



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:04 AM UTC

PDB ID : 2PI5 / pdb_00002pi5
Title : T7 RNA polymerase complexed with a phi10 promoter
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Deposited on : 2007-04-12
Resolution : 2.90 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

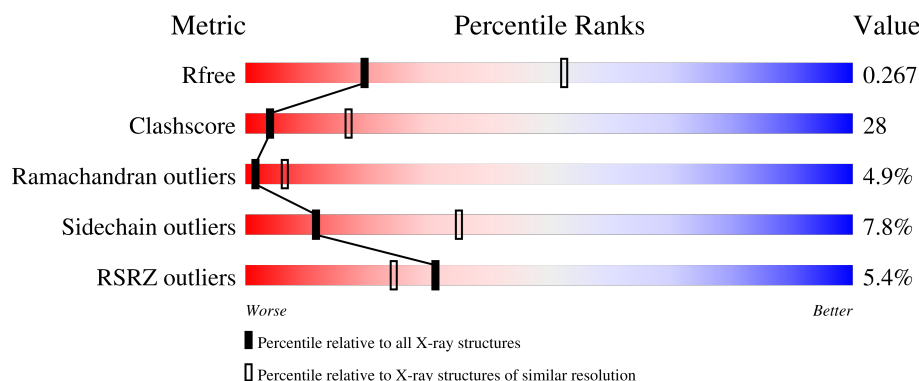
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	T	22	9% 18% 64% 18%
2	P	14	29% 57% 14%
3	A	878	5% 50% 39% 9% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7451 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 5'-D(*CP*TP*TP*C*CP*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	18	Total	C	N	O	P	0	0	0
			368	178	65	108	17			

- Molecule 2 is a DNA chain called 5'-D(*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	14	Total	C	N	O	P	0	0	0
			280	136	50	81	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	862	Total	C	N	O	S	0	0	0
			6803	4334	1178	1254	37			

3 Residue-property plots

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.

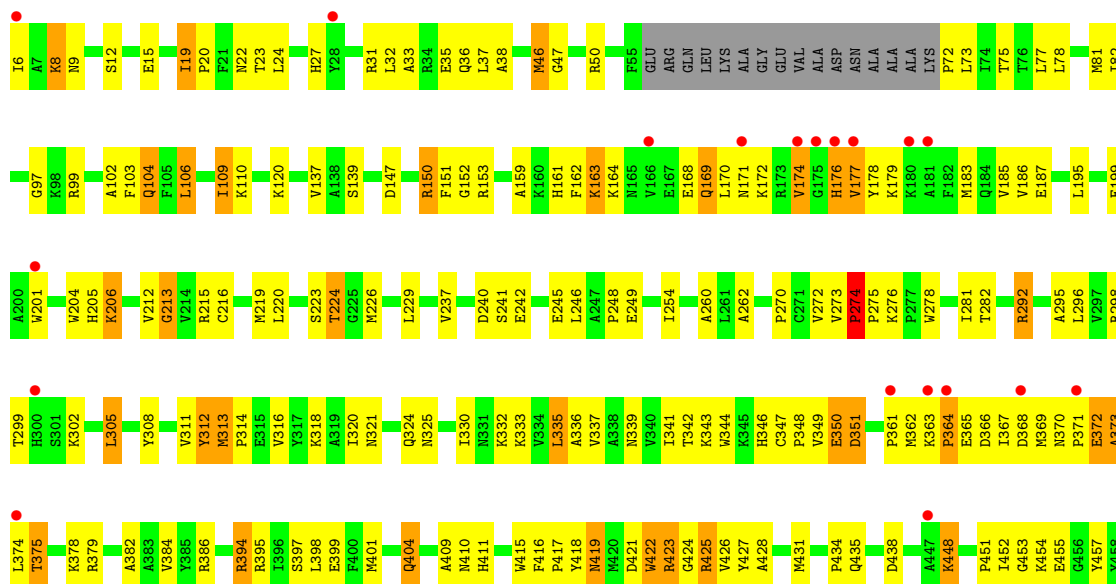
- Molecule 1: 5'-D(*CP*TP*TP*C*CP*TP*AP*TP*AP*GP*TP*GP*AP*GP*TP*CP*GP*TP*AP*TP*TP*A)-3'

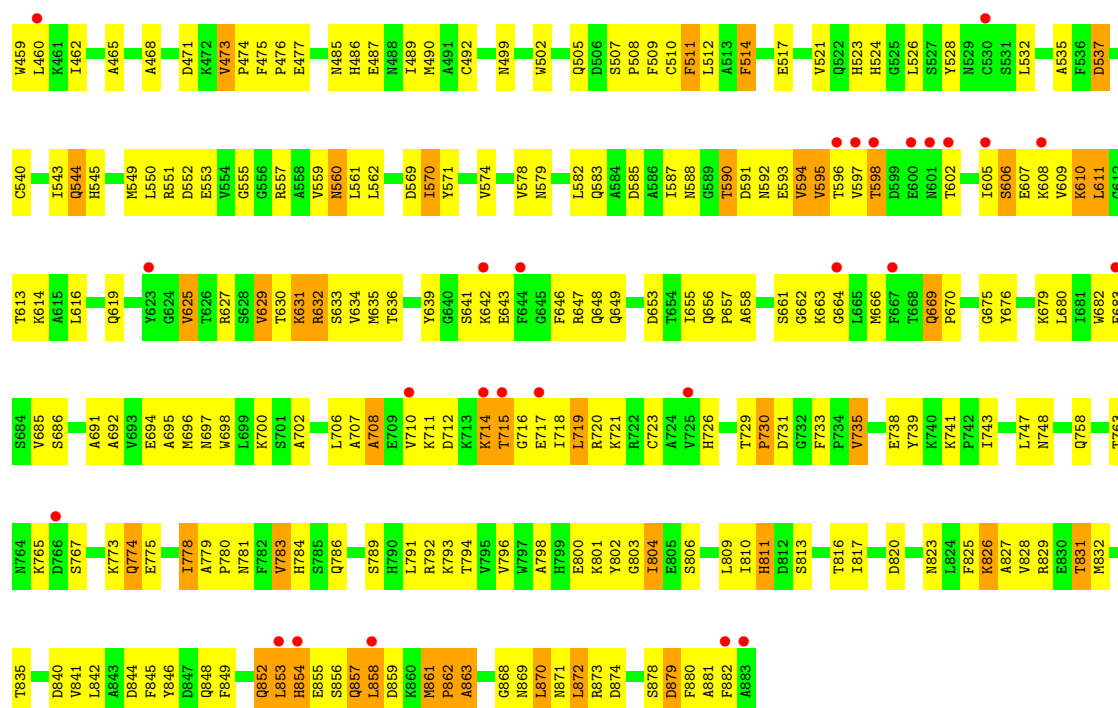


- Molecule 2: 5'-D(*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*T)-3'



- Molecule 3: DNA-directed RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	224.45 Å 73.79 Å 80.31 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.90 39.04 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (39.04-2.90) 89.4 (39.04-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.90 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.249 , 0.268 0.249 , 0.267	Depositor DCC
R_{free} test set	1306 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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

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	0.40	0/412	0.87	0/635
2	P	0.38	0/313	0.95	1/480 (0.2%)
3	A	0.64	1/6959 (0.0%)	0.99	26/9416 (0.3%)
All	All	0.62	1/7684 (0.0%)	0.98	27/10531 (0.3%)

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	3
2	P	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	137	VAL	CA-CB	-5.54	1.47	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	879	ASP	N-CA-C	8.46	120.50	111.28
3	A	150	ARG	N-CA-C	-7.50	99.71	110.59
3	A	161	HIS	N-CA-C	7.35	120.22	111.33
3	A	325	ASN	N-CA-C	7.33	121.13	111.75
3	A	19	ILE	CB-CA-C	-7.26	106.80	113.70
3	A	835	THR	N-CA-C	5.99	117.61	111.14
3	A	220	LEU	N-CA-C	-5.98	103.72	111.02
3	A	778	ILE	N-CA-C	5.96	116.08	110.30
3	A	741	LYS	CA-C-N	5.82	125.58	119.76
3	A	741	LYS	C-N-CA	5.82	125.58	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	511	PHE	N-CA-C	-5.76	104.92	111.14
3	A	535	ALA	N-CA-C	5.67	118.79	109.72
3	A	274	PRO	CA-C-N	5.53	125.45	119.76
3	A	274	PRO	C-N-CA	5.53	125.45	119.76
3	A	669	GLN	CA-C-N	5.52	126.74	119.84
3	A	669	GLN	C-N-CA	5.52	126.74	119.84
3	A	465	ALA	N-CA-C	-5.51	105.18	111.14
3	A	106	LEU	N-CA-C	5.37	117.89	111.71
3	A	719	LEU	N-CA-C	-5.25	105.45	111.07
3	A	468	ALA	N-CA-C	-5.24	102.44	110.14
2	P	103	DA	C5'-C4'-C3'	-5.24	107.05	114.90
3	A	282	THR	N-CA-C	5.15	116.12	108.86
3	A	378	LYS	N-CA-C	-5.14	105.68	111.28
3	A	460	LEU	N-CA-C	-5.12	105.82	111.71
3	A	605	ILE	N-CA-C	-5.11	106.60	112.98
3	A	544	GLN	N-CA-C	-5.09	105.64	111.14
3	A	783	VAL	CB-CA-C	-5.03	105.44	111.88

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	106	DC	Sidechain
1	T	10	DG	Sidechain
1	T	11	DT	Sidechain
1	T	9	DA	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	368	0	207	12	0
2	P	280	0	160	9	0
3	A	6803	0	6764	388	0
All	All	7451	0	7131	405	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 (405) 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:473:VAL:HG22	3:A:474:PRO:HD2	1.20	1.18
3:A:804:ILE:HG12	3:A:820:ASP:HB3	1.48	0.94
3:A:278:TRP:H	3:A:321:ASN:HD21	0.92	0.91
3:A:595:VAL:HG12	3:A:608:LYS:HA	1.51	0.90
3:A:774:GLN:HE21	3:A:774:GLN:HA	1.36	0.90
3:A:816:THR:HG22	3:A:817:ILE:H	1.39	0.87
3:A:425:ARG:HH21	3:A:811:HIS:HB3	1.39	0.87
2:P:103:DA:H2''	2:P:104:DT:H5'	1.57	0.85
3:A:473:VAL:CG2	3:A:474:PRO:HD2	2.06	0.85
3:A:305:LEU:HD22	3:A:305:LEU:O	1.76	0.85
3:A:663:LYS:HG2	3:A:664:GLY:H	1.40	0.85
3:A:595:VAL:HG23	3:A:597:VAL:H	1.40	0.85
3:A:278:TRP:H	3:A:321:ASN:ND2	1.74	0.84
3:A:367:ILE:HD12	3:A:374:LEU:HD21	1.60	0.81
3:A:594:VAL:HG13	3:A:595:VAL:H	1.46	0.81
3:A:278:TRP:N	3:A:321:ASN:HD21	1.76	0.80
3:A:324:GLN:HE21	3:A:418:TYR:H	1.31	0.79
3:A:401:MET:HE3	3:A:431:MET:HE2	1.64	0.78
1:T:5:DC:H4'	3:A:422:TRP:HZ3	1.49	0.78
3:A:170:LEU:O	3:A:174:VAL:HG23	1.84	0.78
2:P:108:DA:H2''	2:P:109:DC:H5'	1.65	0.77
3:A:729:THR:HG22	3:A:733:PHE:O	1.85	0.77
3:A:427:TYR:HA	3:A:435:GLN:HE22	1.50	0.76
3:A:636:THR:HA	3:A:639:TYR:HD2	1.50	0.76
3:A:590:THR:HB	3:A:613:THR:H	1.49	0.75
3:A:846:TYR:HA	3:A:849:PHE:CE1	2.22	0.75
3:A:829:ARG:NH1	3:A:878:SER:O	2.19	0.75
3:A:706:LEU:HD21	3:A:849:PHE:HB2	1.68	0.74
3:A:585:ASP:O	3:A:614:LYS:HA	1.88	0.74
3:A:841:VAL:HG23	3:A:842:LEU:HD22	1.70	0.74
3:A:454:LYS:N	3:A:526:LEU:HD13	2.04	0.73
1:T:5:DC:H4'	3:A:422:TRP:CZ3	2.24	0.72
3:A:544:GLN:HG2	3:A:559:VAL:HG11	1.69	0.72
3:A:729:THR:CG2	3:A:733:PHE:HB3	2.19	0.72
3:A:861:MET:H	3:A:862:PRO:HD2	1.53	0.71
3:A:281:ILE:HD11	3:A:305:LEU:HD13	1.72	0.71
3:A:669:GLN:HE21	3:A:669:GLN:HA	1.54	0.71
3:A:632:ARG:HA	3:A:635:MET:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:594:VAL:HG22	3:A:595:VAL:HG22	1.73	0.70
3:A:106:LEU:HA	3:A:109:ILE:HD12	1.72	0.70
3:A:386:ARG:NH1	3:A:386:ARG:HB2	2.06	0.70
3:A:854:HIS:CG	3:A:855:GLU:N	2.60	0.69
3:A:854:HIS:NE2	3:A:856:SER:C	2.50	0.69
3:A:616:LEU:HD23	3:A:676:TYR:HB2	1.75	0.69
3:A:397:SER:O	3:A:401:MET:HG2	1.93	0.68
3:A:778:ILE:HG23	3:A:779:ALA:H	1.59	0.68
3:A:425:ARG:NH2	3:A:811:HIS:HB3	2.09	0.67
3:A:596:THR:HG23	3:A:607:GLU:HB3	1.76	0.67
3:A:871:ASN:HB3	3:A:874:ASP:OD2	1.95	0.67
3:A:50:ARG:HB2	3:A:50:ARG:NH1	2.08	0.67
3:A:6:ILE:HD12	3:A:8:LYS:HD2	1.76	0.67
3:A:6:ILE:HG21	3:A:8:LYS:HZ3	1.58	0.67
3:A:550:LEU:HD11	3:A:695:ALA:HB2	1.78	0.66
3:A:540:CYS:SG	3:A:543:ILE:HD12	2.35	0.66
3:A:853:LEU:HD13	3:A:854:HIS:HB3	1.77	0.66
3:A:416:PHE:CE2	3:A:434:PRO:HD3	2.30	0.66
3:A:311:VAL:O	3:A:312:TYR:HB3	1.94	0.66
3:A:849:PHE:O	3:A:853:LEU:HB3	1.96	0.65
3:A:692:ALA:O	3:A:696:MET:HG3	1.97	0.65
3:A:164:LYS:HD2	3:A:164:LYS:C	2.21	0.65
3:A:730:PRO:CD	3:A:786:GLN:HE22	2.08	0.65
3:A:731:ASP:OD1	3:A:789:SER:HB2	1.97	0.65
3:A:50:ARG:HB2	3:A:50:ARG:HH11	1.61	0.64
3:A:669:GLN:HA	3:A:669:GLN:NE2	2.11	0.64
3:A:794:THR:OG1	3:A:831:THR:HG21	1.97	0.64
3:A:428:ALA:H	3:A:435:GLN:HE21	1.44	0.64
3:A:630:THR:O	3:A:634:VAL:HG12	1.98	0.64
3:A:729:THR:HG21	3:A:733:PHE:HB3	1.78	0.64
3:A:185:VAL:HG22	3:A:186:VAL:N	2.13	0.64
3:A:366:ASP:HB3	3:A:369:MET:HG2	1.80	0.64
3:A:452:ILE:HG23	3:A:453:GLY:N	2.13	0.63
3:A:169:GLN:HE21	3:A:171:ASN:HB2	1.64	0.63
2:P:108:DA:H2''	2:P:109:DC:C5'	2.28	0.62
3:A:425:ARG:HH21	3:A:811:HIS:CB	2.13	0.62
3:A:8:LYS:O	3:A:9:ASN:HB3	1.98	0.62
3:A:798:ALA:O	3:A:804:ILE:HB	1.99	0.61
3:A:438:ASP:OD2	3:A:509:PHE:HB2	2.00	0.61
3:A:643:GLU:CD	3:A:679:LYS:HD2	2.24	0.61
3:A:647:ARG:HE	3:A:675:GLY:HA2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:594:VAL:HG13	3:A:595:VAL:N	2.14	0.61
3:A:778:ILE:HG23	3:A:779:ALA:N	2.15	0.61
3:A:150:ARG:O	3:A:152:GLY:N	2.34	0.60
3:A:594:VAL:HG22	3:A:595:VAL:N	2.14	0.60
3:A:706:LEU:HG	3:A:853:LEU:HG	1.83	0.60
1:T:19:DA:H1'	1:T:20:DT:H5'	1.84	0.60
2:P:103:DA:H2''	2:P:104:DT:C5'	2.31	0.60
3:A:551:ARG:O	3:A:868:GLY:HA3	2.00	0.60
3:A:853:LEU:HD22	3:A:854:HIS:N	2.16	0.60
1:T:7:DA:H2'	1:T:8:DT:H72	1.84	0.60
3:A:625:VAL:HA	3:A:629:VAL:HG21	1.84	0.60
1:T:5:DC:H2''	1:T:6:DT:H5'	1.83	0.59
3:A:702:ALA:O	3:A:706:LEU:HD12	2.02	0.59
3:A:609:VAL:HG11	3:A:669:GLN:OE1	2.02	0.59
3:A:739:TYR:CD1	3:A:773:LYS:HE3	2.38	0.59
3:A:473:VAL:HG22	3:A:474:PRO:CD	2.12	0.59
3:A:395:ARG:O	3:A:399:GLU:HG2	2.02	0.59
3:A:424:GLY:O	3:A:425:ARG:C	2.46	0.58
3:A:425:ARG:HH11	3:A:784:HIS:CG	2.21	0.58
3:A:452:ILE:HG12	3:A:457:TYR:N	2.18	0.58
3:A:386:ARG:HB2	3:A:386:ARG:HH11	1.67	0.58
3:A:473:VAL:HG21	3:A:477:GLU:CD	2.28	0.58
3:A:594:VAL:HG11	3:A:598:THR:HG21	1.86	0.58
3:A:633:SER:HA	3:A:649:GLN:OE1	2.02	0.58
3:A:743:ILE:HD11	3:A:767:SER:HB3	1.84	0.58
3:A:364:PRO:C	3:A:366:ASP:H	2.09	0.58
3:A:862:PRO:O	3:A:863:ALA:CB	2.52	0.58
3:A:335:LEU:O	3:A:335:LEU:HD22	2.03	0.58
3:A:590:THR:HG22	3:A:591:ASP:N	2.19	0.58
3:A:335:LEU:HD22	3:A:339:ASN:ND2	2.20	0.57
2:P:102:DA:H1'	2:P:103:DA:C8	2.39	0.57
3:A:747:LEU:O	3:A:758:GLN:HA	2.04	0.57
3:A:73:LEU:HG	3:A:260:ALA:HB1	1.86	0.57
3:A:853:LEU:HD22	3:A:854:HIS:H	1.68	0.57
3:A:147:ASP:OD1	3:A:292:ARG:HD2	2.04	0.56
3:A:861:MET:HB3	3:A:862:PRO:CD	2.35	0.56
3:A:862:PRO:O	3:A:863:ALA:HB3	2.05	0.56
3:A:452:ILE:HG23	3:A:453:GLY:H	1.70	0.56
3:A:806:SER:O	3:A:816:THR:HG23	2.04	0.56
3:A:106:LEU:HD21	3:A:212:VAL:HG13	1.88	0.56
3:A:159:ALA:HA	3:A:162:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:560:ASN:O	3:A:881:ALA:HB2	2.05	0.56
3:A:796:VAL:O	3:A:800:GLU:HG3	2.06	0.56
3:A:871:ASN:C	3:A:873:ARG:H	2.14	0.56
3:A:139:SER:OG	3:A:206:LYS:HE2	2.05	0.56
3:A:569:ASP:OD2	3:A:627:ARG:HD2	2.06	0.56
3:A:427:TYR:HA	3:A:435:GLN:NE2	2.19	0.55
3:A:12:SER:OG	3:A:15:GLU:HG3	2.07	0.55
3:A:366:ASP:CB	3:A:369:MET:HG2	2.37	0.55
3:A:639:TYR:HA	3:A:780:PRO:HB3	1.89	0.55
3:A:592:ASN:OD1	3:A:611:LEU:HA	2.07	0.55
3:A:845:PHE:O	3:A:848:GLN:HB2	2.07	0.55
1:T:6:DT:OP2	1:T:7:DA:H4'	2.07	0.55
3:A:763:THR:HG22	3:A:765:LYS:H	1.72	0.55
3:A:311:VAL:O	3:A:312:TYR:CB	2.54	0.54
3:A:551:ARG:HG3	3:A:551:ARG:HH11	1.72	0.54
3:A:281:ILE:HD11	3:A:305:LEU:O	2.07	0.54
3:A:324:GLN:HE21	3:A:418:TYR:N	2.04	0.54
3:A:607:GLU:C	3:A:609:VAL:H	2.15	0.54
3:A:804:ILE:HG23	3:A:816:THR:HG21	1.89	0.54
3:A:176:HIS:CD2	3:A:177:VAL:H	2.25	0.54
3:A:386:ARG:HH11	3:A:386:ARG:CB	2.20	0.54
3:A:647:ARG:HG2	3:A:647:ARG:HH11	1.73	0.54
1:T:17:DG:H1'	1:T:18:DT:H5'	1.89	0.54
3:A:643:GLU:OE1	3:A:679:LYS:HD2	2.08	0.54
3:A:679:LYS:HG3	3:A:683:GLU:OE2	2.08	0.54
3:A:81:MET:HE1	3:A:219:MET:HB3	1.89	0.53
3:A:632:ARG:O	3:A:636:THR:HG23	2.09	0.53
3:A:147:ASP:CG	3:A:292:ARG:HD2	2.34	0.53
3:A:853:LEU:HD13	3:A:853:LEU:C	2.34	0.52
3:A:475:PHE:O	3:A:476:PRO:C	2.52	0.52
3:A:720:ARG:HD2	3:A:721:LYS:O	2.10	0.52
3:A:324:GLN:NE2	3:A:418:TYR:H	2.05	0.52
3:A:619:GLN:NE2	3:A:666:MET:O	2.42	0.52
3:A:6:ILE:HG21	3:A:8:LYS:NZ	2.25	0.52
3:A:459:TRP:HA	3:A:462:ILE:HB	1.91	0.52
3:A:502:TRP:CE3	3:A:512:LEU:HB2	2.45	0.52
3:A:367:ILE:HG23	3:A:368:ASP:OD1	2.10	0.51
3:A:186:VAL:HG12	3:A:187:GLU:N	2.25	0.51
3:A:254:ILE:HG22	3:A:399:GLU:HG3	1.91	0.51
3:A:486:HIS:CE1	3:A:490:MET:HG3	2.45	0.51
3:A:570:ILE:HG23	3:A:571:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:861:MET:HB3	3:A:862:PRO:HD3	1.92	0.51
3:A:272:VAL:O	3:A:415:TRP:HZ3	1.93	0.51
3:A:711:LYS:HG2	3:A:712:ASP:N	2.25	0.51
3:A:729:THR:HG23	3:A:733:PHE:H	1.75	0.51
3:A:802:TYR:OH	3:A:826:LYS:HE3	2.09	0.51
1:T:14:DG:H1'	1:T:15:DT:H5''	1.93	0.51
3:A:579:ASN:HA	3:A:582:LEU:HD12	1.91	0.51
3:A:153:ARG:HG2	3:A:153:ARG:HH11	1.76	0.51
3:A:370:ASN:ND2	3:A:375:THR:OG1	2.44	0.51
3:A:685:VAL:HG23	3:A:686:SER:N	2.26	0.51
3:A:816:THR:HG22	3:A:817:ILE:N	2.17	0.51
3:A:570:ILE:HG23	3:A:571:TYR:N	2.26	0.51
1:T:14:DG:H2''	1:T:15:DT:H5'	1.92	0.50
3:A:861:MET:O	3:A:862:PRO:O	2.29	0.50
3:A:648:GLN:H	3:A:648:GLN:CD	2.19	0.50
3:A:593:GLU:HG3	3:A:594:VAL:H	1.77	0.50
3:A:636:THR:HA	3:A:639:TYR:CD2	2.40	0.50
3:A:593:GLU:HB3	3:A:610:LYS:CB	2.41	0.50
3:A:710:VAL:HG13	3:A:719:LEU:HB2	1.92	0.50
3:A:507:SER:HB3	3:A:510:CYS:HB2	1.94	0.50
3:A:199:GLU:OE2	3:A:199:GLU:HA	2.11	0.49
3:A:19:ILE:HB	3:A:20:PRO:HD3	1.93	0.49
3:A:99:ARG:HG2	3:A:99:ARG:HH11	1.77	0.49
3:A:574:VAL:O	3:A:578:VAL:HG23	2.12	0.49
3:A:606:SER:O	3:A:607:GLU:C	2.53	0.49
3:A:537:ASP:OD1	3:A:813:SER:OG	2.11	0.49
3:A:163:LYS:NZ	3:A:163:LYS:HA	2.28	0.49
3:A:176:HIS:O	3:A:179:LYS:HE2	2.12	0.49
3:A:861:MET:HE3	3:A:862:PRO:HD3	1.94	0.49
3:A:169:GLN:HG2	3:A:172:LYS:NZ	2.27	0.49
3:A:370:ASN:N	3:A:371:PRO:CD	2.76	0.49
3:A:22:ASN:C	3:A:24:LEU:H	2.20	0.49
3:A:454:LYS:HD3	3:A:454:LYS:C	2.37	0.49
3:A:857:GLN:O	3:A:858:LEU:HB3	2.13	0.49
2:P:107:DG:H2''	2:P:108:DA:H5'	1.94	0.49
3:A:72:PRO:HB3	3:A:262:ALA:HB3	1.93	0.49
3:A:641:SER:HB3	3:A:646:PHE:CE1	2.48	0.49
3:A:421:ASP:OD2	3:A:423:ARG:HD3	2.13	0.48
3:A:846:TYR:C	3:A:848:GLN:H	2.20	0.48
3:A:6:ILE:HD12	3:A:8:LYS:CD	2.42	0.48
3:A:224:THR:O	3:A:226:MET:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:HIS:O	3:A:524:HIS:ND1	2.46	0.48
3:A:22:ASN:C	3:A:24:LEU:N	2.69	0.48
3:A:337:VAL:HG21	3:A:512:LEU:HD21	1.96	0.48
3:A:559:VAL:O	3:A:560:ASN:CG	2.57	0.48
2:P:106:DC:H2"	3:A:748:ASN:HB3	1.96	0.48
3:A:240:ASP:OD1	3:A:241:SER:N	2.46	0.48
3:A:511:PHE:O	3:A:514:PHE:N	2.46	0.48
3:A:871:ASN:C	3:A:873:ARG:N	2.71	0.48
3:A:362:MET:HE3	3:A:363:LYS:H	1.79	0.48
3:A:367:ILE:HD12	3:A:374:LEU:CD2	2.37	0.48
3:A:595:VAL:CG1	3:A:608:LYS:HA	2.34	0.48
3:A:823:ASN:O	3:A:826:LYS:HG2	2.14	0.48
3:A:337:VAL:O	3:A:341:ILE:HG12	2.14	0.48
3:A:729:THR:CG2	3:A:733:PHE:H	2.27	0.48
3:A:229:LEU:HG	3:A:242:GLU:HG3	1.96	0.47
3:A:523:HIS:C	3:A:524:HIS:ND1	2.72	0.47
3:A:544:GLN:CG	3:A:559:VAL:HG11	2.40	0.47
3:A:561:LEU:O	3:A:878:SER:HB2	2.13	0.47
3:A:698:TRP:HZ3	3:A:863:ALA:N	2.12	0.47
3:A:24:LEU:HD11	3:A:273:VAL:HG21	1.96	0.47
3:A:308:TYR:HA	3:A:311:VAL:HG23	1.95	0.47
3:A:344:TRP:C	3:A:346:HIS:H	2.23	0.47
3:A:201:TRP:HB2	3:A:302:LYS:HD3	1.95	0.47
3:A:422:TRP:CD2	3:A:423:ARG:HD2	2.49	0.47
3:A:523:HIS:C	3:A:524:HIS:HD1	2.22	0.47
3:A:6:ILE:HB	3:A:8:LYS:HZ2	1.79	0.47
3:A:36:GLN:NE2	3:A:273:VAL:HG22	2.30	0.47
3:A:201:TRP:HZ2	3:A:299:THR:O	1.98	0.47
3:A:363:LYS:HG2	3:A:364:PRO:HD2	1.96	0.47
3:A:559:VAL:O	3:A:560:ASN:CB	2.63	0.47
3:A:590:THR:HB	3:A:613:THR:N	2.25	0.47
3:A:783:VAL:O	3:A:784:HIS:C	2.55	0.47
3:A:308:TYR:HA	3:A:311:VAL:CG2	2.44	0.47
3:A:783:VAL:HG23	3:A:784:HIS:H	1.79	0.47
3:A:791:LEU:HD23	3:A:791:LEU:C	2.40	0.47
3:A:827:ALA:O	3:A:831:THR:HG22	2.14	0.47
3:A:46:MET:HG3	3:A:47:GLY:N	2.29	0.47
3:A:517:GLU:HG3	3:A:532:LEU:HB2	1.97	0.47
3:A:710:VAL:HG12	3:A:720:ARG:O	2.14	0.47
3:A:663:LYS:HG2	3:A:664:GLY:N	2.20	0.47
3:A:679:LYS:HE2	3:A:683:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:691:ALA:O	3:A:692:ALA:C	2.58	0.47
3:A:361:PRO:HD3	3:A:384:VAL:HG21	1.96	0.46
3:A:451:PRO:HA	3:A:528:TYR:O	2.15	0.46
3:A:719:LEU:HD22	3:A:719:LEU:N	2.30	0.46
3:A:371:PRO:O	3:A:372:GLU:HG2	2.15	0.46
3:A:453:GLY:HA2	3:A:526:LEU:HB3	1.96	0.46
3:A:502:TRP:O	3:A:505:GLN:HG2	2.15	0.46
3:A:726:HIS:HD2	3:A:735:VAL:O	1.98	0.46
3:A:870:LEU:C	3:A:870:LEU:HD23	2.40	0.46
3:A:856:SER:O	3:A:857:GLN:C	2.59	0.46
3:A:32:LEU:O	3:A:33:ALA:C	2.56	0.46
3:A:852:GLN:O	3:A:853:LEU:HB2	2.15	0.46
3:A:159:ALA:O	3:A:163:LYS:HG2	2.15	0.46
3:A:452:ILE:CG2	3:A:453:GLY:N	2.78	0.46
3:A:185:VAL:HG22	3:A:186:VAL:H	1.78	0.46
3:A:562:LEU:HD21	3:A:870:LEU:CD1	2.46	0.46
3:A:632:ARG:HA	3:A:635:MET:CG	2.44	0.46
3:A:272:VAL:O	3:A:272:VAL:HG12	2.15	0.46
3:A:425:ARG:NH1	3:A:784:HIS:CG	2.83	0.46
3:A:593:GLU:HB3	3:A:610:LYS:HB2	1.98	0.46
3:A:775:GLU:O	3:A:778:ILE:HG22	2.16	0.46
3:A:224:THR:O	3:A:224:THR:OG1	2.34	0.46
3:A:455:GLU:HA	3:A:455:GLU:OE1	2.16	0.45
3:A:631:LYS:O	3:A:634:VAL:HG12	2.15	0.45
1:T:6:DT:OP2	1:T:7:DA:C4'	2.63	0.45
3:A:224:THR:C	3:A:226:MET:H	2.25	0.45
3:A:857:GLN:HA	3:A:857:GLN:NE2	2.30	0.45
3:A:347:CYS:SG	3:A:348:PRO:HD2	2.56	0.45
3:A:373:ALA:C	3:A:375:THR:H	2.24	0.45
3:A:169:GLN:HG2	3:A:172:LYS:HZ3	1.80	0.45
3:A:199:GLU:HA	3:A:302:LYS:HZ3	1.80	0.45
3:A:474:PRO:HA	3:A:880:PHE:CZ	2.52	0.45
3:A:664:GLY:HA2	3:A:666:MET:SD	2.56	0.45
3:A:841:VAL:HG23	3:A:842:LEU:N	2.32	0.45
3:A:783:VAL:HG23	3:A:784:HIS:N	2.32	0.45
3:A:12:SER:HG	3:A:15:GLU:HG3	1.82	0.45
3:A:23:THR:O	3:A:27:HIS:HD2	1.98	0.45
3:A:204:TRP:O	3:A:205:HIS:C	2.58	0.45
3:A:656:GLN:HA	3:A:656:GLN:OE1	2.17	0.45
3:A:457:TYR:CD1	3:A:521:VAL:HG11	2.52	0.45
3:A:81:MET:HE1	3:A:219:MET:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:341:ILE:C	3:A:343:LYS:H	2.25	0.45
3:A:663:LYS:CG	3:A:664:GLY:H	2.19	0.45
2:P:111:DC:H2''	2:P:112:DA:C8	2.52	0.44
3:A:186:VAL:HG12	3:A:187:GLU:H	1.82	0.44
3:A:404:GLN:CA	3:A:404:GLN:HE21	2.31	0.44
3:A:246:LEU:HD21	3:A:254:ILE:HD12	1.98	0.44
3:A:825:PHE:CD1	3:A:825:PHE:C	2.95	0.44
1:T:16:DC:H2''	1:T:17:DG:C8	2.53	0.44
3:A:102:ALA:CB	3:A:215:ARG:HG3	2.48	0.44
3:A:295:ALA:O	3:A:296:LEU:C	2.59	0.44
3:A:696:MET:O	3:A:700:LYS:HG3	2.17	0.44
3:A:871:ASN:O	3:A:873:ARG:N	2.50	0.44
3:A:103:PHE:O	3:A:104:GLN:C	2.60	0.44
3:A:557:ARG:NH1	3:A:557:ARG:HG2	2.31	0.44
3:A:729:THR:OG1	3:A:789:SER:HB3	2.18	0.44
3:A:829:ARG:NH2	3:A:882:PHE:HD1	2.15	0.44
1:T:20:DT:O2	3:A:97:GLY:HA2	2.18	0.44
3:A:237:VAL:O	3:A:237:VAL:HG12	2.18	0.44
3:A:316:VAL:O	3:A:320:ILE:HG12	2.18	0.44
3:A:363:LYS:C	3:A:365:GLU:H	2.26	0.44
3:A:594:VAL:HG11	3:A:598:THR:CG2	2.47	0.44
3:A:344:TRP:CE3	3:A:348:PRO:HD3	2.52	0.44
2:P:110:DT:H1'	2:P:111:DC:H5''	2.00	0.43
3:A:37:LEU:O	3:A:38:ALA:C	2.57	0.43
3:A:344:TRP:C	3:A:346:HIS:N	2.76	0.43
3:A:349:VAL:C	3:A:351:ASP:H	2.26	0.43
3:A:561:LEU:N	3:A:561:LEU:HD22	2.33	0.43
3:A:574:VAL:O	3:A:574:VAL:HG12	2.17	0.43
3:A:330:ILE:HB	3:A:409:ALA:HA	1.99	0.43
3:A:333:LYS:O	3:A:336:ALA:HB3	2.19	0.43
3:A:656:GLN:HB3	3:A:657:PRO:CD	2.49	0.43
3:A:707:ALA:O	3:A:708:ALA:C	2.61	0.43
3:A:169:GLN:NE2	3:A:171:ASN:HB2	2.31	0.43
3:A:855:GLU:OE2	3:A:856:SER:HB3	2.18	0.43
3:A:404:GLN:NE2	3:A:404:GLN:HA	2.33	0.43
3:A:739:TYR:H	3:A:774:GLN:HE22	1.66	0.43
3:A:698:TRP:CZ3	3:A:862:PRO:HA	2.54	0.43
3:A:853:LEU:HD13	3:A:854:HIS:CB	2.48	0.43
3:A:781:ASN:HD22	3:A:781:ASN:HA	1.65	0.43
3:A:842:LEU:O	3:A:845:PHE:HB3	2.19	0.43
3:A:881:ALA:O	3:A:882:PHE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:281:ILE:HD11	3:A:305:LEU:CD1	2.44	0.43
3:A:452:ILE:CG2	3:A:453:GLY:H	2.31	0.43
3:A:553:GLU:OE2	3:A:869:ASN:N	2.52	0.43
3:A:715:THR:C	3:A:717:GLU:H	2.26	0.43
3:A:854:HIS:CD2	3:A:858:LEU:N	2.87	0.43
3:A:594:VAL:HG22	3:A:595:VAL:H	1.80	0.43
3:A:803:GLY:O	3:A:804:ILE:C	2.62	0.43
3:A:342:THR:O	3:A:395:ARG:NH2	2.48	0.42
3:A:730:PRO:HD2	3:A:786:GLN:HE22	1.84	0.42
3:A:410:ASN:O	3:A:411:HIS:C	2.62	0.42
3:A:706:LEU:HA	3:A:853:LEU:CD2	2.49	0.42
3:A:570:ILE:HG23	3:A:571:TYR:H	1.84	0.42
3:A:697:ASN:HD22	3:A:697:ASN:HA	1.63	0.42
3:A:779:ALA:N	3:A:780:PRO:HD2	2.34	0.42
3:A:19:ILE:HG22	3:A:195:LEU:HD21	2.00	0.42
3:A:185:VAL:CG2	3:A:186:VAL:N	2.80	0.42
3:A:416:PHE:CD2	3:A:434:PRO:HD3	2.54	0.42
3:A:669:GLN:HA	3:A:670:PRO:HD2	1.85	0.42
3:A:164:LYS:HD2	3:A:164:LYS:O	2.19	0.42
3:A:324:GLN:HE21	3:A:417:PRO:HA	1.83	0.42
3:A:828:VAL:O	3:A:831:THR:HG23	2.19	0.42
3:A:109:ILE:HG22	3:A:110:LYS:N	2.35	0.42
3:A:364:PRO:C	3:A:366:ASP:N	2.78	0.42
3:A:72:PRO:O	3:A:75:THR:OG1	2.37	0.42
3:A:159:ALA:O	3:A:163:LYS:CG	2.68	0.42
3:A:428:ALA:H	3:A:435:GLN:NE2	2.13	0.42
3:A:492:CYS:HA	3:A:499:ASN:HB2	2.02	0.42
3:A:774:GLN:HA	3:A:774:GLN:NE2	2.17	0.42
3:A:792:ARG:O	3:A:793:LYS:C	2.61	0.42
3:A:854:HIS:NE2	3:A:856:SER:O	2.52	0.42
3:A:676:TYR:O	3:A:680:LEU:HD13	2.20	0.42
3:A:176:HIS:CG	3:A:177:VAL:H	2.38	0.42
3:A:212:VAL:O	3:A:213:GLY:C	2.63	0.41
3:A:298:ARG:HH12	3:A:427:TYR:HB2	1.85	0.41
3:A:379:ARG:O	3:A:382:ALA:HB3	2.20	0.41
3:A:551:ARG:HG3	3:A:551:ARG:NH1	2.35	0.41
3:A:717:GLU:O	3:A:719:LEU:HD22	2.20	0.41
3:A:583:GLN:O	3:A:587:ILE:HG12	2.20	0.41
3:A:274:PRO:HA	3:A:275:PRO:HD3	1.76	0.41
3:A:448:LYS:HD2	3:A:448:LYS:H	1.85	0.41
3:A:590:THR:CG2	3:A:591:ASP:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:177:VAL:O	3:A:179:LYS:HG2	2.20	0.41
3:A:215:ARG:O	3:A:216:CYS:C	2.64	0.41
3:A:739:TYR:HD1	3:A:773:LYS:HE3	1.84	0.41
3:A:609:VAL:CG2	3:A:611:LEU:HG	2.50	0.41
3:A:857:GLN:HA	3:A:857:GLN:HE21	1.84	0.41
3:A:78:LEU:O	3:A:82:ILE:HG13	2.20	0.41
3:A:710:VAL:HG13	3:A:710:VAL:O	2.20	0.41
3:A:714:LYS:O	3:A:715:THR:OG1	2.35	0.41
3:A:394:ARG:HG2	3:A:394:ARG:HH11	1.86	0.41
3:A:551:ARG:HE	3:A:872:LEU:HD11	1.86	0.41
3:A:712:ASP:OD2	3:A:715:THR:HB	2.20	0.41
3:A:715:THR:O	3:A:717:GLU:N	2.53	0.41
3:A:6:ILE:HD12	3:A:8:LYS:CE	2.50	0.41
3:A:366:ASP:N	3:A:366:ASP:OD2	2.52	0.41
3:A:551:ARG:HB2	3:A:868:GLY:H	1.86	0.41
3:A:557:ARG:HG2	3:A:557:ARG:HH11	1.85	0.41
3:A:655:ILE:O	3:A:658:ALA:HB3	2.20	0.41
3:A:691:ALA:O	3:A:694:GLU:N	2.54	0.41
3:A:718:ILE:HG21	3:A:721:LYS:HG3	2.03	0.41
3:A:6:ILE:CG2	3:A:8:LYS:NZ	2.84	0.41
3:A:840:ASP:O	3:A:844:ASP:OD2	2.39	0.41
3:A:545:HIS:O	3:A:549:MET:HG2	2.21	0.40
3:A:552:ASP:HB2	3:A:691:ALA:HB2	2.03	0.40
3:A:579:ASN:O	3:A:583:GLN:HG2	2.21	0.40
3:A:419:ASN:HD22	3:A:419:ASN:HA	1.49	0.40
3:A:719:LEU:CD2	3:A:719:LEU:H	2.34	0.40
3:A:831:THR:O	3:A:832:MET:C	2.65	0.40
3:A:485:ASN:O	3:A:489:ILE:HG13	2.20	0.40
3:A:555:GLY:O	3:A:559:VAL:HG23	2.21	0.40
3:A:313:MET:N	3:A:314:PRO:HD3	2.37	0.40
3:A:332:LYS:HE2	3:A:409:ALA:O	2.22	0.40
3:A:398:LEU:C	3:A:398:LEU:HD23	2.46	0.40
3:A:421:ASP:HB3	3:A:427:TYR:CE1	2.57	0.40
3:A:642:LYS:HA	3:A:642:LYS:HD3	1.96	0.40
3:A:661:SER:OG	3:A:662:GLY:N	2.53	0.40
3:A:682:TRP:HA	3:A:685:VAL:HG22	2.03	0.40
3:A:739:TYR:HD2	3:A:774:GLN:NE2	2.18	0.40
3:A:825:PHE:CE1	3:A:829:ARG:NH2	2.90	0.40
3:A:842:LEU:HD13	3:A:842:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	858/878 (98%)	693 (81%)	123 (14%)	42 (5%)	1 6

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	168	GLU
3	A	176	HIS
3	A	373	ALA
3	A	560	ASN
3	A	594	VAL
3	A	606	SER
3	A	611	LEU
3	A	857	GLN
3	A	859	ASP
3	A	862	PRO
3	A	863	ALA
3	A	151	PHE
3	A	372	GLU
3	A	602	THR
3	A	715	THR
3	A	104	GLN
3	A	169	GLN
3	A	174	VAL
3	A	177	VAL
3	A	178	TYR
3	A	270	PRO
3	A	312	TYR
3	A	350	GLU
3	A	508	PRO
3	A	631	LYS
3	A	861	MET
3	A	872	LEU
3	A	248	PRO

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Mol	Chain	Res	Type
3	A	425	ARG
3	A	595	VAL
3	A	708	ALA
3	A	716	GLY
3	A	811	HIS
3	A	858	LEU
3	A	590	THR
3	A	588	ASN
3	A	625	VAL
3	A	629	VAL
3	A	810	ILE
3	A	213	GLY
3	A	364	PRO
3	A	804	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	
3	A	714/724 (99%)	658 (92%)	56 (8%)	11	35

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	8	LYS
3	A	31	ARG
3	A	35	GLU
3	A	46	MET
3	A	77	LEU
3	A	109	ILE
3	A	120	LYS
3	A	163	LYS
3	A	183	MET
3	A	206	LYS
3	A	223	SER
3	A	224	THR

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Mol	Chain	Res	Type
3	A	245	GLU
3	A	249	GLU
3	A	274	PRO
3	A	276	LYS
3	A	292	ARG
3	A	305	LEU
3	A	313	MET
3	A	318	LYS
3	A	335	LEU
3	A	350	GLU
3	A	351	ASP
3	A	375	THR
3	A	394	ARG
3	A	404	GLN
3	A	419	ASN
3	A	422	TRP
3	A	423	ARG
3	A	426	VAL
3	A	448	LYS
3	A	471	ASP
3	A	473	VAL
3	A	487	GLU
3	A	514	PHE
3	A	537	ASP
3	A	570	ILE
3	A	598	THR
3	A	610	LYS
3	A	632	ARG
3	A	653	ASP
3	A	714	LYS
3	A	723	CYS
3	A	730	PRO
3	A	735	VAL
3	A	738	GLU
3	A	774	GLN
3	A	801	LYS
3	A	809	LEU
3	A	826	LYS
3	A	831	THR
3	A	852	GLN
3	A	853	LEU
3	A	854	HIS

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Mol	Chain	Res	Type
3	A	870	LEU
3	A	879	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	22	ASN
3	A	27	HIS
3	A	86	ASN
3	A	131	ASN
3	A	161	HIS
3	A	165	ASN
3	A	169	GLN
3	A	171	ASN
3	A	269	GLN
3	A	289	ASN
3	A	321	ASN
3	A	324	GLN
3	A	370	ASN
3	A	410	ASN
3	A	419	ASN
3	A	435	GLN
3	A	463	HIS
3	A	486	HIS
3	A	488	ASN
3	A	544	GLN
3	A	619	GLN
3	A	649	GLN
3	A	669	GLN
3	A	672	GLN
3	A	697	ASN
3	A	726	HIS
3	A	737	GLN
3	A	754	GLN
3	A	764	ASN
3	A	774	GLN
3	A	781	ASN
3	A	786	GLN
3	A	811	HIS
3	A	823	ASN
3	A	848	GLN
3	A	852	GLN

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Mol	Chain	Res	Type
3	A	857	GLN
3	A	869	ASN

5.3.3 RNA [i](#)

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

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	T	18/22 (81%)	0.36	2 (11%) 10 9	64, 72, 123, 136	0
2	P	14/14 (100%)	-0.03	0 100 100	53, 70, 106, 147	0
3	A	862/878 (98%)	0.50	46 (5%) 32 25	48, 81, 129, 148	0
All	All	894/914 (97%)	0.49	48 (5%) 31 24	48, 81, 129, 148	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	883	ALA	8.5
3	A	6	ILE	4.3
3	A	853	LEU	4.3
3	A	602	THR	3.9
3	A	597	VAL	3.8
3	A	766	ASP	3.7
1	T	5	DC	3.6
3	A	608	LYS	3.5
3	A	710	VAL	3.5
3	A	180	LYS	3.5
3	A	600	GLU	3.4
3	A	300	HIS	3.4
3	A	28	TYR	3.3
3	A	605	ILE	3.2
3	A	364	PRO	3.2
3	A	361	PRO	3.1
3	A	447	ALA	3.0
1	T	6	DT	2.9
3	A	601	ASN	2.8
3	A	176	HIS	2.8
3	A	858	LEU	2.7
3	A	175	GLY	2.7
3	A	854	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	725	VAL	2.6
3	A	664	GLY	2.6
3	A	374	LEU	2.6
3	A	717	GLU	2.6
3	A	181	ALA	2.5
3	A	714	LYS	2.5
3	A	598	THR	2.4
3	A	642	LYS	2.4
3	A	174	VAL	2.3
3	A	368	ASP	2.3
3	A	882	PHE	2.2
3	A	644	PHE	2.2
3	A	683	GLU	2.2
3	A	530	CYS	2.2
3	A	667	PHE	2.2
3	A	371	PRO	2.1
3	A	171	ASN	2.1
3	A	177	VAL	2.1
3	A	715	THR	2.1
3	A	623	TYR	2.1
3	A	166	VAL	2.0
3	A	460	LEU	2.0
3	A	201	TRP	2.0
3	A	596	THR	2.0
3	A	363	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.