB:227:GLN:OE1	2.19	0.43
2:CCC:57:PHE:CE1	2:CCC:59:ILE:HD12	2.53	0.43
2:CCC:1061:GLN:NE2	2:CCC:1240:ASP:OD1	2.51	0.43
2:CCC:1080:ASN:HA	2:CCC:1081:PRO:HD3	1.92	0.43
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD13	2.01	0.43
2:CCC:216:THR:O	2:CCC:220:ILE:HG13	2.19	0.43
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.52	0.43
3:DDD:661:VAL:HG23	3:DDD:685:ILE:HG21	2.00	0.43
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CE2	2.53	0.42
3:DDD:515:ARG:NH1	3:DDD:724:MET:HG2	2.33	0.42
3:DDD:664:ILE:HD13	3:DDD:681:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:333:16:G:H3'	8:333:17:U:H5	1.83	0.42
1:BBB:20:SER:OG	1:BBB:21:SER:N	2.52	0.42
2:CCC:963:GLU:O	2:CCC:967:LEU:HB2	2.19	0.42
2:CCC:1280:ALA:HB1	3:DDD:918:ILE:HG12	2.01	0.42
3:DDD:369:PRO:HB3	3:DDD:444:GLY:O	2.19	0.42
3:DDD:994:SER:O	3:DDD:995:TYR:CG	2.72	0.42
2:CCC:150:HIS:HE1	2:CCC:452:ARG:HH11	1.67	0.42
2:CCC:405:PHE:CE1	2:CCC:409:LEU:HD12	2.55	0.42
2:CCC:512:SER:O	2:CCC:512:SER:OG	2.34	0.42
3:DDD:360:TYR:OH	3:DDD:448:GLN:OE1	2.30	0.42
5:FFF:143:SER:HB3	6:111:41:DT:C7	2.48	0.42
5:FFF:159:MET:SD	5:FFF:172:VAL:CG1	3.03	0.42
1:AAA:158:ARG:HB3	1:AAA:172:LEU:CD2	2.47	0.42
2:CCC:207:THR:CG2	2:CCC:354:ASP:HB2	2.49	0.42
2:CCC:1105:SER:HB3	3:DDD:731:ARG:CG	2.50	0.42
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	2.00	0.42
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.19	0.42
3:DDD:759:ILE:CD1	3:DDD:771:GLN:HB3	2.49	0.42
3:DDD:805:GLN:CG	3:DDD:806:ASP:N	2.82	0.42
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CD1	2.98	0.42
1:AAA:22:THR:OG1	1:AAA:207:THR:O	2.21	0.42
2:CCC:540:ARG:NH1	2:CCC:540:ARG:HB2	2.35	0.42
2:CCC:1269:ARG:HD3	7:222:11:DA:H5'	2.00	0.42
3:DDD:733:SER:H	3:DDD:736:GLN:HG3	1.85	0.42
3:DDD:824:PRO:HG3	3:DDD:835:LEU:HB2	2.02	0.42
3:DDD:925:GLU:HB3	3:DDD:926:PRO:CD	2.50	0.42
5:FFF:143:SER:HB3	6:111:41:DT:H72	1.99	0.42
2:CCC:76:GLY:O	2:CCC:94:ALA:HB1	2.19	0.42
2:CCC:1328:LYS:HA	2:CCC:1328:LYS:HD3	1.91	0.42
3:DDD:110:PRO:O	3:DDD:182:ALA:HB3	2.19	0.42
3:DDD:661:VAL:CG2	3:DDD:685:ILE:HG21	2.49	0.42
2:CCC:540:ARG:HH21	8:333:16:G:P	2.42	0.42
2:CCC:668:ILE:HG12	2:CCC:1069:ARG:O	2.20	0.42
3:DDD:58:CYS:SG	3:DDD:61:ILE:HG13	2.60	0.42
3:DDD:71:LEU:HB2	3:DDD:90:VAL:HG21	2.01	0.42
3:DDD:503:SER:HB2	3:DDD:598:LYS:NZ	2.35	0.42
3:DDD:759:ILE:HG23	3:DDD:771:GLN:CD	2.40	0.42
1:AAA:45:ARG:HH12	2:CCC:1216:ARG:HA	1.85	0.42
1:AAA:75:GLN:O	2:CCC:729:ALA:CB	2.49	0.42
1:AAA:78:ILE:HA	1:AAA:81:ILE:HD12	2.02	0.42
2:CCC:21:VAL:HG21	2:CCC:592:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:160:ASP:HB3	2:CCC:163:LYS:HD3	2.00	0.42
5:FFF:263:LEU:O	5:FFF:271:ARG:HG3	2.20	0.42
2:CCC:155:VAL:HG12	2:CCC:156:PHE:N	2.35	0.42
2:CCC:530:ILE:HD11	2:CCC:575:LEU:HD13	2.02	0.42
2:CCC:857:VAL:HG11	2:CCC:862:LEU:HD21	2.01	0.42
2:CCC:901:LEU:O	2:CCC:905:ILE:CD1	2.67	0.42
3:DDD:332:LYS:O	3:DDD:333:GLY:O	2.38	0.42
3:DDD:357:VAL:HG22	3:DDD:461:PHE:CE2	2.55	0.42
3:DDD:646:ILE:CG1	3:DDD:741:ALA:O	2.67	0.42
3:DDD:1082:ASP:OD1	3:DDD:1082:ASP:C	2.58	0.42
5:FFF:127:LEU:HD23	5:FFF:127:LEU:HA	1.86	0.42
7:222:15:DT:H2'	7:222:16:DC:C6	2.55	0.42
1:AAA:61:ILE:HG12	1:AAA:142:MET:HB3	2.02	0.42
1:BBB:163:GLU:O	1:BBB:163:GLU:HG3	2.19	0.42
2:CCC:15:PHE:O	2:CCC:17:LYS:HE3	2.20	0.42
2:CCC:244:GLU:O	2:CCC:247:ARG:HB2	2.20	0.42
2:CCC:1030:GLU:HG3	2:CCC:1034:ARG:CZ	2.49	0.42
3:DDD:844:THR:HG21	3:DDD:864:LEU:CD2	2.50	0.42
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:N	2.35	0.42
5:FFF:192:GLU:CG	5:FFF:193:PRO:HD2	2.48	0.42
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CE1	2.55	0.41
2:CCC:842:ASP:OD1	2:CCC:1045:GLY:HA2	2.19	0.41
2:CCC:998:LEU:H	2:CCC:998:LEU:HG	1.67	0.41
2:CCC:1247:SER:HB3	3:DDD:375:GLU:O	2.20	0.41
3:DDD:58:CYS:SG	3:DDD:60:ARG:N	2.93	0.41
3:DDD:325:LYS:HE2	3:DDD:330:MET:HG2	2.02	0.41
1:AAA:195:ARG:HD2	1:AAA:198:LEU:CD2	2.50	0.41
2:CCC:409:LEU:HD13	2:CCC:427:ASP:HB3	2.02	0.41
2:CCC:582:ASN:OD1	2:CCC:585:GLY:N	2.52	0.41
2:CCC:670:PHE:CE2	2:CCC:1113:LEU:HB3	2.55	0.41
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.55	0.41
3:DDD:846:GLU:N	3:DDD:860:ARG:CG	2.76	0.41
5:FFF:177:VAL:O	5:FFF:181:THR:OG1	2.33	0.41
5:FFF:204:LYS:HB3	5:FFF:205:PRO:HD2	2.02	0.41
2:CCC:400:VAL:HG22	2:CCC:584:TYR:HD1	1.85	0.41
2:CCC:1017:GLN:HE21	2:CCC:1021:LEU:HG	1.84	0.41
2:CCC:1225:VAL:HA	3:DDD:638:SER:HB3	2.02	0.41
2:CCC:1293:VAL:HG12	2:CCC:1300:GLY:C	2.41	0.41
3:DDD:755:ILE:CD1	3:DDD:774:ILE:HG23	2.50	0.41
3:DDD:844:THR:CG2	3:DDD:864:LEU:HD21	2.50	0.41
5:FFF:259:ILE:HG23	5:FFF:280:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:287:THR:H	5:FFF:290:ASP:HB2	1.85	0.41
1:AAA:218:ARG:HD3	1:BBB:232:VAL:CG2	2.51	0.41
1:BBB:83:LEU:HG	3:DDD:526:VAL:HB	2.02	0.41
3:DDD:364:HIS:CD2	4:EEE:4:VAL:HG13	2.55	0.41
3:DDD:424:ASN:OD1	3:DDD:425:ARG:N	2.53	0.41
3:DDD:849:LEU:CA	3:DDD:857:LEU:HB3	2.41	0.41
1:AAA:20:SER:OG	1:AAA:21:SER:N	2.53	0.41
2:CCC:93:SER:HG	2:CCC:126:GLU:HB3	1.84	0.41
2:CCC:160:ASP:OD1	2:CCC:160:ASP:N	2.53	0.41
2:CCC:201:ARG:CB	2:CCC:369:MET:HE2	2.46	0.41
2:CCC:807:TRP:CZ3	2:CCC:1086:PRO:HG3	2.56	0.41
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:CD	2.41	0.41
2:CCC:1212:LEU:HD23	2:CCC:1212:LEU:HA	1.82	0.41
2:CCC:1246:ARG:NH2	2:CCC:1258:PRO:HB3	2.35	0.41
3:DDD:843:VAL:HG21	3:DDD:897:HIS:CA	2.51	0.41
3:DDD:916:GLY:HA2	3:DDD:1255:VAL:HG11	2.02	0.41
3:DDD:948:SER:O	3:DDD:1020:TRP:O	2.39	0.41
3:DDD:1196:LEU:HD22	3:DDD:1210:ILE:HG22	2.03	0.41
1:BBB:78:ILE:HA	1:BBB:81:ILE:HD12	2.02	0.41
2:CCC:277:LEU:HD12	2:CCC:277:LEU:HA	1.81	0.41
3:DDD:425:ARG:HD3	3:DDD:457:TYR:O	2.20	0.41
5:FFF:142:PHE:CE2	5:FFF:146:ALA:HB2	2.55	0.41
1:BBB:78:ILE:HG22	1:BBB:171:LEU:HD13	2.02	0.41
2:CCC:1119:MET:SD	2:CCC:1210:ILE:HD11	2.60	0.41
3:DDD:290:ILE:HD12	3:DDD:290:ILE:H	1.84	0.41
5:FFF:182:ALA:HB1	5:FFF:193:PRO:CG	2.45	0.41
2:CCC:667:LEU:HD23	2:CCC:704:MET:HB2	2.01	0.41
3:DDD:322:ARG:HA	3:DDD:323:PRO:HD2	1.89	0.41
3:DDD:731:ARG:HD3	3:DDD:731:ARG:HA	1.79	0.41
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HD12	2.03	0.41
1:AAA:233:ASP:O	1:AAA:235:ARG:N	2.53	0.41
1:AAA:235:ARG:HB3	1:BBB:13:LEU:HD23	2.03	0.41
2:CCC:184:LEU:HD23	2:CCC:184:LEU:HA	1.87	0.41
2:CCC:230:PHE:CE1	2:CCC:292:ILE:HD11	2.55	0.41
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.21	0.41
2:CCC:1273:MET:HB3	3:DDD:428:THR:HB	2.03	0.41
2:CCC:1305:TYR:OH	5:FFF:247:GLU:CG	2.68	0.41
2:CCC:1315:MET:O	2:CCC:1316:GLU:HB2	2.21	0.41
3:DDD:380:PHE:HB3	3:DDD:415:VAL:HG11	2.03	0.41
3:DDD:577:ALA:O	3:DDD:580:TRP:HB3	2.21	0.41
3:DDD:679:TYR:HE1	3:DDD:754:ILE:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:795:TYR:CZ	3:DDD:799:ARG:CD	3.03	0.41
3:DDD:822:MET:CE	3:DDD:838:ARG:HG2	2.51	0.41
3:DDD:1061:VAL:O	3:DDD:1104:LYS:N	2.42	0.41
3:DDD:1357:ILE:H	3:DDD:1357:ILE:HG13	1.55	0.41
3:DDD:1370:MET:O	3:DDD:1373:ARG:HB2	2.21	0.41
5:FFF:178:TYR:CD1	5:FFF:202:LEU:CD1	3.04	0.41
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.35	0.41
1:BBB:102:LEU:HB2	1:BBB:115:ILE:HG12	2.03	0.41
2:CCC:237:LEU:HD11	2:CCC:292:ILE:HD12	2.03	0.41
2:CCC:832:HIS:CD2	2:CCC:1058:ARG:HD2	2.56	0.41
2:CCC:848:GLU:OE1	2:CCC:886:LYS:HD3	2.21	0.41
2:CCC:1160:ASP:O	2:CCC:1161:LEU:O	2.39	0.41
2:CCC:1262:LYS:HG2	2:CCC:1263:ALA:N	2.36	0.41
3:DDD:123:ARG:NH2	3:DDD:1334:GLU:HG2	2.36	0.41
5:FFF:277:ARG:HD3	5:FFF:306:GLN:HE21	1.86	0.41
2:CCC:189:ASP:OD1	2:CCC:189:ASP:C	2.59	0.40
2:CCC:453:ILE:CD1	2:CCC:530:ILE:HD13	2.52	0.40
3:DDD:579:LEU:HB3	3:DDD:592:VAL:HG21	2.03	0.40
3:DDD:795:TYR:CZ	3:DDD:799:ARG:NE	2.89	0.40
3:DDD:1165:PHE:HZ	3:DDD:1196:LEU:HD12	1.86	0.40
5:FFF:180:ARG:HH21	7:222:26:DT:H3'	1.87	0.40
2:CCC:887:VAL:CG2	2:CCC:913:VAL:HG11	2.50	0.40
2:CCC:1109:ILE:HD13	2:CCC:1109:ILE:HA	1.92	0.40
3:DDD:197:GLU:OE1	3:DDD:220:ARG:NH2	2.51	0.40
3:DDD:659:ALA:O	3:DDD:663:GLU:HG3	2.21	0.40
3:DDD:964:LYS:H	3:DDD:977:SER:HB3	1.86	0.40
2:CCC:818:VAL:HG23	2:CCC:1079:ILE:HG12	2.02	0.40
2:CCC:975:ILE:HG23	2:CCC:1011:LEU:CD1	2.51	0.40
3:DDD:664:ILE:HG21	3:DDD:681:LYS:HD3	2.04	0.40
3:DDD:746:LEU:HD23	3:DDD:758:PRO:HB3	2.04	0.40
3:DDD:759:ILE:HD13	3:DDD:771:GLN:HB3	2.02	0.40
3:DDD:1152:GLU:HA	3:DDD:1194:ARG:HH22	1.87	0.40
7:222:4:DC:H2"	7:222:5:DC:C6	2.56	0.40
1:AAA:57:THR:HG23	1:AAA:158:ARG:NE	2.37	0.40
1:AAA:167:PRO:O	1:AAA:169:GLY:N	2.54	0.40
2:CCC:44:GLU:HG3	2:CCC:45:GLY:N	2.36	0.40
3:DDD:325:LYS:HE2	3:DDD:330:MET:CG	2.52	0.40
3:DDD:846:GLU:CA	3:DDD:860:ARG:NH2	2.82	0.40
5:FFF:78:TYR:CD2	5:FFF:78:TYR:C	2.95	0.40
1:BBB:101:THR:HG22	1:BBB:143:ARG:HG2	2.02	0.40
2:CCC:244:GLU:O	2:CCC:247:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:517:GLN:N	2:CCC:761:GLN:OE1	2.54	0.40
2:CCC:905:ILE:HG12	5:FFF:310:LEU:HD22	2.04	0.40
2:CCC:1101:LEU:HD21	3:DDD:730:ALA:CB	2.51	0.40
5:FFF:143:SER:O	5:FFF:147:THR:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:67:TYR:O	5:FFF:299:ARG:NH1[3_644]	2.16	0.04

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%)	211 (92%)	11 (5%)	6 (3%)	5	35
1	BBB	226/242 (93%)	206 (91%)	12 (5%)	8 (4%)	3	29
2	CCC	1339/1342 (100%)	1240 (93%)	75 (6%)	24 (2%)	8	42
3	DDD	1360/1407 (97%)	1251 (92%)	91 (7%)	18 (1%)	12	48
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	264/336 (79%)	248 (94%)	14 (5%)	2 (1%)	19	60
All	All	3494/3659 (96%)	3229 (92%)	207 (6%)	58 (2%)	9	43

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN

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Mol	Chain	Res	Type
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	174	ASP
3	DDD	519	ASN
1	AAA	168	ILE
1	AAA	234	LEU
1	BBB	119	GLY
2	CCC	258	ASN
2	CCC	625	GLU
2	CCC	729	ALA
2	CCC	730	SER
2	CCC	756	TYR
2	CCC	981	ALA
3	DDD	122	SER
3	DDD	321	LYS
3	DDD	336	GLY
3	DDD	1053	LEU
3	DDD	1309	ILE
2	CCC	455	SER
2	CCC	867	GLU
2	CCC	1103	VAL
3	DDD	1200	GLU
1	AAA	162	GLU
1	AAA	191	ARG
1	AAA	233	ASP
1	BBB	232	VAL
2	CCC	163	LYS
2	CCC	341	LEU
2	CCC	669	PRO
2	CCC	1135	GLN
3	DDD	847	ASP
3	DDD	986	ASP
3	DDD	1024	THR
3	DDD	1091	PRO
3	DDD	1103	GLY
1	AAA	210	THR
2	CCC	45	GLY
2	CCC	234	ASP

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Mol	Chain	Res	Type
2	CCC	986	ALA
3	DDD	947	GLU
3	DDD	1170	LYS
1	BBB	118	ASP
1	BBB	164	ASP
2	CCC	1297	ASP
3	DDD	854	ALA
3	DDD	1297	LYS
5	FFF	113	GLY
1	BBB	169	GLY
2	CCC	983	GLY
5	FFF	295	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	198/208 (95%)	180 (91%)	18 (9%)	9	32
1	BBB	196/208 (94%)	185 (94%)	11 (6%)	21	48
2	CCC	1156/1157 (100%)	1064 (92%)	92 (8%)	12	38
3	DDD	1135/1168 (97%)	1056 (93%)	79 (7%)	15	41
4	EEE	67/74 (90%)	63 (94%)	4 (6%)	19	46
5	FFF	231/290 (80%)	220 (95%)	11 (5%)	25	52
All	All	2983/3105 (96%)	2768 (93%)	215 (7%)	14	41

All (215) 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

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Mol	Chain	Res	Type
1	AAA	135	ASP
1	AAA	137	ASN
1	AAA	159	ILE
1	AAA	166	ARG
1	AAA	174	ASP
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	70	THR
1	BBB	77	ASP
1	BBB	105	SER
1	BBB	131	CYS
1	BBB	137	ASN
1	BBB	150	ARG
1	BBB	187	VAL
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	209	ILE
2	CCC	237	LEU
2	CCC	241	LEU
2	CCC	244	GLU
2	CCC	256	GLU
2	CCC	264	GLU

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Mol	Chain	Res	Type
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	370	MET
2	CCC	393	ASP
2	CCC	398	SER
2	CCC	403	MET
2	CCC	404	LYS
2	CCC	413	GLU
2	CCC	470	ARG
2	CCC	472	GLU
2	CCC	477	GLU
2	CCC	481	LEU
2	CCC	502	VAL
2	CCC	525	THR
2	CCC	529	ARG
2	CCC	539	THR
2	CCC	574	SER
2	CCC	576	SER
2	CCC	592	ARG
2	CCC	601	ASP
2	CCC	618	GLN
2	CCC	620	ASN
2	CCC	622	ASN
2	CCC	635	THR
2	CCC	648	ASP
2	CCC	678	ARG
2	CCC	685	MET
2	CCC	694	ARG
2	CCC	730	SER
2	CCC	739	ASP
2	CCC	757	THR
2	CCC	759	SER
2	CCC	777	VAL
2	CCC	788	SER
2	CCC	789	THR
2	CCC	799	ASN
2	CCC	800	MET
2	CCC	801	ARG

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Mol	Chain	Res	Type
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	895	LEU
2	CCC	935	THR
2	CCC	942	ASP
2	CCC	995	ASP
2	CCC	998	LEU
2	CCC	1073	LYS
2	CCC	1083	GLU
2	CCC	1088	ASP
2	CCC	1113	LEU
2	CCC	1135	GLN
2	CCC	1143	GLU
2	CCC	1150	ASP
2	CCC	1154	ASP
2	CCC	1174	GLU
2	CCC	1223	ARG
2	CCC	1240	ASP
2	CCC	1248	THR
2	CCC	1262	LYS
2	CCC	1269	ARG
2	CCC	1286	THR
2	CCC	1292	THR
2	CCC	1293	VAL
2	CCC	1296	ASP
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	211	GLU
3	DDD	223	LEU
3	DDD	234	PRO

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Mol	Chain	Res	Type
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	464	ASP
3	DDD	479	GLU
3	DDD	492	SER
3	DDD	504	GLN
3	DDD	505	ASP
3	DDD	516	ASP
3	DDD	543	SER
3	DDD	548	VAL
3	DDD	570	LYS
3	DDD	590	SER
3	DDD	591	ILE
3	DDD	599	LYS
3	DDD	602	SER
3	DDD	610	ARG
3	DDD	619	ILE
3	DDD	627	THR
3	DDD	638	SER
3	DDD	642	ASP
3	DDD	644	MET
3	DDD	646	ILE
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	764	ARG
3	DDD	769	VAL
3	DDD	786	THR
3	DDD	790	THR
3	DDD	792	ASN

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Mol	Chain	Res	Type
3	DDD	793	SER
3	DDD	812	ASP
3	DDD	827	GLU
3	DDD	842	ARG
3	DDD	846	GLU
3	DDD	848	VAL
3	DDD	849	LEU
3	DDD	864	LEU
3	DDD	889	ASP
3	DDD	911	LYS
3	DDD	957	SER
3	DDD	969	SER
3	DDD	970	SER
3	DDD	1021	ASP
3	DDD	1023	HIS
3	DDD	1025	MET
3	DDD	1032	SER
3	DDD	1051	ASP
3	DDD	1064	SER
3	DDD	1073	ASP
3	DDD	1272	SER
3	DDD	1283	SER
3	DDD	1303	SER
3	DDD	1320	ILE
3	DDD	1330	ARG
3	DDD	1345	ARG
4	EEE	8	ASP
4	EEE	46	THR
4	EEE	55	GLU
4	EEE	67	ARG
5	FFF	109	TYR
5	FFF	114	LEU
5	FFF	122	GLU
5	FFF	127	LEU
5	FFF	163	ARG
5	FFF	166	ARG
5	FFF	238	LEU
5	FFF	244	ASN
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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	5/7 (71%)	3 (60%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	16	G
8	333	17	U
8	333	18	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	DPO	DDD	1504	-	6,8,8	0.72	0	13,13,13	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	DPO	DDD	1504	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	DDD	1504	DPO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	230/242 (95%)	0.28	18 (7%) 13 11	232, 313, 353, 393	0
1	BBB	228/242 (94%)	0.11	9 (3%) 39 31	221, 286, 358, 431	0
2	CCC	1341/1342 (99%)	-0.04	42 (3%) 49 39	135, 251, 375, 471	0
3	DDD	1362/1407 (96%)	0.18	89 (6%) 18 15	151, 282, 429, 476	0
4	EEE	79/90 (87%)	0.46	7 (8%) 9 8	238, 294, 444, 493	0
5	FFF	268/336 (79%)	0.54	28 (10%) 6 6	273, 363, 422, 452	0
6	111	29/50 (58%)	0.76	4 (13%) 2 3	281, 404, 468, 485	0
7	222	32/50 (64%)	1.14	7 (21%) 0 1	291, 388, 452, 489	0
8	333	6/7 (85%)	1.43	1 (16%) 1 2	311, 325, 352, 367	0
All	All	3575/3766 (94%)	0.15	205 (5%) 23 20	135, 281, 419, 493	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	1111	ASP	10.0
3	DDD	1130	GLY	9.2
3	DDD	1099	TYR	7.6
3	DDD	1097	ALA	6.8
3	DDD	1110	GLU	6.8
3	DDD	1066	GLU	6.7
3	DDD	1098	GLN	6.6
3	DDD	1078	LEU	6.5
8	333	20	G	6.3
4	EEE	79	GLU	6.1
3	DDD	856	ILE	6.1
5	FFF	263	LEU	6.0
3	DDD	969	SER	5.8
3	DDD	748	ALA	5.7
2	CCC	230	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
7	222	24	DT	5.6
3	DDD	1129	GLY	5.6
3	DDD	1112	GLY	5.6
4	EEE	78	ALA	5.4
3	DDD	997	VAL	5.3
1	AAA	134	THR	5.3
5	FFF	131	VAL	5.1
3	DDD	1128	SER	5.1
1	BBB	164	ASP	5.0
3	DDD	1035	VAL	5.0
3	DDD	1113	VAL	4.9
4	EEE	3	ARG	4.9
7	222	36	DG	4.7
2	CCC	261	VAL	4.5
7	222	25	DA	4.5
2	CCC	169	LYS	4.4
2	CCC	124	MET	4.4
3	DDD	854	ALA	4.2
3	DDD	1198	VAL	4.2
3	DDD	1063	ASP	4.1
3	DDD	880	VAL	4.1
1	AAA	144	ILE	4.1
7	222	37	DA	4.1
1	BBB	165	GLU	4.1
2	CCC	983	GLY	4.0
5	FFF	219	GLY	4.0
7	222	23	DT	4.0
3	DDD	1121	LEU	3.9
3	DDD	69	GLU	3.9
3	DDD	879	ALA	3.9
4	EEE	80	LEU	3.9
2	CCC	982	GLY	3.9
3	DDD	732	GLY	3.8
1	AAA	24	ALA	3.8
2	CCC	1001	GLY	3.6
3	DDD	1058	SER	3.6
3	DDD	1131	THR	3.6
2	CCC	882	ILE	3.6
1	AAA	75	GLN	3.5
3	DDD	743	MET	3.5
2	CCC	1002	LEU	3.5
3	DDD	212	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	CCC	333	ILE	3.5
3	DDD	176	PHE	3.4
1	AAA	164	ASP	3.4
3	DDD	1059	LEU	3.4
3	DDD	671	GLY	3.4
3	DDD	848	VAL	3.4
3	DDD	1054	THR	3.4
3	DDD	1115	ILE	3.3
3	DDD	586	GLY	3.3
7	222	35	DT	3.3
2	CCC	125	GLY	3.3
3	DDD	1079	LYS	3.3
5	FFF	296	GLY	3.2
2	CCC	107	ARG	3.2
6	111	44	DG	3.2
7	222	38	DG	3.2
3	DDD	1036	ARG	3.2
3	DDD	853	THR	3.2
3	DDD	767	LEU	3.2
3	DDD	667	GLN	3.2
6	111	54	DA	3.2
2	CCC	743	PRO	3.2
5	FFF	299	ARG	3.2
3	DDD	1029	THR	3.1
3	DDD	1273	ASP	3.1
4	EEE	2	ALA	3.1
3	DDD	970	SER	3.1
5	FFF	134	PHE	3.1
2	CCC	67	GLU	3.0
6	111	43	DT	3.0
1	AAA	27	THR	3.0
1	AAA	201	LEU	3.0
2	CCC	984	VAL	3.0
5	FFF	291	VAL	2.9
2	CCC	855	PRO	2.9
4	EEE	77	ALA	2.9
5	FFF	133	LYS	2.9
2	CCC	105	TYR	2.9
2	CCC	60	GLN	2.9
1	BBB	166	ARG	2.9
3	DDD	1065	ALA	2.9
1	BBB	107	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	AAA	107	ILE	2.9
3	DDD	1040	MET	2.8
3	DDD	993	GLU	2.8
3	DDD	1159	ILE	2.8
3	DDD	1114	GLN	2.8
3	DDD	1096	PRO	2.8
3	DDD	1107	VAL	2.8
1	AAA	205	MET	2.8
3	DDD	1197	ASN	2.7
2	CCC	153	PRO	2.7
5	FFF	310	LEU	2.7
3	DDD	1196	LEU	2.7
3	DDD	672	LEU	2.7
3	DDD	1090	ILE	2.6
3	DDD	1077	ALA	2.6
6	111	31	DT	2.6
3	DDD	943	ARG	2.6
5	FFF	201	GLN	2.6
5	FFF	302	VAL	2.6
3	DDD	940	ALA	2.6
2	CCC	239	MET	2.6
2	CCC	875	ALA	2.6
1	BBB	47	LEU	2.6
2	CCC	260	LYS	2.5
3	DDD	994	SER	2.5
2	CCC	190	PRO	2.5
3	DDD	1089	LEU	2.5
2	CCC	170	VAL	2.5
1	AAA	133	LEU	2.5
1	AAA	135	ASP	2.5
5	FFF	301	ARG	2.5
5	FFF	312	ARG	2.5
3	DDD	232	ASN	2.5
5	FFF	271	ARG	2.5
3	DDD	1116	SER	2.5
2	CCC	974	ARG	2.5
2	CCC	103	VAL	2.5
3	DDD	750	PRO	2.5
3	DDD	1189	MET	2.5
3	DDD	968	ASN	2.4
3	DDD	958	ILE	2.4
5	FFF	220	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	DDD	881	LYS	2.4
4	EEE	14	GLY	2.4
5	FFF	193	PRO	2.4
3	DDD	1016	THR	2.4
5	FFF	244	ASN	2.4
3	DDD	1272	SER	2.4
1	AAA	213	PRO	2.4
3	DDD	1203	ARG	2.4
3	DDD	995	TYR	2.4
5	FFF	162	THR	2.4
5	FFF	306	GLN	2.3
2	CCC	990	ASP	2.3
5	FFF	198	ILE	2.3
3	DDD	976	THR	2.3
1	AAA	59	VAL	2.3
3	DDD	392	THR	2.3
5	FFF	130	ALA	2.3
2	CCC	871	VAL	2.3
3	DDD	1118	GLY	2.3
1	AAA	18	GLN	2.3
1	BBB	162	GLU	2.3
2	CCC	870	ILE	2.3
2	CCC	977	ALA	2.3
3	DDD	1093	THR	2.3
3	DDD	746	LEU	2.3
3	DDD	971	GLY	2.3
3	DDD	747	MET	2.3
3	DDD	670	SER	2.2
1	BBB	98	VAL	2.2
3	DDD	1266	ILE	2.2
5	FFF	295	ILE	2.2
3	DDD	855	ASP	2.2
5	FFF	305	ILE	2.2
2	CCC	722	GLY	2.2
3	DDD	1037	PHE	2.2
3	DDD	941	ALA	2.2
2	CCC	231	GLU	2.2
1	BBB	214	GLU	2.2
1	AAA	72	GLU	2.2
2	CCC	385	PHE	2.2
5	FFF	124	ASN	2.2
2	CCC	614	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
5	FFF	98	ASN	2.2
2	CCC	773	LEU	2.2
2	CCC	928	VAL	2.2
1	AAA	158	ARG	2.1
1	AAA	73	GLY	2.1
3	DDD	1271	SER	2.1
2	CCC	127	ILE	2.1
1	AAA	189	ALA	2.1
5	FFF	69	PRO	2.1
3	DDD	1080	ILE	2.1
5	FFF	109	TYR	2.1
3	DDD	213	LYS	2.1
5	FFF	303	ARG	2.1
2	CCC	241	LEU	2.1
2	CCC	94	ALA	2.1
3	DDD	965	SER	2.1
1	BBB	205	MET	2.0
3	DDD	980	THR	2.0
3	DDD	949	SER	2.0
2	CCC	292	ILE	2.0
2	CCC	883	LEU	2.0
2	CCC	884	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MG	DDD	1503	1/1	0.44	0.59	192,192,192,192	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	ZN	DDD	1501	1/1	0.92	0.08	304,304,304,304	0
9	MG	CCC	1401	1/1	0.96	0.33	143,143,143,143	0
10	ZN	DDD	1502	1/1	0.96	0.15	269,269,269,269	0
11	DPO	DDD	1504	9/9	0.96	0.45	197,205,216,219	0

6.5 Other polymers [i](#)

There are no such residues in this entry.