



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:57 PM GMT

PDB ID : 1MSW
Title : Structural basis for the transition from initiation to elongation transcription
in T7 RNA polymerase
Authors : Yin, Y.W.; Steitz, T.A.
Deposited on : 2002-09-19
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

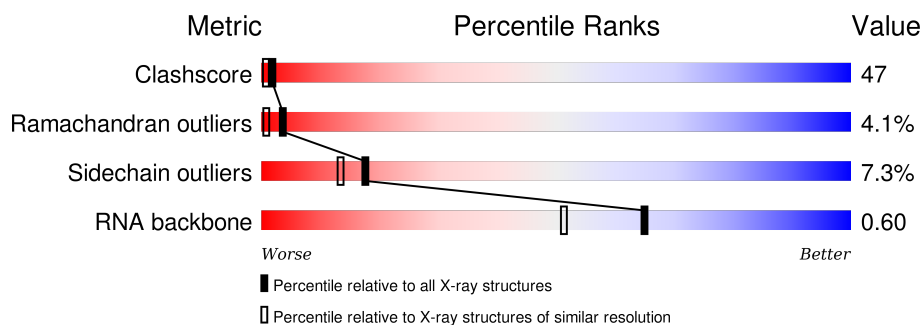
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.


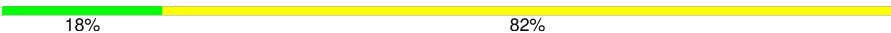


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RNA backbone	2183	1118 (2.80-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	20	
2	N	17	
3	R	10	
4	D	883	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7956 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 DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	20	Total	C	N	O	P	0	0	0
			405	193	71	122	19			

- Molecule 2 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	17	Total	C	N	O	P	0	0	0
			344	165	60	103	16			

- Molecule 3 is a RNA chain called RNA message.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	10	Total	C	N	O	P	0	0	0
			215	97	44	65	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	863	Total	C	N	O	S	0	0	0
			6802	4333	1182	1251	36			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	166	Total	O	0	0
			166	166		
5	N	2	Total	O	0	0
			2	2		
5	R	9	Total	O	0	0
			9	9		
5	T	13	Total	O	0	0
			13	13		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

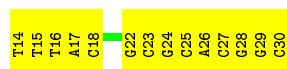
• Molecule 1: Template DNA

Chain T: 



• Molecule 2: Non-Template DNA

Chain N: 



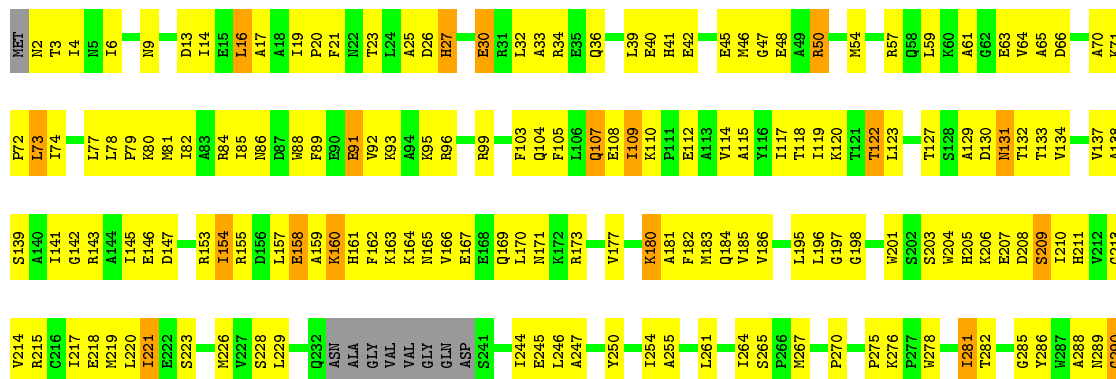
• Molecule 3: RNA message

Chain R: 



• Molecule 4: DNA-directed RNA polymerase

Chain D: 



S856	A779	K697	G613	G538	M439	ASP	R291
Q857	P780	W698	H614	S539	T440	ILE	R292
L858	N781	L699	A615	C540	K441	ASP	P293
D859	F782	K700	L616	G442	G442	MET	L294
	F783			I543	I543	ASN	L295
G868	H784	L706	Q619	G544	L444	PRO	L296
N869		A707	H620	H545	T445	GLU	H300
L870	D787	A708	L621	F546	L446	ALA	S301
N871	G788	E709	A622	M549	P451	T375	K302
L872	S789	V710	G623	L550	L452	A376	K303
R873	H790	K711	G631	R551	G453	K377	A304
D874	L791		H632	D552	K454	K378	
I875		G716	S633	E553		R379	Y308
L876	T794		H634	R557	Y458	A380	
E877	V795	R720	H635			A381	V311
S878	W797	R721	H647	N560	K461	A382	Y312
		C723	Q648	L561	H462	A383	K318
K801		A724	Q649	L562	H463	V384	K319
Y802		V725	V650	T566	G464	K385	I320
G803		H726	B552	V567	A468	R391	I321
I804		W727	D653	Q568	D471	R394	A323
E805		W728	H654	D569	K472	R395	Q324
S806		T729	H655	I570	V473	I396	I325
P807		P730	Q656	V574	P474	S397	I330
			P657	A575	E477	L398	K333
I810		F733	A658	K576	K478	E399	V334
H811		P734	H659	K577	I479	F400	V335
D812		V735	D660	W578	K480	L401	A336
S813		W736	S661	N579	F481	L402	V337
F814			Q662	L582	N488	Q403	A338
G815		K741	L665	Q583	I489	A405	N339
		F742	H666	A584	M490	M406	V340
I816		I743	H667	D585	A491	K407	I341
I817		Q744	H668	A586	S495	F408	
P818		W745	Q669	I587	N410	A409	W344
A819		R746	Q672	N588	N415	H346	K345
D820		L747	H676	G589	T500	C347	P348
		N748	K679	T590	D501	P417	V349
K826		L749		N592		Y418	
A827		F750	H682	V594	P508	N419	I352
V828		L752	H683	V595		M420	A354
R829		Q753	S684	T602	L512	D421	P353
E830		Q754	H685	G603	A513	K422	I355
		R755	Q686	E604	F514	R423	E356
		L757	V687	I605	C515	G424	E357
V833		F758	H688	S606	E517	A428	E358
D834		R759	V689	E607	V429	L360	E359
			H690	K608		P361	L360
E837		Q763	A691	V609		K433	K362
P845		N764		K610		P434	K363
Y846		K765		L611		Q435	PR0
D847		D766		G612		G1U	
Q848		S767					
F849		Q774					
P850		I778					
A851							
D852							
Q853							
H854							
E855							

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	142.91Å 145.46Å 145.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	85.0 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7956	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	T	0.46	0/452	0.90	2/696 (0.3%)
2	N	0.31	0/384	0.67	0/591
3	R	0.47	0/241	0.80	0/375
4	D	0.48	1/6955 (0.0%)	0.65	0/9407
All	All	0.47	1/8032 (0.0%)	0.67	2/11069 (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
1	T	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	407	LYS	CD-CE	5.13	1.64	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	119	DT	N1-C1'-C2'	-5.28	102.57	112.60
1	T	119	DT	C5'-C4'-C3'	-5.10	104.92	114.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	114	DG	Sidechain
1	T	115	DC	Sidechain
1	T	116	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	T	117	DG	Sidechain
1	T	118	DC	Sidechain
1	T	119	DT	Sidechain
1	T	121	DA	Sidechain

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	T	405	0	227	49	0
2	N	344	0	194	17	0
3	R	215	0	112	15	0
4	D	6802	0	6770	645	0
5	D	166	0	0	246	0
5	N	2	0	0	0	0
5	R	9	0	0	8	0
5	T	13	0	0	27	0
All	All	7956	0	7303	715	0

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 47.

All (715) 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)
4:D:360:LEU:HB2	5:D:968:HOH:O	1.29	1.29
4:D:104:GLN:HB3	5:D:979:HOH:O	1.23	1.27
4:D:276:LYS:HE2	5:D:1032:HOH:O	1.22	1.26
4:D:217:ILE:O	4:D:221:ILE:HD13	1.24	1.24
4:D:428:ALA:HA	5:D:944:HOH:O	1.39	1.22
3:R:5:G:H3'	5:R:99:HOH:O	1.43	1.18
4:D:383:ALA:HB3	5:D:986:HOH:O	1.42	1.18
4:D:648:GLN:HA	5:D:1028:HOH:O	1.44	1.17
4:D:647:ARG:HG2	5:D:958:HOH:O	1.42	1.17
4:D:647:ARG:HD3	5:D:913:HOH:O	1.44	1.15
1:T:111:DT:H3'	5:T:132:HOH:O	1.50	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:360:LEU:HD23	5:D:917:HOH:O	1.49	1.11
4:D:386:ARG:HG3	5:D:933:HOH:O	1.52	1.08
4:D:285:GLY:HA2	5:D:928:HOH:O	1.54	1.07
4:D:312:TYR:HB3	5:D:976:HOH:O	1.51	1.06
4:D:735:VAL:HG12	5:D:1012:HOH:O	1.53	1.05
1:T:119:DT:H71	5:T:141:HOH:O	1.55	1.05
1:T:111:DT:C3'	5:T:132:HOH:O	2.02	1.04
4:D:794:THR:HB	5:D:892:HOH:O	1.55	1.04
4:D:330:ILE:HD13	5:D:895:HOH:O	1.54	1.04
4:D:817:ILE:HD11	5:D:947:HOH:O	1.55	1.03
4:D:141:ILE:O	4:D:145:ILE:HD13	1.57	1.03
4:D:344:TRP:CB	5:D:1015:HOH:O	2.06	1.02
4:D:96:ARG:HG3	5:D:891:HOH:O	1.60	1.01
4:D:451:PRO:HD3	5:D:1001:HOH:O	1.59	1.01
4:D:445:THR:HA	5:D:974:HOH:O	1.60	1.00
4:D:4:ILE:HG21	5:D:942:HOH:O	1.60	1.00
4:D:733:PHE:CZ	5:D:1002:HOH:O	2.15	1.00
4:D:344:TRP:HB2	5:D:1015:HOH:O	1.63	0.97
4:D:344:TRP:O	4:D:355:ILE:HD11	1.62	0.97
4:D:177:VAL:O	4:D:180:LYS:HG3	1.64	0.97
4:D:296:LEU:HD21	4:D:320:ILE:HD13	1.45	0.97
4:D:664:GLY:HA2	5:D:1031:HOH:O	1.66	0.95
4:D:65:ALA:HA	5:D:1017:HOH:O	1.65	0.94
4:D:118:THR:O	4:D:122:THR:HG23	1.67	0.94
4:D:664:GLY:CA	5:D:1031:HOH:O	2.14	0.94
4:D:796:VAL:HB	5:D:1016:HOH:O	1.67	0.93
4:D:270:PRO:HD3	5:D:935:HOH:O	1.69	0.93
4:D:795:VAL:N	5:D:892:HOH:O	2.00	0.93
4:D:816:THR:CG2	5:D:989:HOH:O	2.18	0.92
4:D:132:THR:CG2	5:D:983:HOH:O	2.17	0.92
4:D:464:GLY:HA3	5:D:1036:HOH:O	1.69	0.91
4:D:289:ASN:C	5:D:960:HOH:O	2.07	0.91
4:D:74:ILE:HG13	5:D:1017:HOH:O	1.70	0.90
4:D:355:ILE:HD13	4:D:355:ILE:H	1.35	0.90
3:R:10:G:N3	5:R:46:HOH:O	2.05	0.90
3:R:9:A:H1'	4:D:756:ARG:NH2	1.87	0.90
4:D:433:ASN:HD22	4:D:435:GLN:H	1.15	0.90
4:D:746:ARG:HE	4:D:754:GLN:HE22	1.14	0.89
4:D:816:THR:HG22	5:D:989:HOH:O	1.72	0.89
4:D:302:LYS:O	4:D:304:ALA:N	2.04	0.89
4:D:378:LYS:HD2	4:D:379:ARG:N	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:830:GLU:HB2	5:D:910:HOH:O	1.71	0.88
4:D:270:PRO:CG	5:D:935:HOH:O	2.21	0.88
4:D:137:VAL:HG21	4:D:244:ILE:HD11	1.54	0.88
4:D:491:ALA:HB1	4:D:499:ASN:ND2	1.90	0.87
4:D:419:ASN:C	5:D:957:HOH:O	2.10	0.87
3:R:10:G:C2	5:R:46:HOH:O	2.26	0.87
4:D:217:ILE:N	5:D:1005:HOH:O	2.08	0.87
4:D:546:PHE:HB3	5:D:909:HOH:O	1.74	0.86
4:D:118:THR:CA	5:D:955:HOH:O	2.23	0.86
4:D:468:ALA:HB2	5:D:987:HOH:O	1.74	0.86
4:D:118:THR:HA	5:D:955:HOH:O	1.74	0.85
4:D:129:ALA:HB3	5:D:1045:HOH:O	1.75	0.85
4:D:292:ARG:HA	4:D:292:ARG:HE	1.40	0.85
4:D:720:ARG:CZ	5:D:1029:HOH:O	2.22	0.85
4:D:359:GLU:HA	5:D:917:HOH:O	1.75	0.85
3:R:9:A:H1'	4:D:756:ARG:HH21	1.42	0.85
4:D:118:THR:N	5:D:955:HOH:O	2.10	0.84
4:D:441:LYS:N	5:D:967:HOH:O	2.11	0.84
3:R:3:C:H5'	5:R:91:HOH:O	1.76	0.83
4:D:876:LEU:HD12	5:D:1018:HOH:O	1.78	0.83
4:D:360:LEU:N	5:D:917:HOH:O	2.02	0.83
4:D:3:THR:HA	5:D:985:HOH:O	1.78	0.83
4:D:361:PRO:HD2	5:D:968:HOH:O	1.78	0.83
4:D:441:LYS:HG3	5:D:967:HOH:O	1.80	0.82
1:T:126:DT:H2''	1:T:125:DG:H5'	1.58	0.82
4:D:780:PRO:CD	5:D:1010:HOH:O	2.26	0.82
4:D:59:LEU:HD12	4:D:64:VAL:HG22	1.60	0.82
4:D:875:ILE:HG13	5:D:1014:HOH:O	1.80	0.82
4:D:428:ALA:CB	5:D:944:HOH:O	2.24	0.81
4:D:270:PRO:CD	5:D:935:HOH:O	2.26	0.81
4:D:359:GLU:CA	5:D:917:HOH:O	2.27	0.81
4:D:632:ARG:HB3	5:D:916:HOH:O	1.80	0.81
4:D:281:ILE:HG12	4:D:282:THR:HG23	1.62	0.81
4:D:873:ARG:HD3	5:D:1018:HOH:O	1.79	0.81
4:D:361:PRO:CD	5:D:968:HOH:O	2.29	0.81
4:D:741:LYS:HZ2	4:D:742:PRO:HD3	1.45	0.81
4:D:270:PRO:HG3	5:D:935:HOH:O	1.81	0.81
4:D:780:PRO:HG3	5:D:1010:HOH:O	1.81	0.80
4:D:733:PHE:HZ	5:D:1002:HOH:O	1.53	0.80
1:T:121:DA:H1'	5:T:135:HOH:O	1.81	0.80
4:D:473:VAL:HG22	4:D:474:PRO:HD2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:276:LYS:HG2	5:D:1032:HOH:O	1.80	0.80
4:D:856:SER:HB3	5:D:884:HOH:O	1.82	0.80
4:D:157:LEU:HG	4:D:158:GLU:HG2	1.63	0.80
4:D:115:ALA:O	4:D:119:ILE:HG13	1.82	0.80
4:D:780:PRO:CG	5:D:1010:HOH:O	2.31	0.79
4:D:741:LYS:HZ2	4:D:741:LYS:HA	1.47	0.79
4:D:790:HIS:CD2	5:D:995:HOH:O	2.36	0.79
4:D:505:GLN:OE1	5:D:1046:HOH:O	2.00	0.78
1:T:128:DC:H1'	1:T:127:DG:N7	1.97	0.78
4:D:561:LEU:O	5:D:1014:HOH:O	2.01	0.78
4:D:361:PRO:N	5:D:968:HOH:O	2.17	0.78
4:D:119:ILE:O	4:D:123:LEU:HB2	1.85	0.77
4:D:756:ARG:HH11	4:D:756:ARG:HG3	1.48	0.77
3:R:5:G:C8	5:R:99:HOH:O	2.37	0.77
4:D:716:GLY:O	5:D:1013:HOH:O	2.02	0.77
4:D:214:VAL:O	4:D:218:GLU:HG3	1.85	0.77
1:T:121:DA:C1'	5:T:135:HOH:O	2.33	0.76
4:D:454:LYS:HE3	5:D:948:HOH:O	1.85	0.76
4:D:433:ASN:ND2	4:D:435:GLN:H	1.84	0.76
4:D:817:ILE:CD1	5:D:947:HOH:O	2.23	0.76
1:T:127:DG:H1'	1:T:126:DT:H5'	1.66	0.76
4:D:255:ALA:HA	5:D:942:HOH:O	1.84	0.76
4:D:514:PHE:CE2	5:D:1036:HOH:O	2.39	0.76
4:D:137:VAL:O	4:D:141:ILE:HD12	1.85	0.76
4:D:791:LEU:O	5:D:892:HOH:O	2.04	0.75
4:D:289:ASN:CA	5:D:960:HOH:O	2.33	0.75
1:T:125:DG:H1'	1:T:124:DC:H5'	1.67	0.75
4:D:741:LYS:NZ	4:D:742:PRO:HD3	2.01	0.75
4:D:820:ASP:OD2	5:D:989:HOH:O	2.05	0.75
4:D:117:ILE:C	5:D:955:HOH:O	2.25	0.75
4:D:428:ALA:CA	5:D:944:HOH:O	2.08	0.74
5:T:139:HOH:O	4:D:780:PRO:HB2	1.87	0.74
4:D:468:ALA:CB	5:D:987:HOH:O	2.33	0.74
4:D:688:THR:O	5:D:1007:HOH:O	2.04	0.74
4:D:594:VAL:O	4:D:607:GLU:HB2	1.87	0.74
4:D:873:ARG:CA	5:D:1018:HOH:O	2.35	0.74
4:D:103:PHE:HB3	5:D:946:HOH:O	1.87	0.74
4:D:291:ARG:O	4:D:293:PRO:HD3	1.88	0.74
4:D:748:ASN:OD1	4:D:754:GLN:HB3	1.86	0.74
4:D:453:GLY:HA3	5:D:980:HOH:O	1.86	0.74
4:D:213:GLY:O	4:D:217:ILE:HG12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:729:THR:HA	5:D:1041:HOH:O	1.88	0.73
4:D:441:LYS:CG	5:D:967:HOH:O	2.35	0.73
4:D:691:ALA:HB1	5:D:909:HOH:O	1.87	0.73
1:T:128:DC:O2	5:T:134:HOH:O	2.05	0.73
4:D:454:LYS:O	5:D:951:HOH:O	2.06	0.73
4:D:129:ALA:O	5:D:983:HOH:O	2.04	0.73
4:D:552:ASP:HB2	4:D:691:ALA:HB2	1.68	0.73
4:D:787:ASP:HB3	5:D:1026:HOH:O	1.87	0.73
4:D:587:ILE:O	4:D:588:ASN:HB2	1.88	0.73
4:D:54:MET:HG3	4:D:57:ARG:NH2	2.04	0.73
4:D:352:ILE:HG22	4:D:352:ILE:O	1.89	0.73
4:D:355:ILE:H	4:D:355:ILE:CD1	1.97	0.73
4:D:360:LEU:H	4:D:360:LEU:HD23	1.53	0.72
4:D:88:TRP:O	4:D:92:VAL:HG12	1.89	0.72
4:D:289:ASN:N	5:D:960:HOH:O	2.21	0.72
4:D:452:ILE:O	5:D:980:HOH:O	2.07	0.72
4:D:819:ALA:HB3	5:D:947:HOH:O	1.88	0.72
4:D:804:ILE:HD11	5:D:1004:HOH:O	1.88	0.72
4:D:141:ILE:O	4:D:145:ILE:CD1	2.36	0.72
4:D:247:ALA:HB3	4:D:250:TYR:HD2	1.55	0.72
4:D:795:VAL:HG23	5:D:892:HOH:O	1.90	0.71
4:D:420:MET:HE2	4:D:424:GLY:HA2	1.73	0.71
4:D:682:TRP:O	4:D:686:SER:HB2	1.91	0.71
3:R:5:G:O5'	5:R:99:HOH:O	2.09	0.71
4:D:875:ILE:N	5:D:1014:HOH:O	2.23	0.71
4:D:594:VAL:HA	4:D:608:LYS:O	1.90	0.71
4:D:107:GLN:OE1	5:D:1011:HOH:O	2.09	0.70
4:D:117:ILE:HG22	5:D:955:HOH:O	1.91	0.70
4:D:585:ASP:O	4:D:614:LYS:HG2	1.91	0.70
4:D:217:ILE:O	4:D:221:ILE:CD1	2.20	0.70
4:D:70:ALA:O	4:D:74:ILE:HG12	1.90	0.70
4:D:741:LYS:HD3	4:D:742:PRO:HD2	1.73	0.70
4:D:577:LYS:NZ	4:D:577:LYS:HB2	2.06	0.70
4:D:73:LEU:HD23	4:D:74:ILE:N	2.06	0.69
4:D:454:LYS:CD	5:D:948:HOH:O	2.40	0.69
4:D:278:TRP:H	4:D:321:ASN:HD21	1.38	0.69
4:D:423:ARG:HH12	4:D:784:HIS:HD2	1.39	0.69
1:T:111:DT:C2'	5:T:132:HOH:O	2.36	0.69
4:D:4:ILE:N	5:D:985:HOH:O	2.05	0.69
4:D:538:GLY:O	5:D:984:HOH:O	2.09	0.69
4:D:488:ASN:ND2	5:D:993:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:14:DT:H2"	2:N:15:DT:OP1	1.93	0.69
4:D:859:ASP:O	5:D:988:HOH:O	2.11	0.69
4:D:420:MET:CB	5:D:957:HOH:O	2.41	0.69
4:D:873:ARG:HA	5:D:1018:HOH:O	1.92	0.69
4:D:93:LYS:NZ	5:D:1011:HOH:O	2.26	0.69
4:D:473:VAL:CG2	4:D:474:PRO:HD2	2.23	0.69
4:D:146:GLU:OE2	5:D:971:HOH:O	2.10	0.69
4:D:730:PRO:HD3	5:D:1041:HOH:O	1.93	0.68
4:D:709:GLU:CA	5:D:940:HOH:O	2.41	0.68
3:R:1:A:H5"	5:R:75:HOH:O	1.93	0.68
4:D:324:GLN:HB3	4:D:418:TYR:HD1	1.58	0.68
4:D:765:LYS:HD3	4:D:766:ASP:N	2.09	0.68
4:D:587:ILE:HA	4:D:614:LYS:HE3	1.76	0.68
4:D:324:GLN:NE2	5:D:928:HOH:O	2.27	0.67
4:D:546:PHE:O	5:D:909:HOH:O	2.11	0.67
4:D:709:GLU:HA	5:D:940:HOH:O	1.93	0.67
4:D:109:ILE:HD13	4:D:114:VAL:CG2	2.25	0.67
4:D:803:GLY:O	5:D:966:HOH:O	2.13	0.67
4:D:755:PHE:HB2	5:D:1024:HOH:O	1.95	0.67
4:D:74:ILE:CG1	5:D:1017:HOH:O	2.36	0.67
4:D:281:ILE:HD13	4:D:281:ILE:H	1.59	0.67
1:T:130:DG:HO5'	1:T:130:DG:H8	1.41	0.67
4:D:804:ILE:HD12	4:D:820:ASP:CG	2.15	0.66
4:D:81:MET:O	4:D:85:ILE:HG12	1.95	0.66
4:D:354:ALA:HB3	4:D:391:ARG:HD2	1.77	0.66
4:D:458:TYR:O	4:D:462:ILE:HD12	1.95	0.66
4:D:655:ILE:HD12	4:D:655:ILE:H	1.60	0.66
4:D:78:LEU:HD13	4:D:119:ILE:HD12	1.77	0.66
1:T:127:DG:C5	5:T:134:HOH:O	2.47	0.66
4:D:209:SER:OG	5:D:971:HOH:O	2.12	0.66
4:D:137:VAL:HG12	4:D:141:ILE:HD11	1.78	0.66
4:D:546:PHE:C	5:D:909:HOH:O	2.33	0.66
4:D:857:GLN:HA	4:D:857:GLN:OE1	1.95	0.66
4:D:134:VAL:HG12	4:D:244:ILE:HG23	1.77	0.66
4:D:797:TRP:N	5:D:1016:HOH:O	2.27	0.66
4:D:756:ARG:NH1	4:D:756:ARG:HG3	2.07	0.66
4:D:95:LYS:O	5:D:902:HOH:O	2.12	0.66
4:D:505:GLN:HB3	5:D:952:HOH:O	1.94	0.66
4:D:807:PHE:O	5:D:941:HOH:O	2.13	0.66
4:D:4:ILE:CG2	5:D:942:HOH:O	2.30	0.66
4:D:196:LEU:H	4:D:196:LEU:HD22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:344:TRP:CE3	5:D:1015:HOH:O	2.50	0.65
4:D:537:ASP:OD2	5:D:984:HOH:O	2.13	0.65
4:D:217:ILE:HD13	5:D:1005:HOH:O	1.95	0.65
4:D:352:ILE:O	4:D:353:PRO:O	2.15	0.65
4:D:54:MET:HG3	4:D:57:ARG:HH21	1.61	0.65
4:D:308:TYR:O	4:D:311:VAL:HG12	1.97	0.65
4:D:779:ALA:O	4:D:783:VAL:HG23	1.96	0.65
5:T:139:HOH:O	4:D:780:PRO:HG2	1.97	0.65
4:D:829:ARG:NH2	4:D:882:PHE:HA	2.11	0.65
1:T:119:DT:O4'	5:T:139:HOH:O	2.13	0.65
4:D:25:ALA:HA	5:D:937:HOH:O	1.96	0.65
4:D:593:GLU:HG2	4:D:594:VAL:H	1.62	0.65
4:D:500:THR:OG1	5:D:1009:HOH:O	2.15	0.65
4:D:228:SER:HB3	4:D:245:GLU:OE1	1.96	0.64
4:D:488:ASN:CG	5:D:993:HOH:O	2.36	0.64
4:D:360:LEU:N	4:D:360:LEU:HD23	2.13	0.64
4:D:650:VAL:HG12	4:D:655:ILE:CD1	2.27	0.64
4:D:669:GLN:HG3	4:D:672:GLN:HB2	1.79	0.64
4:D:355:ILE:HD13	4:D:355:ILE:N	2.09	0.64
4:D:250:TYR:O	4:D:254:ILE:HD12	1.97	0.64
5:T:139:HOH:O	4:D:780:PRO:CG	2.46	0.63
4:D:787:ASP:CB	5:D:1026:HOH:O	2.43	0.63
4:D:490:MET:HE3	5:D:926:HOH:O	1.97	0.63
1:T:126:DT:C4	5:T:134:HOH:O	2.51	0.63
4:D:99:ARG:O	5:D:982:HOH:O	2.15	0.63
4:D:71:LYS:HA	5:D:1034:HOH:O	1.98	0.63
4:D:595:VAL:HB	4:D:607:GLU:HA	1.81	0.63
4:D:664:GLY:HA3	5:D:1031:HOH:O	1.88	0.63
4:D:746:ARG:HE	4:D:754:GLN:NE2	1.92	0.63
4:D:720:ARG:NH2	5:D:1029:HOH:O	2.31	0.63
4:D:353:PRO:HG3	4:D:394:ARG:HB2	1.80	0.63
4:D:532:LEU:O	4:D:818:PRO:HD3	1.99	0.63
4:D:423:ARG:HH12	4:D:784:HIS:CD2	2.16	0.62
4:D:579:ASN:HA	4:D:582:LEU:HB2	1.81	0.62
4:D:74:ILE:CD1	5:D:1017:HOH:O	2.47	0.62
1:T:119:DT:P	5:T:141:HOH:O	2.57	0.62
4:D:806:SER:O	4:D:816:THR:HG23	1.99	0.62
1:T:119:DT:OP2	5:T:141:HOH:O	2.16	0.62
4:D:445:THR:CB	5:D:974:HOH:O	2.47	0.62
4:D:207:GLU:HG2	4:D:211:HIS:HE1	1.65	0.62
1:T:123:DG:H2''	1:T:122:DC:H5'	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:562:LEU:HD21	4:D:870:LEU:CD1	2.30	0.62
4:D:180:LYS:HD2	4:D:181:ALA:N	2.15	0.61
4:D:14:ILE:HG23	4:D:288:ALA:HB1	1.81	0.61
1:T:126:DT:C5	5:T:134:HOH:O	2.52	0.61
4:D:725:VAL:HG23	4:D:774:GLN:NE2	2.15	0.61
4:D:340:VAL:CG2	4:D:341:ILE:N	2.64	0.61
4:D:117:ILE:HG21	4:D:145:ILE:HD12	1.80	0.61
4:D:25:ALA:O	4:D:26:ASP:HB2	2.00	0.61
4:D:50:ARG:NH2	4:D:267:MET:HG2	2.15	0.61
4:D:104:GLN:N	5:D:946:HOH:O	2.17	0.61
1:T:120:DT:H1'	1:T:119:DT:H71	1.81	0.61
4:D:330:ILE:HD12	4:D:330:ILE:N	2.16	0.61
4:D:710:VAL:HG13	4:D:720:ARG:H	1.64	0.60
4:D:330:ILE:HD13	4:D:408:PHE:O	1.99	0.60
4:D:666:MET:HE1	5:D:1031:HOH:O	2.01	0.60
4:D:790:HIS:HD2	5:D:995:HOH:O	1.80	0.60
4:D:420:MET:N	5:D:957:HOH:O	2.28	0.60
4:D:797:TRP:CE2	5:D:910:HOH:O	2.51	0.60
4:D:264:ILE:HB	4:D:292:ARG:HD2	1.83	0.60
2:N:25:DC:H1'	2:N:26:DA:H5''	1.83	0.60
3:R:4:G:O3'	4:D:394:ARG:NH1	2.33	0.60
4:D:873:ARG:O	5:D:1018:HOH:O	2.17	0.60
4:D:746:ARG:NE	4:D:754:GLN:HE22	1.94	0.60
4:D:445:THR:CA	5:D:974:HOH:O	2.33	0.60
4:D:292:ARG:HA	4:D:292:ARG:NE	2.14	0.60
4:D:19:ILE:HB	4:D:20:PRO:HD3	1.82	0.60
1:T:119:DT:C4'	5:T:139:HOH:O	2.49	0.60
4:D:816:THR:HG21	5:D:989:HOH:O	1.94	0.60
4:D:141:ILE:CD1	4:D:217:ILE:HD11	2.32	0.60
4:D:82:ILE:HG12	4:D:112:GLU:HA	1.83	0.59
1:T:117:DG:H2''	1:T:116:DC:H5'	1.82	0.59
4:D:360:LEU:HB3	4:D:384:VAL:HG21	1.83	0.59
4:D:320:ILE:HD11	4:D:420:MET:SD	2.41	0.59
4:D:157:LEU:HD23	4:D:196:LEU:HD12	1.83	0.59
4:D:765:LYS:HA	4:D:765:LYS:HZ3	1.68	0.59
4:D:539:SER:O	4:D:540:CYS:HB2	2.03	0.59
4:D:796:VAL:CB	5:D:1016:HOH:O	2.36	0.59
4:D:16:LEU:HG	4:D:20:PRO:HB2	1.85	0.59
4:D:141:ILE:HD13	4:D:217:ILE:HD11	1.84	0.59
4:D:439:MET:HB2	5:D:934:HOH:O	2.03	0.59
4:D:857:GLN:HE22	4:D:859:ASP:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:119:DT:H6	5:T:141:HOH:O	1.85	0.58
4:D:655:ILE:O	4:D:658:ALA:N	2.34	0.58
4:D:404:GLN:N	5:D:973:HOH:O	2.35	0.58
1:T:119:DT:C7	5:T:141:HOH:O	2.32	0.58
3:R:9:A:H2	5:D:991:HOH:O	1.86	0.58
4:D:157:LEU:O	4:D:159:ALA:N	2.35	0.58
4:D:13:ASP:CG	4:D:14:ILE:HD12	2.24	0.58
4:D:169:GLN:H	4:D:169:GLN:CD	2.07	0.58
4:D:826:LYS:HE2	4:D:830:GLU:OE2	2.04	0.58
4:D:85:ILE:HA	4:D:219:MET:HE1	1.86	0.58
2:N:17:DA:H3'	2:N:18:DC:H5''	1.85	0.58
4:D:337:VAL:HG11	4:D:512:LEU:HD21	1.86	0.58
4:D:562:LEU:HD21	4:D:870:LEU:HD12	1.84	0.58
4:D:80:LYS:O	5:D:1048:HOH:O	2.16	0.58
4:D:85:ILE:HA	4:D:219:MET:CE	2.34	0.58
3:R:10:G:H8	4:D:301:SER:OG	1.87	0.58
4:D:153:ARG:C	4:D:155:ARG:H	2.06	0.58
4:D:153:ARG:O	4:D:157:LEU:HB3	2.04	0.58
4:D:812:ASP:OD2	5:D:984:HOH:O	2.17	0.58
4:D:25:ALA:CA	5:D:937:HOH:O	2.52	0.58
4:D:340:VAL:HG23	4:D:341:ILE:N	2.19	0.58
4:D:344:TRP:HB3	5:D:1015:HOH:O	1.88	0.57
4:D:130:ASP:C	4:D:132:THR:H	2.07	0.57
4:D:318:LYS:O	4:D:322:ILE:HG12	2.03	0.57
4:D:137:VAL:HG12	4:D:141:ILE:CD1	2.34	0.57
4:D:420:MET:HB3	5:D:957:HOH:O	2.04	0.57
4:D:454:LYS:CE	5:D:948:HOH:O	2.45	0.57
4:D:557:ARG:O	4:D:568:GLN:HG3	2.04	0.57
4:D:729:THR:HG22	5:D:1041:HOH:O	2.03	0.57
4:D:611:LEU:HD22	4:D:615:ALA:HB1	1.85	0.57
4:D:633:SER:HA	4:D:649:GLN:HE22	1.69	0.57
4:D:420:MET:CE	4:D:424:GLY:HA2	2.34	0.57
4:D:154:ILE:HD11	4:D:183:MET:CE	2.33	0.57
4:D:727:TRP:NE1	5:D:1037:HOH:O	2.38	0.57
4:D:404:GLN:CA	5:D:973:HOH:O	2.53	0.57
4:D:335:LEU:HD22	4:D:339:ASN:ND2	2.19	0.57
4:D:420:MET:HE3	4:D:424:GLY:O	2.05	0.57
4:D:797:TRP:CZ3	4:D:801:LYS:HE3	2.40	0.57
4:D:589:GLY:C	4:D:614:LYS:HG3	2.25	0.57
4:D:110:LYS:HB3	4:D:112:GLU:OE2	2.05	0.57
4:D:689:VAL:C	5:D:972:HOH:O	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:851:ASP:O	4:D:853:LEU:N	2.38	0.57
4:D:14:ILE:HG13	4:D:290:GLY:HA2	1.87	0.57
4:D:407:LYS:HB2	5:D:973:HOH:O	2.04	0.56
1:T:120:DT:H1'	5:T:141:HOH:O	2.04	0.56
2:N:22:DG:H2''	2:N:23:DC:C6	2.40	0.56
4:D:710:VAL:N	5:D:940:HOH:O	2.38	0.56
4:D:440:THR:HG22	5:D:967:HOH:O	2.04	0.56
4:D:208:ASP:C	4:D:210:ILE:H	2.09	0.56
4:D:25:ALA:HB2	5:D:937:HOH:O	2.03	0.56
4:D:30:GLU:N	5:D:937:HOH:O	2.38	0.56
4:D:147:ASP:HB3	4:D:751:PHE:HE2	1.70	0.56
4:D:344:TRP:HE3	5:D:1015:HOH:O	1.87	0.56
4:D:281:ILE:CD1	4:D:281:ILE:H	2.19	0.56
1:T:111:DT:OP2	1:T:111:DT:H3'	2.05	0.56
5:T:139:HOH:O	4:D:780:PRO:CB	2.50	0.56
4:D:517:GLU:HG3	4:D:532:LEU:HB2	1.86	0.56
4:D:360:LEU:CB	5:D:968:HOH:O	2.12	0.56
4:D:780:PRO:CB	5:D:975:HOH:O	2.54	0.56
4:D:797:TRP:NE1	5:D:910:HOH:O	2.38	0.56
4:D:325:ASN:HB3	5:D:919:HOH:O	2.06	0.56
4:D:684:SER:O	4:D:687:VAL:HG22	2.06	0.56
4:D:454:LYS:HD3	5:D:948:HOH:O	2.05	0.56
4:D:221:ILE:CD1	4:D:221:ILE:N	2.69	0.55
4:D:255:ALA:CA	5:D:942:HOH:O	2.49	0.55
4:D:25:ALA:CB	5:D:937:HOH:O	2.54	0.55
4:D:134:VAL:HG11	4:D:229:LEU:CD2	2.36	0.55
4:D:300:HIS:O	4:D:301:SER:HB2	2.06	0.55
1:T:114:DG:H4'	4:D:396:ILE:HG21	1.88	0.55
4:D:710:VAL:CG1	4:D:720:ARG:HB3	2.37	0.55
4:D:726:HIS:HB2	4:D:736:TRP:CD1	2.41	0.55
4:D:804:ILE:CD1	5:D:1004:HOH:O	2.50	0.55
4:D:264:ILE:HD12	4:D:264:ILE:O	2.05	0.55
4:D:471:ASP:OD1	4:D:472:LYS:HE2	2.06	0.55
1:T:127:DG:H1'	1:T:126:DT:C5'	2.36	0.55
4:D:593:GLU:HG2	4:D:594:VAL:N	2.22	0.55
4:D:619:GLN:OE1	4:D:667:PHE:HA	2.06	0.55
3:R:10:G:N2	5:R:46:HOH:O	2.31	0.55
4:D:16:LEU:CG	4:D:20:PRO:HB2	2.37	0.55
4:D:689:VAL:O	4:D:689:VAL:HG23	2.06	0.55
4:D:830:GLU:CB	5:D:910:HOH:O	2.43	0.55
4:D:154:ILE:HD11	4:D:183:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:779:ALA:O	4:D:783:VAL:CG2	2.55	0.55
4:D:428:ALA:HB1	5:D:944:HOH:O	1.97	0.55
4:D:829:ARG:NH1	4:D:878:SER:O	2.40	0.55
4:D:420:MET:CG	5:D:957:HOH:O	2.54	0.55
4:D:655:ILE:O	4:D:656:GLN:C	2.44	0.54
4:D:543:ILE:HD12	4:D:543:ILE:H	1.71	0.54
4:D:590:THR:HG22	4:D:591:ASP:N	2.22	0.54
4:D:853:LEU:O	4:D:854:HIS:HB2	2.08	0.54
4:D:160:LYS:HD3	4:D:163:LYS:HD2	1.88	0.54
4:D:651:LEU:HG	4:D:656:GLN:HE21	1.73	0.54
4:D:545:HIS:O	4:D:549:MET:HG2	2.07	0.54
4:D:157:LEU:CD2	4:D:196:LEU:HD12	2.37	0.54
4:D:553:GLU:HB3	5:D:893:HOH:O	2.06	0.54
4:D:347:CYS:HA	5:D:1015:HOH:O	2.06	0.54
4:D:13:ASP:OD2	4:D:14:ILE:HD12	2.07	0.54
4:D:400:PHE:O	4:D:404:GLN:HB2	2.07	0.54
4:D:570:ILE:O	4:D:574:VAL:HG23	2.08	0.54
4:D:160:LYS:HZ3	4:D:160:LYS:HB2	1.73	0.53
4:D:810:ILE:HD12	4:D:810:ILE:N	2.23	0.53
4:D:292:ARG:CA	4:D:292:ARG:HE	2.18	0.53
4:D:806:SER:HB2	5:D:1008:HOH:O	2.07	0.53
4:D:410:ASN:N	5:D:903:HOH:O	2.21	0.53
4:D:92:VAL:HG11	4:D:103:PHE:CD1	2.43	0.53
4:D:791:LEU:HA	4:D:814:PHE:HE2	1.73	0.53
4:D:335:LEU:CD2	4:D:339:ASN:ND2	2.72	0.53
4:D:160:LYS:CD	4:D:163:LYS:HD2	2.39	0.53
1:T:126:DT:C2'	1:T:125:DG:H5'	2.33	0.53
4:D:2:ASN:O	4:D:127:THR:HA	2.09	0.53
4:D:196:LEU:HD22	4:D:196:LEU:N	2.23	0.53
4:D:790:HIS:HD2	5:D:904:HOH:O	1.92	0.53
4:D:141:ILE:C	4:D:145:ILE:HD13	2.25	0.52
4:D:810:ILE:CD1	5:D:932:HOH:O	2.57	0.52
4:D:6:ILE:HD12	4:D:6:ILE:N	2.24	0.52
4:D:153:ARG:NH2	4:D:201:TRP:HB2	2.24	0.52
1:T:120:DT:H2''	5:T:141:HOH:O	2.09	0.52
5:T:131:HOH:O	4:D:421:ASP:HB2	2.08	0.52
4:D:6:ILE:H	4:D:6:ILE:HD12	1.75	0.52
4:D:780:PRO:CA	5:D:975:HOH:O	2.58	0.52
1:T:122:DC:H2''	1:T:121:DA:O5'	2.10	0.52
4:D:650:VAL:HG12	4:D:655:ILE:HD11	1.91	0.52
4:D:421:ASP:O	5:D:1002:HOH:O	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:335:LEU:HD21	4:D:406:ASN:OD1	2.10	0.52
4:D:727:TRP:CZ3	5:D:1012:HOH:O	2.54	0.52
4:D:226:MET:HA	4:D:250:TYR:CD2	2.44	0.52
4:D:147:ASP:HB3	4:D:751:PHE:CE2	2.45	0.52
4:D:380:ALA:C	5:D:986:HOH:O	2.47	0.52
4:D:533:PRO:CD	5:D:974:HOH:O	2.57	0.52
4:D:610:LYS:HA	4:D:672:GLN:OE1	2.09	0.52
4:D:360:LEU:C	5:D:968:HOH:O	2.44	0.51
4:D:181:ALA:O	4:D:185:VAL:HG23	2.10	0.51
3:R:10:G:C8	4:D:301:SER:OG	2.63	0.51
4:D:41:HIS:O	4:D:45:GLU:HG3	2.10	0.51
1:T:111:DT:H3'	1:T:111:DT:P	2.49	0.51
4:D:709:GLU:C	5:D:940:HOH:O	2.49	0.51
4:D:65:ALA:CA	5:D:1017:HOH:O	2.39	0.51
4:D:577:LYS:HZ3	4:D:577:LYS:HB2	1.75	0.51
4:D:461:LYS:HA	5:D:1036:HOH:O	2.11	0.51
4:D:2:ASN:OD1	4:D:245:GLU:HB2	2.11	0.51
1:T:120:DT:C2'	5:T:141:HOH:O	2.59	0.51
4:D:182:PHE:O	4:D:186:VAL:HG23	2.11	0.51
4:D:595:VAL:CG2	4:D:608:LYS:H	2.23	0.51
4:D:118:THR:HG22	4:D:220:LEU:HD12	1.93	0.51
4:D:652:GLU:O	4:D:657:PRO:HD3	2.11	0.51
4:D:433:ASN:HB2	4:D:434:PRO:CD	2.41	0.51
4:D:255:ALA:N	5:D:942:HOH:O	2.44	0.50
4:D:706:LEU:HA	5:D:1029:HOH:O	2.11	0.50
4:D:709:GLU:CG	5:D:940:HOH:O	2.60	0.50
4:D:32:LEU:HG	5:D:1047:HOH:O	2.11	0.50
4:D:215:ARG:O	4:D:219:MET:HG3	2.11	0.50
4:D:804:ILE:HD12	4:D:820:ASP:HB3	1.93	0.50
4:D:30:GLU:HG3	4:D:34:ARG:HH21	1.76	0.50
4:D:339:ASN:OD1	4:D:402:LEU:HD11	2.11	0.50
4:D:550:LEU:HB2	4:D:691:ALA:HB1	1.92	0.50
4:D:210:ILE:O	4:D:214:VAL:HG23	2.11	0.50
4:D:33:ALA:HB3	5:D:937:HOH:O	2.12	0.50
4:D:85:ILE:HG22	4:D:89:PHE:CE2	2.46	0.50
4:D:804:ILE:HD12	4:D:820:ASP:CB	2.42	0.50
4:D:30:GLU:HA	5:D:937:HOH:O	2.12	0.50
4:D:341:ILE:HD11	4:D:348:PRO:CG	2.40	0.50
4:D:143:ARG:HH11	4:D:143:ARG:HG2	1.76	0.50
4:D:778:ILE:HG23	4:D:779:ALA:N	2.26	0.50
1:T:119:DT:C6	5:T:141:HOH:O	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:655:ILE:HG23	4:D:659:ILE:HD13	1.93	0.50
4:D:551:ARG:HB2	4:D:868:GLY:H	1.76	0.50
4:D:276:LYS:CE	5:D:1032:HOH:O	2.07	0.50
4:D:217:ILE:CA	5:D:1005:HOH:O	2.57	0.50
4:D:711:LYS:NZ	5:D:1013:HOH:O	2.45	0.50
4:D:707:ALA:O	4:D:722:ARG:HG2	2.10	0.50
4:D:631:LYS:HD3	4:D:635:MET:SD	2.51	0.50
4:D:417:PRO:HG2	4:D:429:VAL:HB	1.94	0.50
4:D:651:LEU:HG	4:D:656:GLN:NE2	2.26	0.50
4:D:379:ARG:C	4:D:381:ALA:H	2.15	0.49
4:D:379:ARG:C	4:D:381:ALA:N	2.65	0.49
4:D:312:TYR:HD2	5:D:976:HOH:O	1.94	0.49
4:D:727:TRP:CE3	5:D:1012:HOH:O	2.64	0.49
4:D:404:GLN:HA	5:D:973:HOH:O	2.12	0.49
4:D:117:ILE:HG12	4:D:752:LEU:HD12	1.95	0.49
4:D:157:LEU:HD12	4:D:158:GLU:H	1.78	0.49
4:D:875:ILE:CG1	5:D:1014:HOH:O	2.50	0.49
4:D:254:ILE:C	5:D:942:HOH:O	2.49	0.49
4:D:710:VAL:HG13	4:D:720:ARG:N	2.28	0.49
4:D:159:ALA:HA	4:D:195:LEU:HD21	1.94	0.49
4:D:291:ARG:C	4:D:293:PRO:HD3	2.32	0.49
4:D:495:SER:HA	5:D:929:HOH:O	2.13	0.49
4:D:417:PRO:O	5:D:944:HOH:O	2.20	0.49
4:D:653:ASP:O	4:D:657:PRO:HG3	2.12	0.49
1:T:127:DG:H2"	1:T:126:DT:OP2	2.13	0.49
4:D:593:GLU:CG	4:D:594:VAL:H	2.25	0.49
4:D:854:HIS:O	4:D:855:GLU:O	2.31	0.49
4:D:352:ILE:CG2	4:D:352:ILE:O	2.61	0.49
4:D:47:GLY:HA3	4:D:265:SER:O	2.12	0.49
4:D:654:THR:O	4:D:657:PRO:HG2	2.13	0.48
4:D:473:VAL:HG11	4:D:477:GLU:OE2	2.13	0.48
4:D:195:LEU:C	4:D:197:GLY:H	2.16	0.48
4:D:13:ASP:OD1	4:D:14:ILE:HD12	2.12	0.48
4:D:873:ARG:CB	5:D:1018:HOH:O	2.57	0.48
4:D:620:TRP:O	4:D:623:TYR:HB3	2.13	0.48
4:D:207:GLU:HG2	4:D:211:HIS:CE1	2.45	0.48
4:D:543:ILE:N	4:D:543:ILE:HD12	2.27	0.48
4:D:833:VAL:O	4:D:837:GLU:HB2	2.12	0.48
4:D:744:GLN:NE2	4:D:758:GLN:NE2	2.61	0.48
4:D:360:LEU:N	4:D:360:LEU:CD2	2.76	0.48
4:D:88:TRP:O	4:D:91:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:584:ALA:O	4:D:588:ASN:HB3	2.14	0.48
4:D:349:VAL:HG13	4:D:508:PRO:HG3	1.96	0.48
4:D:330:ILE:CD1	5:D:895:HOH:O	2.33	0.48
4:D:729:THR:CB	5:D:1041:HOH:O	2.61	0.48
4:D:162:PHE:C	4:D:164:LYS:H	2.17	0.48
4:D:533:PRO:HA	4:D:816:THR:O	2.13	0.48
4:D:707:ALA:O	4:D:722:ARG:NH1	2.43	0.48
2:N:28:DG:H2''	2:N:29:DG:H8	1.79	0.48
4:D:468:ALA:HA	5:D:952:HOH:O	2.13	0.48
4:D:828:VAL:HG11	4:D:882:PHE:O	2.13	0.48
2:N:22:DG:H2''	2:N:23:DC:C5	2.48	0.48
4:D:276:LYS:CD	5:D:1032:HOH:O	2.55	0.48
4:D:286:TYR:CZ	4:D:417:PRO:HG3	2.48	0.48
4:D:320:ILE:O	4:D:324:GLN:HG2	2.14	0.48
1:T:117:DG:H2''	1:T:116:DC:C5'	2.43	0.48
4:D:595:VAL:CB	4:D:607:GLU:HA	2.43	0.47
4:D:278:TRP:CH2	4:D:294:LEU:HB3	2.50	0.47
4:D:650:VAL:O	4:D:655:ILE:HD12	2.14	0.47
4:D:375:THR:O	4:D:376:ALA:HB3	2.14	0.47
1:T:128:DC:H42	2:N:27:DC:H42	1.61	0.47
4:D:537:ASP:N	4:D:882:PHE:HD1	2.13	0.47
4:D:25:ALA:C	4:D:27:HIS:H	2.17	0.47
4:D:669:GLN:HG2	4:D:672:GLN:NE2	2.30	0.47
4:D:46:MET:O	4:D:267:MET:HE2	2.15	0.47
3:R:6:C:H5'	4:D:171:ASN:O	2.15	0.47
4:D:690:VAL:N	5:D:972:HOH:O	2.48	0.47
4:D:93:LYS:HE3	4:D:103:PHE:HZ	1.79	0.47
4:D:109:ILE:HD12	4:D:109:ILE:H	1.80	0.47
4:D:735:VAL:CG2	5:D:1037:HOH:O	2.63	0.47
4:D:330:ILE:CD1	4:D:330:ILE:N	2.78	0.47
4:D:20:PRO:O	4:D:23:THR:HB	2.14	0.47
4:D:254:ILE:HG22	5:D:942:HOH:O	2.15	0.46
4:D:676:TYR:O	4:D:679:LYS:HB3	2.16	0.46
4:D:828:VAL:CG1	4:D:882:PHE:O	2.63	0.46
4:D:577:LYS:HD3	4:D:687:VAL:CG2	2.45	0.46
4:D:700:LYS:NZ	4:D:700:LYS:HB3	2.30	0.46
4:D:85:ILE:HD13	4:D:219:MET:SD	2.55	0.46
4:D:226:MET:O	4:D:246:LEU:HD12	2.16	0.46
4:D:4:ILE:HD13	4:D:254:ILE:HG21	1.98	0.46
4:D:473:VAL:HG22	4:D:474:PRO:CD	2.40	0.46
4:D:696:MET:O	4:D:700:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:296:LEU:CD2	4:D:320:ILE:HD13	2.32	0.46
4:D:802:TYR:OH	4:D:826:LYS:HD3	2.15	0.46
4:D:817:ILE:CG1	5:D:947:HOH:O	2.60	0.46
2:N:27:DC:H2''	2:N:28:DG:H5''	1.98	0.46
4:D:70:ALA:HB1	5:D:1017:HOH:O	2.15	0.46
4:D:481:PHE:HE2	5:D:987:HOH:O	1.98	0.46
4:D:765:LYS:HD3	4:D:766:ASP:H	1.78	0.46
4:D:379:ARG:O	5:D:986:HOH:O	2.21	0.45
1:T:126:DT:H1'	1:T:125:DG:H5''	1.98	0.45
4:D:855:GLU:HB3	4:D:856:SER:H	1.44	0.45
4:D:669:GLN:HG2	4:D:672:GLN:HE21	1.81	0.45
4:D:421:ASP:C	4:D:421:ASP:OD1	2.54	0.45
4:D:157:LEU:HG	4:D:196:LEU:HD12	1.98	0.45
4:D:763:THR:CG2	5:D:962:HOH:O	0.76	0.45
4:D:360:LEU:O	4:D:362:MET:SD	2.75	0.45
1:T:112:DG:N3	1:T:112:DG:O4'	2.50	0.45
4:D:505:GLN:CA	5:D:952:HOH:O	2.64	0.45
1:T:113:DT:H2'	4:D:57:ARG:NH1	2.31	0.45
4:D:577:LYS:HZ2	4:D:577:LYS:HB2	1.80	0.45
4:D:659:ILE:HD11	4:D:667:PHE:HD2	1.81	0.45
4:D:169:GLN:CD	4:D:169:GLN:N	2.69	0.45
4:D:105:PHE:O	4:D:108:GLU:HG2	2.17	0.45
4:D:330:ILE:HD11	4:D:408:PHE:CB	2.47	0.45
4:D:74:ILE:HD11	5:D:1017:HOH:O	2.11	0.45
4:D:461:LYS:HE2	4:D:479:ILE:HD12	1.97	0.45
4:D:875:ILE:CA	5:D:1014:HOH:O	2.64	0.45
4:D:655:ILE:CG2	4:D:659:ILE:HD13	2.47	0.45
4:D:621:LEU:C	4:D:623:TYR:H	2.19	0.45
4:D:398:LEU:O	4:D:402:LEU:HB2	2.17	0.45
4:D:816:THR:HG22	4:D:817:ILE:H	1.82	0.45
4:D:270:PRO:CB	5:D:935:HOH:O	2.62	0.45
1:T:126:DT:H1'	1:T:125:DG:C5'	2.46	0.45
4:D:655:ILE:N	4:D:655:ILE:HD12	2.30	0.45
4:D:162:PHE:O	4:D:167:GLU:N	2.49	0.45
4:D:229:LEU:HD23	4:D:244:ILE:HG23	1.98	0.45
4:D:321:ASN:O	4:D:325:ASN:HB2	2.17	0.45
4:D:160:LYS:C	4:D:162:PHE:N	2.68	0.45
1:T:115:DC:O5'	1:T:115:DC:H2'	2.17	0.45
4:D:727:TRP:CZ2	4:D:782:PHE:HA	2.52	0.45
4:D:533:PRO:HD2	5:D:974:HOH:O	2.16	0.44
4:D:706:LEU:O	4:D:723:CYS:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:123:DG:H2"	1:T:122:DC:C5'	2.47	0.44
4:D:633:SER:CA	4:D:649:GLN:HE22	2.30	0.44
4:D:276:LYS:CG	5:D:1032:HOH:O	2.50	0.44
4:D:416:PHE:HE1	5:D:935:HOH:O	2.01	0.44
4:D:73:LEU:O	4:D:77:LEU:HG	2.17	0.44
4:D:651:LEU:HA	4:D:655:ILE:HD13	1.99	0.44
2:N:17:DA:C3'	2:N:18:DC:H5"	2.46	0.44
4:D:154:ILE:HG22	4:D:196:LEU:HD21	2.00	0.44
4:D:395:ARG:O	4:D:399:GLU:HG3	2.17	0.44
4:D:655:ILE:HG22	4:D:656:GLN:N	2.33	0.44
4:D:566:THR:HG23	4:D:568:GLN:HE22	1.83	0.44
4:D:145:ILE:N	4:D:145:ILE:HD12	2.32	0.44
4:D:873:ARG:HH11	4:D:873:ARG:HG3	1.83	0.44
4:D:278:TRP:HH2	4:D:294:LEU:HB3	1.81	0.44
4:D:727:TRP:CD1	5:D:1037:HOH:O	2.56	0.44
1:T:123:DG:H1'	1:T:122:DC:H5"	1.99	0.44
4:D:655:ILE:HG23	4:D:659:ILE:CD1	2.48	0.44
1:T:118:DC:H2"	1:T:117:DG:OP2	2.18	0.44
4:D:9:ASN:OD1	4:D:48:GLU:OE2	2.35	0.44
4:D:281:ILE:HD13	4:D:281:ILE:N	2.30	0.44
4:D:221:ILE:H	4:D:221:ILE:CD1	2.30	0.44
2:N:24:DG:H2"	2:N:25:DC:C6	2.53	0.44
4:D:208:ASP:O	4:D:210:ILE:N	2.51	0.44
4:D:33:ALA:CB	5:D:937:HOH:O	2.64	0.44
4:D:78:LEU:HB3	4:D:79:PRO:HD3	2.00	0.43
4:D:153:ARG:C	4:D:155:ARG:N	2.71	0.43
4:D:452:ILE:HG23	4:D:453:GLY:N	2.32	0.43
4:D:109:ILE:CD1	4:D:109:ILE:H	2.30	0.43
4:D:275:PRO:HD3	4:D:415:TRP:HB3	2.00	0.43
4:D:661:SER:C	4:D:663:LYS:H	2.21	0.43
4:D:117:ILE:CG2	4:D:145:ILE:HD12	2.46	0.43
4:D:353:PRO:HG3	4:D:394:ARG:CB	2.47	0.43
4:D:846:TYR:HA	4:D:849:PHE:CE1	2.53	0.43
4:D:157:LEU:O	4:D:158:GLU:C	2.55	0.43
4:D:157:LEU:CG	4:D:196:LEU:HD12	2.48	0.43
4:D:356:GLU:HG2	4:D:357:ARG:N	2.33	0.43
4:D:652:GLU:OE2	5:D:1028:HOH:O	2.21	0.43
4:D:744:GLN:HE21	4:D:758:GLN:NE2	2.17	0.43
4:D:39:LEU:HD12	4:D:39:LEU:HA	1.73	0.43
4:D:180:LYS:O	4:D:184:GLN:HG3	2.18	0.43
4:D:109:ILE:HD13	4:D:114:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:386:ARG:CG	5:D:933:HOH:O	2.34	0.43
4:D:17:ALA:O	4:D:21:PHE:HB2	2.18	0.43
1:T:119:DT:H4'	5:T:139:HOH:O	2.15	0.42
2:N:27:DC:C2'	2:N:28:DG:H5''	2.49	0.42
4:D:632:ARG:HE	4:D:632:ARG:HA	1.84	0.42
4:D:324:GLN:CD	5:D:928:HOH:O	2.53	0.42
4:D:579:ASN:O	4:D:583:GLN:HG2	2.18	0.42
4:D:582:LEU:HB3	4:D:621:LEU:HD21	2.01	0.42
4:D:439:MET:O	4:D:443:LEU:HD22	2.18	0.42
4:D:612:GLY:O	4:D:615:ALA:N	2.52	0.42
4:D:204:TRP:O	4:D:205:HIS:CB	2.66	0.42
4:D:593:GLU:CG	4:D:594:VAL:N	2.82	0.42
4:D:160:LYS:NZ	4:D:160:LYS:HA	2.34	0.42
4:D:463:HIS:CB	4:D:534:LEU:HD22	2.48	0.42
4:D:138:ALA:O	4:D:213:GLY:HA3	2.19	0.42
4:D:464:GLY:CA	5:D:1036:HOH:O	2.44	0.42
4:D:302:LYS:HG2	4:D:303:LYS:N	2.35	0.42
4:D:78:LEU:HA	4:D:119:ILE:HD11	2.02	0.42
4:D:166:VAL:HG12	4:D:166:VAL:O	2.20	0.42
4:D:575:ALA:O	4:D:578:VAL:HB	2.19	0.42
4:D:64:VAL:HG21	4:D:127:THR:OG1	2.20	0.42
4:D:32:LEU:O	4:D:33:ALA:C	2.58	0.42
4:D:154:ILE:HD11	4:D:183:MET:HE1	1.99	0.42
4:D:84:ARG:HB2	4:D:223:SER:HB3	2.00	0.42
4:D:729:THR:OG1	4:D:733:PHE:HB3	2.20	0.42
4:D:729:THR:HB	4:D:789:SER:HB2	2.02	0.42
4:D:130:ASP:C	4:D:132:THR:N	2.71	0.42
2:N:26:DA:H2''	2:N:27:DC:O5'	2.19	0.42
1:T:128:DC:H42	2:N:27:DC:N4	2.17	0.42
2:N:16:DT:H2''	2:N:17:DA:O5'	2.20	0.42
4:D:758:GLN:HA	4:D:759:PRO:HD3	1.85	0.42
4:D:735:VAL:C	5:D:1012:HOH:O	2.57	0.42
4:D:446:LEU:HD13	4:D:806:SER:HB3	2.02	0.42
4:D:65:ALA:HB2	4:D:123:LEU:HD23	2.01	0.42
2:N:29:DG:H2''	2:N:30:DC:H5	1.85	0.42
4:D:537:ASP:CG	5:D:984:HOH:O	2.55	0.42
4:D:828:VAL:HG21	4:D:883:ALA:HA	2.01	0.42
4:D:611:LEU:HD22	4:D:615:ALA:CB	2.48	0.42
4:D:698:TRP:HZ3	4:D:845:PHE:HD2	1.68	0.42
4:D:330:ILE:HD11	4:D:408:PHE:HB2	2.02	0.41
4:D:17:ALA:C	4:D:20:PRO:HD2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:GLU:O	4:D:66:ASP:HB2	2.19	0.41
4:D:141:ILE:HG23	4:D:145:ILE:HD11	2.02	0.41
4:D:221:ILE:HD13	4:D:221:ILE:H	1.85	0.41
4:D:157:LEU:HG	4:D:158:GLU:N	2.36	0.41
4:D:41:HIS:CE1	4:D:45:GLU:OE2	2.72	0.41
4:D:86:ASN:HA	4:D:86:ASN:HD22	1.69	0.41
4:D:790:HIS:CD2	5:D:904:HOH:O	2.70	0.41
4:D:208:ASP:C	4:D:210:ILE:N	2.74	0.41
4:D:869:ASN:N	5:D:893:HOH:O	2.15	0.41
4:D:749:LEU:HD23	4:D:749:LEU:HA	1.89	0.41
4:D:710:VAL:HG12	4:D:720:ARG:HB3	2.02	0.41
4:D:16:LEU:HD21	4:D:20:PRO:HB2	2.02	0.41
4:D:690:VAL:HG22	5:D:972:HOH:O	2.20	0.41
4:D:560:ASN:HA	5:D:938:HOH:O	2.19	0.41
4:D:561:LEU:HD12	4:D:561:LEU:HA	1.88	0.41
4:D:605:ILE:O	4:D:606:SER:HB3	2.21	0.41
2:N:27:DC:H2"	2:N:28:DG:OP1	2.21	0.41
4:D:744:GLN:HB3	4:D:757:LEU:O	2.21	0.41
4:D:71:LYS:N	4:D:72:PRO:HD2	2.36	0.41
1:T:127:DG:N7	5:T:134:HOH:O	2.50	0.41
4:D:608:LYS:HG3	4:D:609:VAL:N	2.36	0.41
4:D:333:LYS:HB3	4:D:516:PHE:CE1	2.56	0.41
4:D:378:LYS:HD2	4:D:379:ARG:H	1.77	0.41
4:D:550:LEU:HD11	4:D:695:ALA:HB2	2.02	0.41
4:D:828:VAL:CG2	4:D:883:ALA:HA	2.50	0.41
4:D:88:TRP:CZ2	4:D:215:ARG:HD3	2.55	0.41
4:D:285:GLY:CA	5:D:928:HOH:O	2.35	0.41
4:D:622:ALA:O	4:D:666:MET:HG2	2.21	0.41
4:D:595:VAL:HG23	4:D:608:LYS:H	1.84	0.41
2:N:17:DA:H2'	4:D:173:ARG:NH2	2.35	0.41
4:D:139:SER:O	4:D:143:ARG:HG2	2.20	0.41
4:D:551:ARG:HD3	4:D:551:ARG:HA	1.84	0.41
4:D:131:ASN:C	4:D:133:THR:H	2.24	0.41
4:D:142:GLY:HA3	5:D:924:HOH:O	2.21	0.41
4:D:161:HIS:CE1	4:D:165:ASN:HB2	2.55	0.41
4:D:42:GLU:CD	5:D:1035:HOH:O	2.59	0.41
4:D:360:LEU:CD2	5:D:917:HOH:O	2.31	0.41
4:D:577:LYS:HD3	4:D:687:VAL:HG21	2.03	0.41
4:D:857:GLN:NE2	4:D:859:ASP:HB2	2.34	0.41
4:D:404:GLN:NE2	4:D:404:GLN:HA	2.36	0.41
4:D:817:ILE:O	4:D:817:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:GLN:HE21	4:D:40:GLU:CG	2.34	0.40
4:D:330:ILE:CD1	4:D:330:ILE:H	2.34	0.40
1:T:125:DG:H2"	1:T:124:DC:OP2	2.20	0.40
4:D:590:THR:CG2	4:D:591:ASP:N	2.83	0.40
4:D:647:ARG:CD	5:D:913:HOH:O	2.29	0.40
4:D:74:ILE:HB	5:D:1034:HOH:O	2.21	0.40
4:D:765:LYS:C	4:D:765:LYS:HZ2	2.24	0.40

There are no symmetry-related clashes.

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
4	D	857/883 (97%)	736 (86%)	86 (10%)	35 (4%)	3 1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	16	LEU
4	D	158	GLU
4	D	302	LYS
4	D	303	LYS
4	D	353	PRO
4	D	588	ASN
4	D	592	ASN
4	D	655	ILE
4	D	852	GLN
4	D	854	HIS
4	D	855	GLU
4	D	61	ALA
4	D	203	SER
4	D	206	LYS

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Mol	Chain	Res	Type
4	D	209	SER
4	D	290	GLY
4	D	358	GLU
4	D	404	GLN
4	D	595	VAL
4	D	602	THR
4	D	606	SER
4	D	767	SER
4	D	851	ASP
4	D	198	GLY
4	D	376	ALA
4	D	853	LEU
4	D	30	GLU
4	D	859	ASP
4	D	882	PHE
4	D	656	GLN
4	D	662	GLY
4	D	766	ASP
4	D	154	ILE
4	D	603	GLY
4	D	664	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	711/729 (98%)	659 (93%)	52 (7%)	17 13

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	27	HIS
4	D	50	ARG
4	D	73	LEU
4	D	91	GLU
4	D	107	GLN

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Mol	Chain	Res	Type
4	D	109	ILE
4	D	120	LYS
4	D	122	THR
4	D	131	ASN
4	D	160	LYS
4	D	170	LEU
4	D	180	LYS
4	D	221	ILE
4	D	261	LEU
4	D	281	ILE
4	D	292	ARG
4	D	296	LEU
4	D	335	LEU
4	D	337	VAL
4	D	340	VAL
4	D	346	HIS
4	D	353	PRO
4	D	355	ILE
4	D	358	GLU
4	D	360	LEU
4	D	362	MET
4	D	378	LYS
4	D	402	LEU
4	D	433	ASN
4	D	443	LEU
4	D	514	PHE
4	D	561	LEU
4	D	577	LYS
4	D	616	LEU
4	D	666	MET
4	D	672	GLN
4	D	686	SER
4	D	741	LYS
4	D	743	ILE
4	D	754	GLN
4	D	757	LEU
4	D	765	LYS
4	D	783	VAL
4	D	787	ASP
4	D	805	GLU
4	D	816	THR
4	D	834	ASP

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Mol	Chain	Res	Type
4	D	837	GLU
4	D	847	ASP
4	D	857	GLN
4	D	859	ASP
4	D	871	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	9	ASN
4	D	41	HIS
4	D	86	ASN
4	D	107	GLN
4	D	131	ASN
4	D	161	HIS
4	D	184	GLN
4	D	321	ASN
4	D	433	ASN
4	D	544	GLN
4	D	568	GLN
4	D	649	GLN
4	D	656	GLN
4	D	697	ASN
4	D	726	HIS
4	D	744	GLN
4	D	754	GLN
4	D	758	GLN
4	D	772	HIS
4	D	781	ASN
4	D	784	HIS
4	D	811	HIS
4	D	848	GLN
4	D	871	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	8	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.