



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:47 AM UTC

PDB ID : 1CEZ / pdb_00001cez
Title : CRYSTAL STRUCTURE OF A T7 RNA POLYMERASE-T7 PROMOTER COMPLEX
Authors : Cheetham, G.M.T.; Jeruzalmi, D.; Steitz, T.A.
Deposited on : 1999-03-11
Resolution : 2.40 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

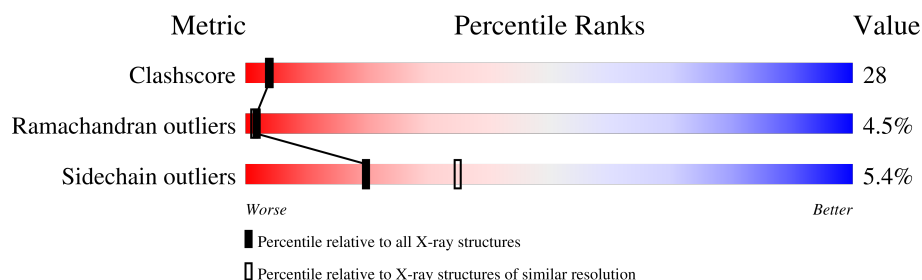
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	17	24% 65% 12%
2	N	15	27% 60% 13%
3	A	883	57% 32% 8% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7766 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 DNA (5'-D(P*TP*AP*TP*AP*GP*TP*GP*AP*GP*TP*CP*GP*TP*AP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	17	Total	C	N	O	P	0	0	0
			352	169	62	104	17			

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	15	Total	C	N	O	P	0	0	0
			304	146	55	88	15			

- Molecule 3 is a protein called PROTEIN (BACTERIOPHAGE T7 RNA POLYMERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	862	Total	C	N	O	S	0	0	0
			6639	4228	1164	1211	36			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	T	14	Total	O	0	0
			14	14		
4	N	18	Total	O	0	0
			18	18		
4	A	439	Total	O	0	0
			439	439		

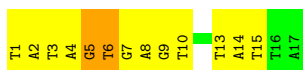
3 Residue-property plots [i](#)

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. 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. 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.

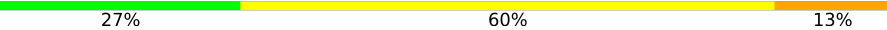
Note EDS was not executed.

- Molecule 1: DNA (5'-D(P*TP*AP*TP*AP*GP*TP*GP*AP*GP*TP*CP*GP*TP*AP*TP*T P*A)-3')

Chain T: 



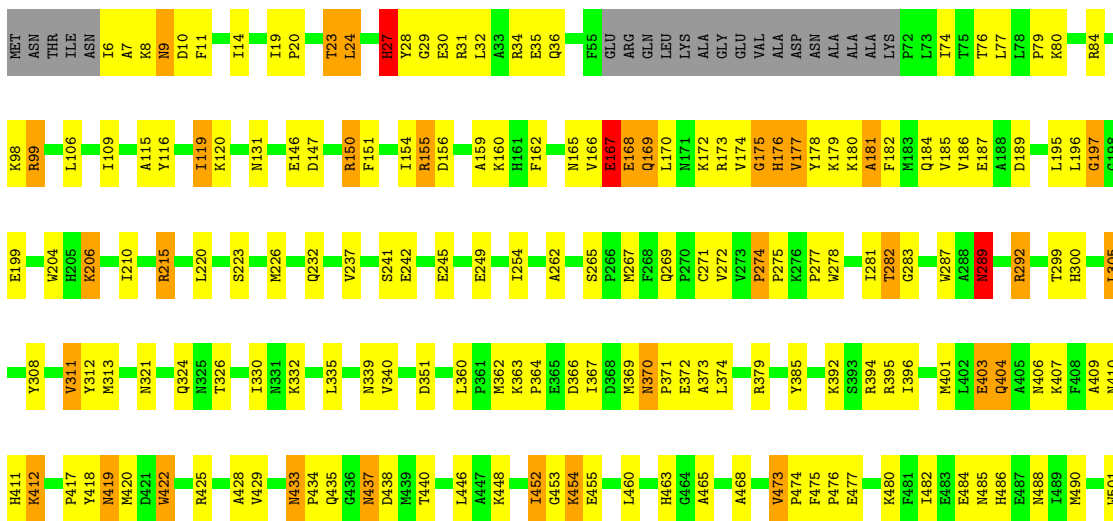
- Molecule 2: DNA (5'-D(P*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*TP*A)-3')

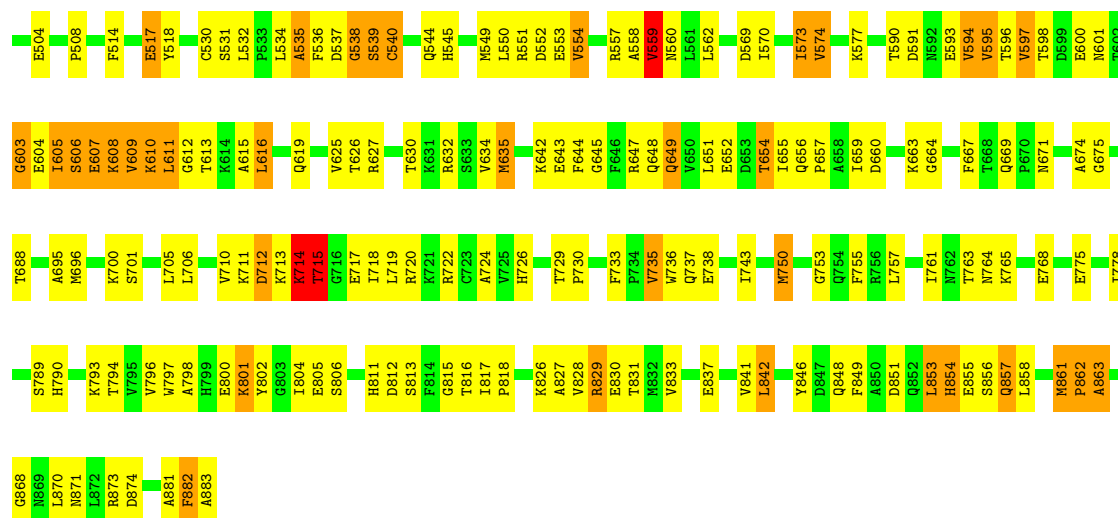
Chain N: 



- Molecule 3: PROTEIN (BACTERIOPHAGE T7 RNA POLYMERASE)

Chain A: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	220.10Å 73.30Å 80.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	81.3 (40.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.224 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7766	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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	0.37	0/394	0.82	0/607
2	N	0.74	0/340	1.07	2/521 (0.4%)
3	A	0.60	0/6791	1.06	42/9207 (0.5%)
All	All	0.60	0/7525	1.05	44/10335 (0.4%)

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	2
2	N	0	1
All	All	0	3

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	452	ILE	N-CA-C	8.72	118.79	110.42
3	A	882	PHE	N-CA-C	-8.62	99.14	110.43
3	A	313	MET	CA-C-N	8.28	127.85	119.24
3	A	313	MET	C-N-CA	8.28	127.85	119.24
3	A	540	CYS	N-CA-C	-7.90	96.80	109.76
3	A	429	VAL	N-CA-C	7.52	119.20	111.00
3	A	610	LYS	N-CA-C	-7.39	103.85	114.12
3	A	167	GLU	N-CA-C	7.07	119.99	109.59
3	A	150	ARG	N-CA-C	-6.97	101.14	110.55
3	A	181	ALA	N-CA-C	-6.87	96.16	110.80
3	A	535	ALA	N-CA-C	6.71	120.34	109.40
3	A	559	VAL	N-CA-C	-6.41	96.01	109.34
3	A	559	VAL	CA-C-N	-6.30	112.60	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	559	VAL	C-N-CA	-6.30	112.60	123.25
2	N	115	DA	C4'-C3'-O3'	6.25	119.37	110.00
3	A	605	ILE	N-CA-C	-6.19	105.24	112.98
3	A	715	THR	N-CA-C	-6.09	97.82	110.80
3	A	649	GLN	N-CA-C	-5.92	106.61	113.88
3	A	311	VAL	N-CA-C	5.86	116.90	111.45
3	A	168	GLU	N-CA-C	5.85	123.26	110.80
3	A	538	GLY	N-CA-C	-5.75	104.32	112.37
3	A	635	MET	N-CA-C	5.73	118.47	111.82
2	N	106	DC	N1-C1'-C2'	5.71	122.06	113.50
3	A	340	VAL	N-CA-C	5.66	116.72	111.45
3	A	750	MET	N-CA-C	-5.63	101.32	109.59
3	A	433	ASN	N-CA-C	5.59	114.57	108.14
3	A	607	GLU	N-CA-C	-5.50	104.64	111.90
3	A	274	PRO	CA-C-N	5.44	125.74	119.92
3	A	274	PRO	C-N-CA	5.44	125.74	119.92
3	A	27	HIS	N-CA-C	-5.37	101.82	110.14
3	A	287	TRP	N-CA-C	5.33	119.85	112.45
3	A	409	ALA	N-CA-C	5.30	118.54	111.75
3	A	861	MET	CA-C-N	5.28	126.44	119.84
3	A	861	MET	C-N-CA	5.28	126.44	119.84
3	A	778	ILE	N-CA-C	5.25	115.88	110.36
3	A	802	TYR	N-CA-C	-5.24	102.26	110.17
3	A	574	VAL	N-CA-C	-5.23	105.44	110.72
3	A	131	ASN	N-CA-C	5.17	121.81	110.80
3	A	289	ASN	N-CA-C	-5.17	107.00	113.72
3	A	282	THR	N-CA-C	5.16	116.13	108.86
3	A	119	ILE	CB-CA-C	-5.14	105.38	111.81
3	A	841	VAL	N-CA-C	5.13	116.47	110.62
3	A	468	ALA	N-CA-C	-5.08	99.98	110.80
3	A	460	LEU	N-CA-C	-5.05	105.78	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	106	DC	Sidechain
1	T	5	DG	Sidechain
1	T	6	DT	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	352	0	195	22	0
2	N	304	0	170	20	0
3	A	6639	0	6470	368	0
4	A	439	0	0	30	0
4	N	18	0	0	0	0
4	T	14	0	0	0	0
All	All	7766	0	6835	402	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 28.

All (402) 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:A:281:ILE:HG23	3:A:282:THR:HG23	1.30	1.13
2:N:113:DC:H3'	2:N:115:DA:OP1	1.49	1.11
3:A:710:VAL:HG11	3:A:720:ARG:H	1.10	1.08
3:A:829:ARG:HG3	3:A:829:ARG:HH11	1.16	1.07
3:A:763:THR:HG22	3:A:765:LYS:H	1.15	1.05
3:A:663:LYS:HG2	3:A:664:GLY:H	1.15	1.03
3:A:473:VAL:HG22	3:A:474:PRO:HD2	1.45	0.99
3:A:714:LYS:HE2	3:A:714:LYS:HA	1.47	0.96
3:A:155:ARG:HH11	3:A:155:ARG:HG3	1.28	0.95
3:A:595:VAL:HA	3:A:608:LYS:HA	1.44	0.94
2:N:103:DA:H2''	2:N:104:DT:H5'	1.50	0.93
3:A:537:ASP:O	3:A:882:PHE:HB2	1.67	0.93
3:A:560:ASN:O	3:A:881:ALA:HB2	1.71	0.90
3:A:269:GLN:HE22	3:A:407:LYS:NZ	1.68	0.90
3:A:647:ARG:HD2	3:A:675:GLY:HA2	1.53	0.89
3:A:710:VAL:CG1	3:A:720:ARG:H	1.86	0.87
3:A:324:GLN:HE21	3:A:418:TYR:H	1.21	0.86
3:A:710:VAL:HG11	3:A:720:ARG:N	1.89	0.86
3:A:816:THR:HG22	3:A:817:ILE:H	1.38	0.86
3:A:19:ILE:HG22	3:A:20:PRO:HD3	1.57	0.85
3:A:713:LYS:HD3	3:A:714:LYS:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:362:MET:HE3	3:A:363:LYS:H	1.42	0.84
3:A:663:LYS:HG2	3:A:664:GLY:N	1.93	0.84
3:A:794:THR:OG1	3:A:831:THR:HG21	1.78	0.83
3:A:485:ASN:HD22	3:A:488:ASN:HD22	1.25	0.83
3:A:710:VAL:HG21	3:A:719:LEU:HB3	1.60	0.83
3:A:278:TRP:H	3:A:321:ASN:HD21	1.26	0.83
3:A:729:THR:CG2	3:A:733:PHE:H	1.92	0.82
3:A:269:GLN:HE22	3:A:407:LYS:HZ2	1.20	0.81
3:A:711:LYS:HG2	3:A:712:ASP:H	1.45	0.81
3:A:713:LYS:HD3	3:A:714:LYS:H	1.46	0.81
3:A:861:MET:N	3:A:862:PRO:HD2	1.94	0.81
3:A:395:ARG:HD3	4:A:1290:HOH:O	1.81	0.81
3:A:696:MET:O	3:A:700:LYS:HG3	1.80	0.80
3:A:34:ARG:HH22	3:A:165:ASN:HD22	1.27	0.80
3:A:798:ALA:HB1	3:A:804:ILE:HD12	1.62	0.80
3:A:846:TYR:HA	3:A:849:PHE:CE1	2.15	0.80
1:T:14:DA:H1'	1:T:15:DT:H5''	1.62	0.80
3:A:763:THR:HG22	3:A:765:LYS:N	1.96	0.79
3:A:711:LYS:HA	4:A:1295:HOH:O	1.83	0.79
3:A:729:THR:HG21	3:A:733:PHE:HB3	1.64	0.78
3:A:705:LEU:HD11	3:A:861:MET:HB2	1.65	0.78
3:A:632:ARG:HH21	3:A:654:THR:HG23	1.50	0.77
3:A:156:ASP:OD1	3:A:160:LYS:HE2	1.85	0.76
3:A:29:GLY:HA3	3:A:175:GLY:HA3	1.68	0.76
3:A:829:ARG:HG3	3:A:829:ARG:NH1	1.95	0.76
3:A:816:THR:HG22	3:A:817:ILE:N	2.00	0.76
3:A:147:ASP:O	3:A:150:ARG:O	2.05	0.75
3:A:170:LEU:O	3:A:174:VAL:HG23	1.86	0.75
3:A:19:ILE:O	3:A:23:THR:HG22	1.87	0.75
3:A:24:LEU:O	3:A:27:HIS:O	2.05	0.74
3:A:871:ASN:HB3	3:A:874:ASP:OD2	1.87	0.73
3:A:729:THR:HG22	3:A:733:PHE:H	1.55	0.72
2:N:114:DT:OP1	2:N:114:DT:H2'	1.90	0.72
3:A:177:VAL:O	3:A:179:LYS:N	2.23	0.72
3:A:729:THR:CG2	3:A:733:PHE:HB3	2.19	0.72
3:A:615:ALA:O	3:A:619:GLN:HG3	1.89	0.72
3:A:829:ARG:HH11	3:A:829:ARG:CG	1.94	0.72
3:A:706:LEU:HD21	3:A:849:PHE:HB2	1.72	0.71
3:A:713:LYS:HA	4:A:1219:HOH:O	1.88	0.71
3:A:169:GLN:HG2	3:A:172:LYS:HE3	1.71	0.71
3:A:517:GLU:HG3	3:A:530:CYS:SG	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:177:VAL:O	3:A:179:LYS:HG3	1.90	0.71
3:A:371:PRO:C	3:A:373:ALA:H	1.98	0.71
3:A:364:PRO:C	3:A:366:ASP:H	1.98	0.70
2:N:113:DC:O3'	2:N:114:DT:H3'	1.91	0.70
3:A:281:ILE:CG2	3:A:282:THR:HG23	2.15	0.69
3:A:635:MET:HA	4:A:1137:HOH:O	1.91	0.69
3:A:485:ASN:HD22	3:A:488:ASN:ND2	1.91	0.69
3:A:155:ARG:HG3	3:A:155:ARG:NH1	2.06	0.69
3:A:147:ASP:OD1	3:A:292:ARG:HD2	1.94	0.68
3:A:23:THR:HG21	3:A:195:LEU:HD11	1.73	0.68
3:A:29:GLY:HA3	3:A:175:GLY:CA	2.23	0.68
3:A:710:VAL:HG11	3:A:719:LEU:N	2.08	0.68
2:N:103:DA:H2''	2:N:104:DT:C5'	2.23	0.68
3:A:184:GLN:HE21	3:A:185:VAL:HG12	1.59	0.68
3:A:553:GLU:CD	4:A:1176:HOH:O	2.36	0.68
3:A:729:THR:HG22	3:A:733:PHE:N	2.08	0.68
3:A:369:MET:C	3:A:371:PRO:HD2	2.20	0.67
3:A:311:VAL:O	3:A:312:TYR:HB3	1.94	0.67
3:A:642:LYS:HA	3:A:649:GLN:HE22	1.59	0.67
2:N:113:DC:C3'	2:N:115:DA:OP1	2.36	0.67
3:A:550:LEU:HD11	3:A:695:ALA:HB2	1.76	0.66
1:T:4:DA:N1	3:A:206:LYS:HE2	2.11	0.66
3:A:463:HIS:HE1	4:A:1101:HOH:O	1.78	0.66
3:A:630:THR:O	3:A:634:VAL:HG23	1.95	0.66
3:A:790:HIS:NE2	3:A:831:THR:HG23	2.11	0.66
2:N:113:DC:H3'	2:N:115:DA:P	2.36	0.66
2:N:113:DC:H2''	2:N:115:DA:OP2	1.96	0.65
3:A:34:ARG:HH22	3:A:165:ASN:ND2	1.93	0.65
3:A:647:ARG:C	3:A:649:GLN:H	2.05	0.65
3:A:710:VAL:HG11	3:A:719:LEU:H	1.60	0.65
3:A:797:TRP:CZ2	3:A:801:LYS:HG3	2.31	0.65
3:A:701:SER:HB3	3:A:861:MET:HG2	1.79	0.64
3:A:32:LEU:HD22	3:A:272:VAL:HG12	1.80	0.64
3:A:362:MET:HE3	3:A:363:LYS:N	2.12	0.64
3:A:573:ILE:HD11	3:A:688:THR:HG23	1.78	0.64
2:N:113:DC:H4'	2:N:114:DT:OP2	1.96	0.64
3:A:438:ASP:OD2	3:A:508:PRO:HG2	1.97	0.64
3:A:169:GLN:HB3	3:A:172:LYS:HD2	1.78	0.63
1:T:9:DG:H2''	1:T:10:DT:C5'	2.28	0.63
3:A:23:THR:O	3:A:27:HIS:HD2	1.81	0.63
3:A:861:MET:H	3:A:862:PRO:HD2	1.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:651:LEU:HD23	3:A:651:LEU:O	1.99	0.63
3:A:826:LYS:O	3:A:830:GLU:HG3	1.98	0.63
3:A:116:TYR:CZ	3:A:120:LYS:HD2	2.33	0.63
1:T:2:DA:H1'	1:T:3:DT:H5'	1.80	0.62
3:A:486:HIS:O	3:A:490:MET:HG2	1.99	0.62
3:A:35:GLU:OE2	3:A:411:HIS:HE1	1.82	0.62
3:A:159:ALA:HA	3:A:162:PHE:CE2	2.34	0.62
2:N:114:DT:H3'	2:N:114:DT:P	2.39	0.62
3:A:115:ALA:O	3:A:119:ILE:HG12	1.99	0.62
3:A:36:GLN:NE2	3:A:272:VAL:H	1.97	0.61
3:A:412:LYS:HE2	3:A:412:LYS:HA	1.82	0.61
3:A:713:LYS:O	3:A:714:LYS:C	2.43	0.61
3:A:595:VAL:CA	3:A:608:LYS:HA	2.23	0.61
3:A:610:LYS:O	3:A:611:LEU:O	2.18	0.61
3:A:750:MET:HE2	3:A:753:GLY:C	2.26	0.61
3:A:612:GLY:O	3:A:616:LEU:HD22	2.01	0.60
3:A:19:ILE:CG2	3:A:20:PRO:HD3	2.30	0.60
3:A:179:LYS:O	3:A:181:ALA:N	2.35	0.60
3:A:321:ASN:HB3	4:A:1138:HOH:O	2.01	0.60
3:A:330:ILE:HG21	3:A:335:LEU:HD12	1.84	0.60
3:A:714:LYS:HA	3:A:714:LYS:CE	2.26	0.59
3:A:120:LYS:HE2	3:A:265:SER:O	2.00	0.59
3:A:179:LYS:HG2	4:A:1025:HOH:O	2.01	0.59
3:A:647:ARG:HD2	3:A:675:GLY:CA	2.29	0.59
3:A:715:THR:HG22	3:A:715:THR:O	2.02	0.59
3:A:480:LYS:O	3:A:484:GLU:HG3	2.03	0.59
3:A:710:VAL:CG1	3:A:719:LEU:H	2.16	0.58
3:A:169:GLN:HG2	3:A:172:LYS:CE	2.33	0.58
1:T:9:DG:H1'	1:T:10:DT:H5''	1.84	0.58
3:A:663:LYS:CG	3:A:664:GLY:H	2.00	0.58
3:A:215:ARG:NH2	3:A:750:MET:O	2.37	0.58
3:A:278:TRP:H	3:A:321:ASN:ND2	2.00	0.58
3:A:858:LEU:N	4:A:1062:HOH:O	2.36	0.58
3:A:155:ARG:HH11	3:A:155:ARG:CG	2.06	0.57
3:A:242:GLU:HG2	3:A:757:LEU:HD11	1.86	0.57
3:A:403:GLU:CD	4:A:1208:HOH:O	2.47	0.57
3:A:36:GLN:HE22	3:A:271:CYS:HA	1.70	0.57
3:A:632:ARG:HH21	3:A:654:THR:CG2	2.16	0.57
3:A:540:CYS:O	3:A:544:GLN:HG3	2.05	0.57
3:A:485:ASN:ND2	3:A:488:ASN:HD22	1.99	0.56
3:A:448:LYS:HE3	3:A:805:GLU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:655:ILE:HG23	3:A:667:PHE:CD2	2.40	0.56
3:A:335:LEU:CD2	3:A:339:ASN:ND2	2.69	0.56
3:A:816:THR:CG2	3:A:817:ILE:H	2.13	0.56
3:A:167:GLU:HA	4:A:1156:HOH:O	2.05	0.56
1:T:2:DA:H2''	1:T:3:DT:OP2	2.06	0.56
3:A:177:VAL:HB	3:A:179:LYS:HE3	1.86	0.56
3:A:608:LYS:O	3:A:609:VAL:HB	2.05	0.56
3:A:166:VAL:HG13	3:A:173:ARG:CD	2.36	0.56
3:A:729:THR:OG1	3:A:789:SER:HB3	2.06	0.56
1:T:13:DT:H2''	1:T:14:DA:C8	2.41	0.55
3:A:632:ARG:NH2	3:A:654:THR:HG23	2.20	0.55
1:T:9:DG:H2''	1:T:10:DT:H5'	1.88	0.55
3:A:379:ARG:HD3	3:A:660:ASP:OD2	2.06	0.55
3:A:412:LYS:NZ	4:A:985:HOH:O	2.34	0.55
3:A:750:MET:HE2	3:A:753:GLY:CA	2.36	0.55
3:A:829:ARG:NH1	3:A:829:ARG:CG	2.58	0.55
3:A:645:GLY:O	3:A:649:GLN:HG3	2.05	0.55
3:A:166:VAL:HG13	3:A:173:ARG:HD2	1.89	0.55
3:A:232:GLN:HB2	3:A:241:SER:OG	2.07	0.55
1:T:5:DG:C5	3:A:237:VAL:HG13	2.42	0.54
3:A:486:HIS:HD2	3:A:518:TYR:OH	1.89	0.54
3:A:651:LEU:O	3:A:656:GLN:HB2	2.06	0.54
3:A:750:MET:HE2	3:A:753:GLY:HA2	1.89	0.54
1:T:1:DT:H2''	1:T:2:DA:OP1	2.08	0.54
3:A:711:LYS:O	3:A:712:ASP:HB2	2.07	0.54
3:A:729:THR:HG22	3:A:733:PHE:CA	2.37	0.54
3:A:743:ILE:O	3:A:763:THR:HB	2.07	0.54
3:A:6:ILE:O	3:A:7:ALA:C	2.51	0.54
3:A:272:VAL:HG12	3:A:272:VAL:O	2.08	0.53
3:A:862:PRO:O	3:A:863:ALA:HB3	2.08	0.53
3:A:607:GLU:O	3:A:609:VAL:N	2.36	0.53
3:A:729:THR:HG22	3:A:733:PHE:O	2.09	0.53
3:A:738:GLU:HG3	3:A:738:GLU:O	2.08	0.53
3:A:364:PRO:C	3:A:366:ASP:N	2.66	0.53
3:A:562:LEU:HD21	3:A:870:LEU:HD12	1.90	0.53
3:A:19:ILE:O	3:A:23:THR:CG2	2.55	0.53
3:A:463:HIS:HD2	3:A:535:ALA:H	1.56	0.53
3:A:647:ARG:C	3:A:649:GLN:N	2.66	0.53
3:A:603:GLY:O	3:A:605:ILE:N	2.42	0.53
3:A:626:THR:O	3:A:630:THR:HG23	2.09	0.53
2:N:115:DA:OP2	2:N:115:DA:H2'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:LEU:HB2	4:A:930:HOH:O	2.08	0.53
3:A:392:LYS:O	3:A:396:ILE:HG12	2.09	0.53
3:A:433:ASN:HB2	3:A:434:PRO:CD	2.39	0.53
3:A:185:VAL:CG2	3:A:277:PRO:HG3	2.39	0.52
3:A:367:ILE:O	3:A:374:LEU:HD22	2.09	0.52
3:A:570:ILE:O	3:A:574:VAL:HG23	2.09	0.52
3:A:609:VAL:CG2	3:A:611:LEU:HG	2.38	0.52
3:A:609:VAL:HG11	3:A:669:GLN:OE1	2.09	0.52
3:A:35:GLU:OE2	3:A:272:VAL:HG21	2.10	0.52
3:A:32:LEU:HD22	3:A:272:VAL:CG1	2.40	0.52
3:A:722:ARG:NH1	3:A:768:GLU:CD	2.67	0.52
3:A:562:LEU:HD21	3:A:870:LEU:CD1	2.39	0.52
3:A:701:SER:CB	3:A:861:MET:HG2	2.40	0.52
3:A:713:LYS:HA	3:A:713:LYS:HE2	1.91	0.52
3:A:199:GLU:HA	3:A:199:GLU:OE1	2.09	0.52
2:N:113:DC:C3'	2:N:115:DA:P	2.97	0.52
3:A:557:ARG:HB2	3:A:562:LEU:HD12	1.92	0.52
3:A:278:TRP:HE1	3:A:324:GLN:HE22	1.56	0.51
3:A:446:LEU:HD22	3:A:806:SER:HB3	1.91	0.51
3:A:452:ILE:HG23	3:A:453:GLY:N	2.25	0.51
3:A:454:LYS:HE3	3:A:455:GLU:N	2.24	0.51
3:A:871:ASN:OD1	3:A:873:ARG:HB2	2.10	0.51
3:A:537:ASP:H	3:A:882:PHE:HD2	1.59	0.51
3:A:31:ARG:HD3	3:A:176:HIS:CE1	2.44	0.51
3:A:856:SER:O	3:A:857:GLN:C	2.52	0.51
3:A:80:LYS:O	3:A:223:SER:HB2	2.11	0.51
1:T:1:DT:O4	3:A:738:GLU:N	2.40	0.51
3:A:335:LEU:HD23	3:A:335:LEU:O	2.11	0.51
3:A:816:THR:CG2	3:A:817:ILE:N	2.71	0.51
2:N:113:DC:C3'	2:N:114:DT:H3'	2.40	0.51
3:A:710:VAL:CG1	3:A:718:ILE:HG23	2.41	0.51
3:A:428:ALA:H	3:A:435:GLN:NE2	2.09	0.51
3:A:437:ASN:C	3:A:437:ASN:HD22	2.18	0.50
3:A:711:LYS:CG	3:A:712:ASP:H	2.15	0.50
3:A:729:THR:HG23	3:A:733:PHE:H	1.73	0.50
3:A:185:VAL:HG22	3:A:186:VAL:N	2.27	0.50
3:A:197:GLY:HA3	3:A:283:GLY:HA3	1.92	0.50
3:A:552:ASP:OD1	3:A:554:VAL:HG13	2.10	0.50
3:A:790:HIS:CD2	3:A:831:THR:HG23	2.47	0.50
3:A:99:ARG:HD2	3:A:99:ARG:N	2.26	0.50
3:A:371:PRO:HG2	3:A:373:ALA:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:9:DG:C2'	1:T:10:DT:H5''	2.41	0.50
3:A:729:THR:OG1	3:A:789:SER:CB	2.60	0.50
3:A:176:HIS:O	3:A:177:VAL:O	2.29	0.50
3:A:501:TRP:HA	3:A:504:GLU:OE1	2.11	0.50
3:A:609:VAL:HG11	3:A:669:GLN:CD	2.37	0.49
3:A:269:GLN:NE2	3:A:407:LYS:HZ2	2.00	0.49
3:A:881:ALA:O	3:A:882:PHE:C	2.54	0.49
3:A:269:GLN:HE22	3:A:407:LYS:HZ3	1.56	0.49
3:A:437:ASN:ND2	3:A:440:THR:H	2.10	0.49
3:A:446:LEU:HB2	3:A:531:SER:O	2.12	0.49
3:A:861:MET:O	3:A:862:PRO:O	2.30	0.49
3:A:422:TRP:CD1	3:A:422:TRP:C	2.90	0.49
3:A:655:ILE:HD12	3:A:674:ALA:HB2	1.95	0.49
3:A:717:GLU:HG2	3:A:718:ILE:N	2.28	0.49
3:A:722:ARG:HH11	3:A:768:GLU:CD	2.19	0.49
3:A:308:TYR:HA	3:A:311:VAL:CG2	2.42	0.49
3:A:351:ASP:O	3:A:394:ARG:NH2	2.44	0.49
3:A:420:MET:HA	3:A:425:ARG:O	2.12	0.49
3:A:643:GLU:HA	4:A:1168:HOH:O	2.12	0.49
3:A:763:THR:CG2	3:A:764:ASN:N	2.75	0.49
3:A:606:SER:C	3:A:608:LYS:N	2.68	0.49
3:A:710:VAL:O	3:A:710:VAL:HG13	2.12	0.49
3:A:106:LEU:HA	3:A:109:ILE:CD1	2.43	0.48
3:A:710:VAL:HG12	3:A:720:ARG:O	2.13	0.48
3:A:278:TRP:NE1	3:A:324:GLN:HE22	2.11	0.48
3:A:789:SER:O	3:A:793:LYS:HG3	2.13	0.48
3:A:881:ALA:C	3:A:882:PHE:O	2.52	0.48
3:A:206:LYS:O	3:A:210:ILE:HG12	2.13	0.48
3:A:534:LEU:HD11	3:A:818:PRO:HG3	1.95	0.48
3:A:150:ARG:O	3:A:151:PHE:HB2	2.14	0.48
3:A:517:GLU:HG2	3:A:532:LEU:HB2	1.96	0.48
3:A:473:VAL:HG13	3:A:477:GLU:HB2	1.96	0.48
2:N:108:DA:H1'	2:N:109:DC:H5''	1.95	0.47
3:A:155:ARG:NH1	3:A:155:ARG:CG	2.70	0.47
2:N:105:DA:N3	3:A:98:LYS:HE2	2.29	0.47
3:A:569:ASP:OD2	3:A:627:ARG:NE	2.48	0.47
3:A:360:LEU:HD11	3:A:385:TYR:OH	2.15	0.47
3:A:448:LYS:HG2	4:A:947:HOH:O	2.15	0.47
3:A:651:LEU:HD23	3:A:651:LEU:C	2.40	0.47
3:A:332:LYS:NZ	3:A:410:ASN:HD22	2.12	0.46
3:A:371:PRO:C	3:A:373:ALA:N	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1:DT:OP1	1:T:1:DT:H3'	2.16	0.46
3:A:281:ILE:HG23	3:A:282:THR:CG2	2.22	0.46
3:A:324:GLN:NE2	3:A:418:TYR:H	2.01	0.46
3:A:833:VAL:O	3:A:837:GLU:HG3	2.14	0.46
2:N:112:DA:H1'	2:N:113:DC:H5''	1.96	0.46
3:A:269:GLN:HE21	3:A:404:GLN:HE22	1.63	0.46
3:A:724:ALA:HB1	3:A:737:GLN:O	2.16	0.46
1:T:9:DG:H2''	1:T:10:DT:H5''	1.97	0.46
3:A:335:LEU:HD21	3:A:406:ASN:OD1	2.14	0.46
3:A:573:ILE:O	3:A:577:LYS:HG3	2.16	0.46
3:A:590:THR:HB	3:A:613:THR:H	1.80	0.46
3:A:596:THR:O	3:A:597:VAL:C	2.58	0.46
3:A:711:LYS:O	3:A:712:ASP:CB	2.62	0.46
2:N:102:DA:H1'	2:N:103:DA:C8	2.51	0.46
3:A:649:GLN:HA	3:A:652:GLU:HG2	1.96	0.46
3:A:861:MET:N	3:A:862:PRO:CD	2.75	0.46
3:A:711:LYS:HG2	3:A:712:ASP:N	2.24	0.45
3:A:364:PRO:O	3:A:366:ASP:N	2.49	0.45
3:A:84:ARG:HB2	3:A:223:SER:HB3	1.98	0.45
3:A:169:GLN:HG2	3:A:172:LYS:CD	2.46	0.45
3:A:590:THR:HG22	3:A:591:ASP:N	2.31	0.45
3:A:729:THR:HG1	3:A:789:SER:CB	2.30	0.45
3:A:846:TYR:C	3:A:848:GLN:H	2.24	0.45
3:A:593:GLU:O	3:A:594:VAL:O	2.35	0.45
3:A:326:THR:HA	4:A:1161:HOH:O	2.16	0.45
3:A:729:THR:CG2	3:A:733:PHE:N	2.67	0.45
3:A:806:SER:O	3:A:816:THR:HG23	2.17	0.45
1:T:1:DT:O2	3:A:300:HIS:N	2.50	0.45
3:A:534:LEU:O	3:A:815:GLY:HA2	2.16	0.45
3:A:242:GLU:HG2	3:A:757:LEU:CD1	2.46	0.45
3:A:254:ILE:HD13	3:A:396:ILE:HD12	1.99	0.45
3:A:551:ARG:NH1	4:A:1148:HOH:O	2.45	0.45
3:A:851:ASP:CB	4:A:1059:HOH:O	2.64	0.45
3:A:36:GLN:HE22	3:A:272:VAL:H	1.65	0.44
3:A:465:ALA:HB2	3:A:482:ILE:CD1	2.47	0.44
3:A:729:THR:OG1	3:A:730:PRO:HD2	2.17	0.44
3:A:30:GLU:OE1	3:A:166:VAL:HG12	2.16	0.44
3:A:324:GLN:HG3	3:A:417:PRO:HA	1.99	0.44
3:A:371:PRO:O	3:A:373:ALA:N	2.50	0.44
3:A:545:HIS:O	3:A:549:MET:HG2	2.16	0.44
3:A:669:GLN:NE2	3:A:669:GLN:HA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:177:VAL:HG21	4:A:1248:HOH:O	2.16	0.44
3:A:551:ARG:O	3:A:868:GLY:HA3	2.18	0.44
3:A:536:PHE:O	3:A:813:SER:HA	2.18	0.44
1:T:7:DG:H2''	1:T:8:DA:OP2	2.17	0.44
3:A:538:GLY:CA	3:A:883:ALA:HB3	2.47	0.44
3:A:553:GLU:CD	3:A:553:GLU:H	2.26	0.44
3:A:729:THR:CG2	3:A:733:PHE:CB	2.93	0.44
1:T:4:DA:H4'	1:T:5:DG:OP2	2.18	0.44
3:A:473:VAL:CG2	3:A:474:PRO:HD2	2.32	0.44
3:A:750:MET:HE1	3:A:755:PHE:N	2.33	0.44
1:T:5:DG:C6	3:A:237:VAL:HG22	2.53	0.44
3:A:8:LYS:O	3:A:9:ASN:CB	2.65	0.44
3:A:401:MET:HE2	3:A:401:MET:HA	1.99	0.43
3:A:448:LYS:HE3	3:A:805:GLU:CB	2.47	0.43
3:A:74:ILE:HG13	3:A:74:ILE:O	2.18	0.43
3:A:281:ILE:HD11	3:A:305:LEU:O	2.18	0.43
3:A:419:ASN:HD22	3:A:419:ASN:HA	1.46	0.43
3:A:538:GLY:O	3:A:539:SER:O	2.35	0.43
2:N:114:DT:P	2:N:114:DT:C3'	3.06	0.43
3:A:14:ILE:HG13	4:A:975:HOH:O	2.17	0.43
3:A:610:LYS:O	3:A:611:LEU:C	2.61	0.43
3:A:827:ALA:O	3:A:831:THR:HG22	2.18	0.43
3:A:308:TYR:CZ	3:A:736:TRP:HZ3	2.36	0.43
3:A:558:ALA:C	3:A:559:VAL:O	2.58	0.43
3:A:656:GLN:HB3	3:A:657:PRO:CD	2.49	0.43
3:A:715:THR:C	3:A:717:GLU:H	2.26	0.43
3:A:182:PHE:CE1	3:A:448:LYS:HB3	2.54	0.43
2:N:113:DC:C2'	2:N:115:DA:OP2	2.66	0.43
3:A:189:ASP:CA	4:A:1116:HOH:O	2.65	0.43
3:A:369:MET:C	3:A:371:PRO:CD	2.91	0.43
3:A:761:ILE:O	3:A:761:ILE:HG13	2.18	0.43
3:A:146:GLU:HG3	3:A:204:TRP:CE2	2.54	0.43
3:A:269:GLN:HE21	3:A:404:GLN:NE2	2.16	0.43
3:A:454:LYS:HE3	3:A:455:GLU:HA	2.01	0.43
3:A:729:THR:HG22	3:A:733:PHE:HB3	1.99	0.43
1:T:5:DG:C8	1:T:6:DT:H72	2.54	0.42
1:T:5:DG:N7	3:A:237:VAL:HG13	2.34	0.42
3:A:463:HIS:CD2	3:A:534:LEU:HA	2.53	0.42
3:A:540:CYS:HB3	3:A:559:VAL:HG12	2.01	0.42
3:A:557:ARG:NE	4:A:1048:HOH:O	2.50	0.42
3:A:595:VAL:HA	3:A:608:LYS:CA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:553:GLU:CG	4:A:1176:HOH:O	2.65	0.42
3:A:553:GLU:HA	3:A:870:LEU:HD13	2.01	0.42
3:A:796:VAL:O	3:A:800:GLU:HG3	2.19	0.42
3:A:274:PRO:HA	3:A:275:PRO:HD3	1.82	0.42
3:A:332:LYS:HZ1	3:A:410:ASN:HD22	1.67	0.42
3:A:454:LYS:HE3	3:A:455:GLU:CA	2.49	0.42
3:A:106:LEU:HA	3:A:109:ILE:HD12	2.01	0.42
3:A:174:VAL:CG1	3:A:177:VAL:HG22	2.49	0.42
3:A:360:LEU:HD21	3:A:385:TYR:CZ	2.54	0.42
3:A:842:LEU:HA	3:A:842:LEU:HD12	1.82	0.42
3:A:448:LYS:HG3	4:A:894:HOH:O	2.20	0.42
3:A:463:HIS:CD2	3:A:535:ALA:H	2.36	0.42
3:A:154:ILE:O	3:A:154:ILE:CG2	2.67	0.42
3:A:19:ILE:CG2	3:A:20:PRO:CD	2.97	0.42
3:A:182:PHE:HE2	3:A:412:LYS:HD3	1.83	0.42
3:A:289:ASN:HD22	3:A:289:ASN:HA	1.59	0.42
3:A:154:ILE:O	3:A:154:ILE:HG22	2.18	0.41
3:A:335:LEU:HD23	3:A:335:LEU:C	2.44	0.41
3:A:486:HIS:HE1	4:A:1087:HOH:O	2.03	0.41
3:A:659:ILE:HA	3:A:663:LYS:O	2.20	0.41
3:A:726:HIS:HD2	3:A:735:VAL:O	2.03	0.41
3:A:853:LEU:O	3:A:854:HIS:C	2.62	0.41
3:A:370:ASN:N	3:A:371:PRO:CD	2.83	0.41
3:A:606:SER:O	3:A:607:GLU:C	2.61	0.41
3:A:324:GLN:HE21	3:A:418:TYR:N	2.00	0.41
3:A:332:LYS:NZ	3:A:410:ASN:ND2	2.68	0.41
3:A:475:PHE:N	3:A:476:PRO:HD2	2.36	0.41
3:A:189:ASP:HA	4:A:1116:HOH:O	2.20	0.41
3:A:554:VAL:HG11	4:A:1319:HOH:O	2.20	0.41
3:A:569:ASP:CG	3:A:627:ARG:HE	2.28	0.41
3:A:27:HIS:O	3:A:28:TYR:CB	2.69	0.41
3:A:186:VAL:HG12	3:A:187:GLU:N	2.36	0.41
3:A:651:LEU:HD12	3:A:671:ASN:HA	2.03	0.41
3:A:27:HIS:O	3:A:28:TYR:HB2	2.21	0.41
3:A:76:THR:O	3:A:79:PRO:HG2	2.20	0.41
3:A:150:ARG:NE	4:A:1244:HOH:O	2.52	0.41
3:A:308:TYR:HA	3:A:311:VAL:HG23	2.02	0.41
3:A:412:LYS:HE2	3:A:412:LYS:CA	2.48	0.41
3:A:609:VAL:HG13	3:A:609:VAL:O	2.20	0.41
3:A:711:LYS:C	4:A:1295:HOH:O	2.64	0.41
2:N:108:DA:H2''	2:N:109:DC:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:763:THR:HG22	3:A:764:ASN:N	2.36	0.41
1:T:1:DT:O2	3:A:299:THR:HA	2.21	0.40
1:T:2:DA:H1'	1:T:3:DT:C5'	2.47	0.40
3:A:120:LYS:NZ	3:A:267:MET:SD	2.94	0.40
3:A:714:LYS:HE2	3:A:714:LYS:CA	2.33	0.40
3:A:849:PHE:HE2	3:A:861:MET:HE2	1.86	0.40
3:A:9:ASN:O	3:A:11:PHE:N	2.55	0.40
3:A:593:GLU:C	3:A:594:VAL:O	2.64	0.40
3:A:648:GLN:HG3	4:A:993:HOH:O	2.21	0.40
3:A:220:LEU:HD21	3:A:226:MET:HE2	2.04	0.40
3:A:594:VAL:O	3:A:595:VAL:C	2.64	0.40
3:A:816:THR:HG22	3:A:817:ILE:HG12	2.04	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
3	A	858/883 (97%)	754 (88%)	65 (8%)	39 (4%)	2 1

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	168	GLU
3	A	178	TYR
3	A	180	LYS
3	A	539	SER
3	A	594	VAL
3	A	597	VAL
3	A	600	GLU
3	A	604	GLU
3	A	606	SER

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Mol	Chain	Res	Type
3	A	609	VAL
3	A	611	LEU
3	A	644	PHE
3	A	712	ASP
3	A	714	LYS
3	A	715	THR
3	A	854	HIS
3	A	857	GLN
3	A	862	PRO
3	A	169	GLN
3	A	598	THR
3	A	603	GLY
3	A	811	HIS
3	A	812	ASP
3	A	10	ASP
3	A	175	GLY
3	A	197	GLY
3	A	372	GLU
3	A	608	LYS
3	A	853	LEU
3	A	855	GLU
3	A	863	ALA
3	A	9	ASN
3	A	177	VAL
3	A	262	ALA
3	A	601	ASN
3	A	370	ASN
3	A	559	VAL
3	A	595	VAL
3	A	625	VAL

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	
3	A	666/729 (91%)	630 (95%)	36 (5%)	20	35

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	23	THR
3	A	24	LEU
3	A	27	HIS
3	A	77	LEU
3	A	99	ARG
3	A	155	ARG
3	A	167	GLU
3	A	176	HIS
3	A	206	LYS
3	A	215	ARG
3	A	245	GLU
3	A	249	GLU
3	A	289	ASN
3	A	292	ARG
3	A	305	LEU
3	A	403	GLU
3	A	404	GLN
3	A	412	LYS
3	A	419	ASN
3	A	422	TRP
3	A	437	ASN
3	A	454	LYS
3	A	473	VAL
3	A	514	PHE
3	A	517	GLU
3	A	554	VAL
3	A	573	ILE
3	A	616	LEU
3	A	654	THR
3	A	714	LYS
3	A	735	VAL
3	A	775	GLU
3	A	801	LYS
3	A	828	VAL
3	A	829	ARG
3	A	842	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	22	ASN

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Mol	Chain	Res	Type
3	A	27	HIS
3	A	36	GLN
3	A	86	ASN
3	A	107	GLN
3	A	165	ASN
3	A	171	ASN
3	A	184	GLN
3	A	230	HIS
3	A	239	GLN
3	A	269	GLN
3	A	289	ASN
3	A	300	HIS
3	A	321	ASN
3	A	324	GLN
3	A	410	ASN
3	A	411	HIS
3	A	419	ASN
3	A	435	GLN
3	A	437	ASN
3	A	463	HIS
3	A	486	HIS
3	A	488	ASN
3	A	505	GLN
3	A	588	ASN
3	A	619	GLN
3	A	649	GLN
3	A	669	GLN
3	A	671	ASN
3	A	697	ASN
3	A	726	HIS
3	A	737	GLN
3	A	744	GLN
3	A	764	ASN
3	A	786	GLN
3	A	823	ASN
3	A	869	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.