



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:18 PM UTC

PDB ID : 1TUP / pdb_00001tup
Title : TUMOR SUPPRESSOR P53 COMPLEXED WITH DNA
Authors : Cho, Y.; Gorina, S.; Jeffrey, P.D.; Pavletich, N.P.
Deposited on : 1995-07-11
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

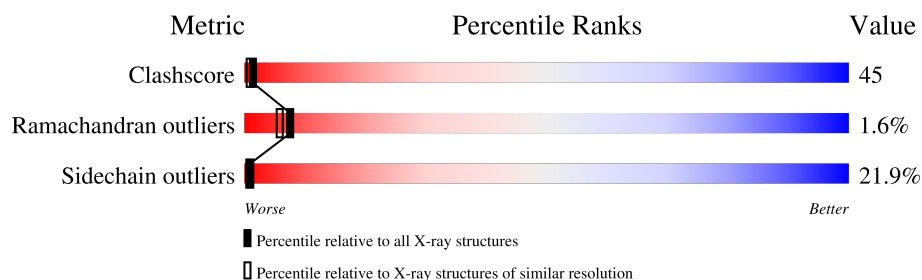
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	E	21	10% 38% 52%
2	F	21	10% 62% 29%
3	A	219	47% 32% 8% • 11%
3	B	219	32% 42% 13% • 11%
3	C	219	24% 41% 20% • 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5828 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(*TP*TP*TP*CP*CP*TP*AP*GP*AP*CP*TP*TP*GP*CP*CP*CP*A P*AP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	21	Total	C	N	O	P	0	0	0
			420	204	69	127	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	21	Total	C	N	O	P	0	0	0
			435	208	86	121	20			

- Molecule 3 is a protein called PROTEIN (P53 TUMOR SUPPRESSOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	196	Total	C	N	O	S	0	0	0
			1535	945	283	291	16			
3	B	194	Total	C	N	O	S	0	0	0
			1522	939	281	286	16			
3	C	195	Total	C	N	O	S	0	0	0
			1529	942	282	289	16			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	22	Total 22	O 22	0	0
5	F	14	Total 14	O 14	0	0
5	A	198	Total 198	O 198	0	0
5	B	70	Total 70	O 70	0	0
5	C	80	Total 80	O 80	0	0

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. 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(*TP*TP*TP*CP*CP*TP*AP*GP*AP*CP*TP*TP*GP*CP*CP*CP*A P*AP*TP*TP*A)-3')

Chain E: 



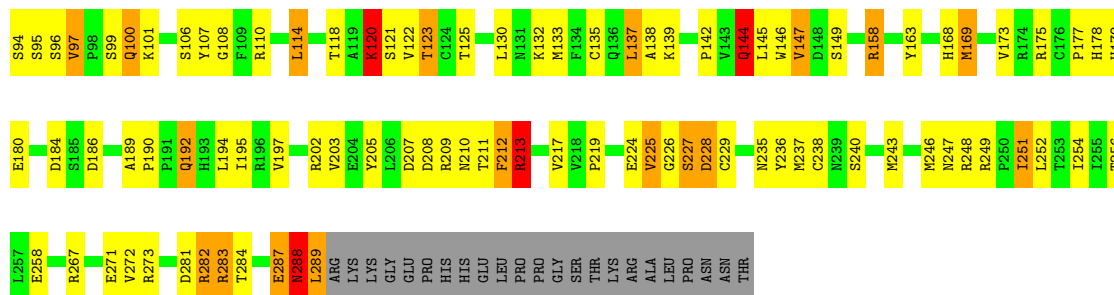
- Molecule 2: DNA (5'-D(*AP*TP*AP*AP*TP*TP*GP*GP*GP*CP*AP*AP*GP*TP*CP*TP*A P*GP*GP*AP*A)-3')

Chain F: 



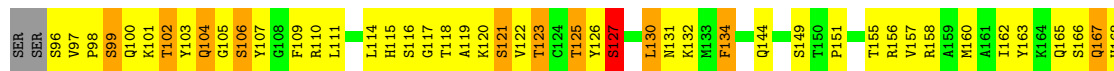
- Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

Chain A: 



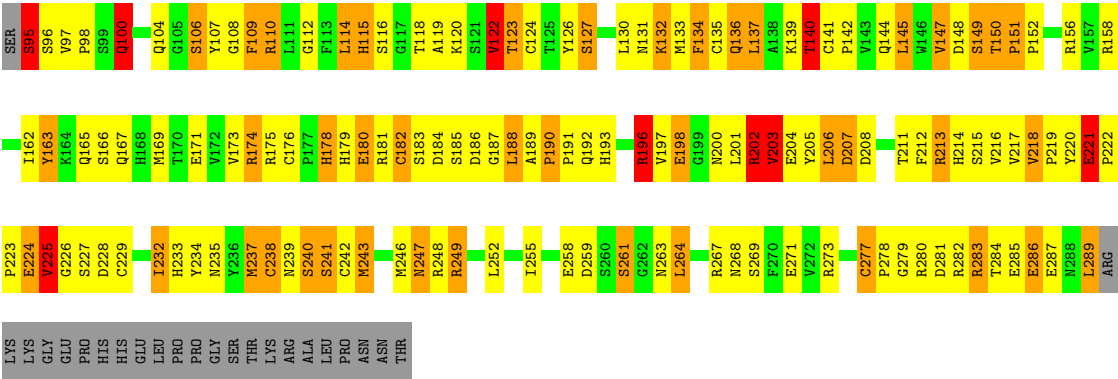
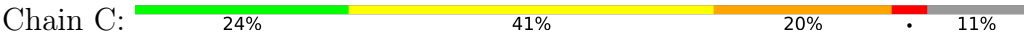
- Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

Chain B: 





● Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.50Å 67.90Å 108.80Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, TNT	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5828	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.51	0/468	1.42	12/719 (1.7%)
2	F	0.53	0/490	1.45	9/756 (1.2%)
3	A	0.98	0/1570	1.60	24/2129 (1.1%)
3	B	0.99	0/1557	1.81	35/2112 (1.7%)
3	C	0.96	0/1564	1.78	37/2121 (1.7%)
All	All	0.91	0/5649	1.68	117/7837 (1.5%)

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
3	A	1	0
3	C	1	0
All	All	2	0

There are no bond length outliers.

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	116	SER	N-CA-C	12.27	124.73	111.36
3	B	218	VAL	N-CA-CB	-10.78	104.39	111.83
3	B	214	HIS	CA-CB-CG	9.76	123.56	113.80
3	B	104	GLN	N-CA-C	-9.64	90.27	110.80
3	B	117	GLY	N-CA-C	-9.52	102.91	111.95
3	C	96	SER	N-CA-CB	9.31	123.94	110.16
3	C	212	PHE	CA-CB-CG	-8.85	104.95	113.80
3	B	222	PRO	N-CA-CB	8.40	107.89	103.19
1	E	1015	DC	P-O3'-C3'	8.39	132.79	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	237	MET	N-CA-C	8.31	122.84	112.87
3	C	178	HIS	CA-CB-CG	-8.23	105.57	113.80
3	C	95	SER	CA-C-N	-8.05	108.86	120.29
3	C	95	SER	C-N-CA	-8.05	108.86	120.29
3	C	247	ASN	N-CA-C	7.99	122.17	111.30
3	C	220	TYR	N-CA-CB	7.81	121.62	109.83
3	B	259	ASP	N-CA-CB	7.64	122.47	110.56
2	F	1107	DG	P-O3'-C3'	7.63	131.65	120.20
3	A	237	MET	N-CA-C	7.63	121.42	112.72
2	F	1118	DG	P-O3'-C3'	7.52	131.49	120.20
2	F	1114	DT	P-O5'-C5'	-7.48	108.77	120.00
3	C	169	MET	N-CA-C	7.47	120.36	111.33
2	F	1116	DT	P-O3'-C3'	7.32	131.19	120.20
3	C	151	PRO	CA-C-N	7.23	124.94	119.66
3	C	151	PRO	C-N-CA	7.23	124.94	119.66
3	C	148	ASP	CA-CB-CG	-7.23	105.37	112.60
3	A	97	VAL	N-CA-CB	-7.08	104.09	111.87
2	F	1118	DG	C4'-C3'-O3'	6.99	120.49	110.00
3	C	247	ASN	N-CA-CB	6.98	121.60	111.62
1	E	1003	DT	P-O3'-C3'	6.97	130.66	120.20
3	B	237	MET	N-CA-C	6.90	121.55	113.20
3	B	123	THR	N-CA-C	6.87	118.42	111.07
3	A	186	ASP	N-CA-C	-6.78	104.88	113.02
3	A	226	GLY	N-CA-C	-6.74	106.03	115.32
3	A	249	ARG	CA-C-N	6.70	126.93	119.90
3	A	249	ARG	C-N-CA	6.70	126.93	119.90
3	C	221	GLU	CA-C-N	6.64	124.51	119.66
3	C	221	GLU	C-N-CA	6.64	124.51	119.66
3	A	179	HIS	N-CA-C	6.60	118.14	111.07
3	C	106	SER	N-CA-C	6.58	120.90	112.34
1	E	1010	DC	P-O3'-C3'	-6.51	110.43	120.20
3	A	288	ASN	CA-CB-CG	6.47	119.07	112.60
3	B	265	LEU	N-CA-CB	6.30	119.43	110.67
3	A	243	MET	CA-C-N	-6.28	112.64	122.51
3	A	243	MET	C-N-CA	-6.28	112.64	122.51
1	E	1011	DT	P-O5'-C5'	6.22	129.34	120.00
3	B	235	ASN	CA-CB-CG	6.22	118.82	112.60
3	C	243	MET	CA-C-N	-6.14	112.43	122.20
3	C	243	MET	C-N-CA	-6.14	112.43	122.20
3	A	235	ASN	CA-CB-CG	6.12	118.72	112.60
3	B	206	LEU	N-CA-C	6.11	119.36	109.40
3	A	123	THR	N-CA-CB	-6.09	101.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	213	ARG	CG-CD-NE	-6.05	98.69	112.00
2	F	1112	DA	P-O3'-C3'	-6.05	111.13	120.20
3	B	276	ALA	N-CA-C	-6.03	99.83	109.96
1	E	1007	DA	P-O5'-C5'	6.00	129.00	120.00
3	B	104	GLN	CA-C-N	-5.99	115.58	122.83
3	B	104	GLN	C-N-CA	-5.99	115.58	122.83
1	E	1003	DT	O4'-C1'-N1	5.97	117.36	108.40
3	B	283	ARG	CA-C-N	5.93	129.03	120.79
3	B	283	ARG	C-N-CA	5.93	129.03	120.79
1	E	1005	DC	P-O3'-C3'	5.84	128.96	120.20
3	B	115	HIS	CA-CB-CG	-5.83	107.97	113.80
1	E	1017	DA	P-O3'-C3'	5.83	128.94	120.20
3	B	208	ASP	N-CA-CB	5.82	118.70	109.51
3	A	144	GLN	N-CA-C	5.74	118.59	109.24
3	C	196	ARG	N-CA-CB	5.68	121.43	111.55
3	C	152	PRO	O-C-N	5.67	123.92	121.31
3	A	213	ARG	CD-NE-CZ	5.64	132.29	124.40
3	C	122	VAL	N-CA-CB	5.63	118.08	111.66
3	A	283	ARG	CA-C-N	5.62	128.07	120.65
3	A	283	ARG	C-N-CA	5.62	128.07	120.65
3	C	140	THR	N-CA-C	5.59	117.85	108.96
3	C	163	TYR	N-CA-CB	5.54	118.15	110.17
1	E	1012	DT	P-O3'-C3'	5.54	128.51	120.20
3	C	277	CYS	CA-C-N	5.53	126.75	119.84
3	C	277	CYS	C-N-CA	5.53	126.75	119.84
3	B	211	THR	N-CA-C	-5.52	107.80	114.75
3	B	206	LEU	N-CA-CB	5.51	120.42	110.83
3	C	203	VAL	CB-CA-C	-5.46	104.19	111.13
3	A	195	ILE	N-CA-C	5.46	115.82	108.17
3	B	287	GLU	N-CA-C	-5.43	105.47	111.71
3	B	100	GLN	N-CA-C	-5.39	103.51	111.81
3	A	212	PHE	CA-CB-CG	5.37	119.17	113.80
3	B	134	PHE	CA-CB-CG	5.35	119.15	113.80
3	B	127	SER	CA-C-N	5.32	125.38	119.32
3	B	127	SER	C-N-CA	5.32	125.38	119.32
3	B	216	VAL	CA-CB-CG2	5.31	119.42	110.40
3	B	263	ASN	CA-CB-CG	-5.30	107.30	112.60
2	F	1113	DG	P-O3'-C3'	5.29	128.14	120.20
2	F	1119	DG	C1'-O4'-C4'	-5.27	101.80	109.70
3	C	213	ARG	N-CA-CB	5.26	117.71	109.97
3	A	158	ARG	N-CA-CB	-5.26	101.68	110.83
3	C	100	GLN	CB-CG-CD	5.24	121.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1006	DT	C5'-C4'-C3'	-5.24	107.04	114.90
3	B	252	LEU	CB-CA-C	-5.24	99.36	109.37
3	C	264	LEU	N-CA-C	5.23	117.81	110.23
3	C	184	ASP	CB-CA-C	5.21	118.40	110.37
3	A	120	LYS	N-CA-C	5.20	118.72	112.38
3	B	218	VAL	CA-C-N	-5.20	114.60	119.85
3	B	218	VAL	C-N-CA	-5.20	114.60	119.85
3	B	102	THR	N-CA-CB	5.19	117.53	109.48
3	C	109	PHE	CB-CA-C	5.17	117.60	110.16
3	A	190	PRO	N-CA-CB	5.15	108.08	103.08
3	B	187	GLY	N-CA-C	-5.15	108.22	114.92
3	C	190	PRO	CA-C-N	5.13	125.42	119.47
3	C	190	PRO	C-N-CA	5.13	125.42	119.47
1	E	1004	DC	N1-C1'-C2'	5.12	121.17	113.50
3	C	224	GLU	N-CA-C	5.11	117.96	110.30
2	F	1119	DG	C5'-C4'-O4'	5.10	117.05	109.40
1	E	1016	DC	P-O5'-C5'	-5.06	112.41	120.00
3	A	207	ASP	N-CA-C	-5.05	97.53	107.69
3	B	99	SER	N-CA-C	5.05	117.95	110.48
3	B	117	GLY	CA-C-O	-5.03	118.95	122.22
3	C	267	ARG	CD-NE-CZ	5.02	131.43	124.40
3	C	96	SER	CB-CA-C	5.02	119.38	110.85
3	C	202	ARG	N-CA-C	5.00	118.96	113.21
3	A	247	ASN	CA-CB-CG	5.00	117.60	112.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	211	THR	CB
3	C	247	ASN	CA

There are no planarity outliers.

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	E	420	0	241	51	0
2	F	435	0	238	40	0
3	A	1535	0	1490	78	0
3	B	1522	0	1477	134	0
3	C	1529	0	1485	171	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	198	0	0	16	0
5	B	70	0	0	7	0
5	C	80	0	0	14	1
5	E	22	0	0	1	0
5	F	14	0	0	3	0
All	All	5828	0	4931	459	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1113:DG:H2''	2:F:1114:DT:H5''	1.33	1.08
3:B:166:SER:HB2	3:C:114:LEU:HD21	1.29	1.07
3:A:211:THR:HG23	3:A:213:ARG:HB2	1.40	1.03
1:E:1004:DC:H2'	1:E:1005:DC:C6	1.99	0.97
3:C:119:ALA:HB3	3:C:122:VAL:HG13	1.45	0.96
3:B:264:LEU:HD11	3:B:267:ARG:HG3	1.50	0.94
3:A:211:THR:CG2	3:A:213:ARG:HB2	1.96	0.94
1:E:1008:DG:H1	2:F:1115:DC:H42	0.92	0.91
3:B:163:TYR:CE1	3:B:173:VAL:HG22	2.06	0.90
3:A:209:ARG:HG3	3:A:209:ARG:HH11	1.37	0.89
3:C:280:ARG:HG2	3:C:283:ARG:NH1	1.88	0.88
3:B:104:GLN:NE2	3:B:110:ARG:HD3	1.89	0.88
3:C:197:VAL:HG12	3:C:234:TYR:CD1	2.08	0.88
2:F:1110:DC:H2''	2:F:1111:DA:C8	2.09	0.87
3:B:162:ILE:HD11	3:B:252:LEU:HD12	1.55	0.87
3:A:133:MET:HE1	3:A:236:TYR:CE1	2.11	0.86
1:E:1008:DG:H1	2:F:1115:DC:N4	1.73	0.86
3:B:273:ARG:NH1	3:B:281:ASP:OD2	2.06	0.86
3:C:175:ARG:HH12	3:C:183:SER:HB2	1.38	0.85
3:A:211:THR:HG23	3:A:213:ARG:H	1.41	0.85
3:C:224:GLU:O	3:C:227:SER:N	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:MET:SD	3:A:251:ILE:HD13	2.18	0.83
3:B:166:SER:CB	3:C:114:LEU:HD21	2.08	0.83
3:C:136:GLN:OE1	3:C:278:PRO:HD2	1.80	0.81
3:C:132:LYS:CD	3:C:271:GLU:HG2	2.11	0.81
3:C:132:LYS:HD3	3:C:271:GLU:HG2	1.63	0.81
3:C:175:ARG:HH22	3:C:183:SER:HB2	1.46	0.80
3:C:130:LEU:HD13	3:C:286:GLU:HG3	1.64	0.80
1:E:1004:DC:H2'	1:E:1005:DC:H6	1.47	0.79
2:F:1117:DA:H2''	2:F:1118:DG:OP2	1.80	0.79
3:B:101:LYS:HB3	3:B:267:ARG:NH2	1.98	0.78
3:C:175:ARG:NH1	3:C:183:SER:HB2	1.98	0.78
3:C:283:ARG:HH11	3:C:283:ARG:HB3	1.48	0.78
2:F:1113:DG:C2'	2:F:1114:DT:H5''	2.12	0.78
3:B:240:SER:O	3:B:246:MET:HB3	1.83	0.78
1:E:1001:DT:H1'	5:C:2299:HOH:O	1.82	0.78
3:C:186:ASP:O	3:C:188:LEU:N	2.16	0.78
3:C:196:ARG:HD3	3:C:237:MET:HE2	1.65	0.77
3:A:133:MET:HE1	3:A:236:TYR:HE1	1.50	0.77
3:B:119:ALA:O	3:B:279:GLY:HA3	1.85	0.77
3:C:196:ARG:HB3	3:C:205:TYR:OH	1.85	0.76
1:E:1002:DT:H3	2:F:1121:DA:H61	1.31	0.76
3:C:104:GLN:HG2	3:C:109:PHE:O	1.86	0.76
3:C:95:SER:N	3:C:211:THR:HG21	2.00	0.76
3:C:158:ARG:HH21	3:C:217:VAL:HG21	1.50	0.76
3:C:127:SER:OG	3:C:130:LEU:HB2	1.86	0.76
2:F:1106:DT:H2''	2:F:1107:DG:O5'	1.86	0.76
3:B:127:SER:HB3	3:B:130:LEU:HB2	1.67	0.75
3:C:186:ASP:O	3:C:188:LEU:HD22	1.86	0.75
3:B:121:SER:HA	3:B:277:CYS:HA	1.68	0.75
3:C:156:ARG:HD2	3:C:217:VAL:HG12	1.69	0.75
3:A:208:ASP:HB3	3:A:211:THR:HG22	1.69	0.74
3:B:207:ASP:OD1	3:B:214:HIS:ND1	2.20	0.74
3:C:119:ALA:HB3	3:C:122:VAL:CG1	2.17	0.74
3:C:156:ARG:HD2	3:C:217:VAL:CG1	2.17	0.74
3:C:140:THR:OG1	3:C:198:GLU:OE2	2.06	0.74
3:C:110:ARG:HH11	3:C:110:ARG:HB2	1.52	0.74
2:F:1120:DA:OP1	2:F:1120:DA:H3'	1.88	0.73
2:F:1108:DG:H1'	2:F:1109:DG:H5'	1.69	0.73
3:C:175:ARG:NH2	3:C:183:SER:HB2	2.04	0.73
3:A:192:GLN:HG2	5:A:2073:HOH:O	1.87	0.73
1:E:1004:DC:N4	2:F:1119:DG:O6	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:114:LEU:HD22	3:A:142:PRO:HG2	1.71	0.72
3:C:130:LEU:HD21	3:C:285:GLU:HB3	1.72	0.71
3:C:188:LEU:N	3:C:188:LEU:HD13	2.05	0.71
3:A:108:GLY:O	3:A:110:ARG:NH1	2.24	0.71
3:C:188:LEU:HD22	3:C:188:LEU:H	1.56	0.70
3:C:206:LEU:CD1	3:C:207:ASP:H	2.04	0.70
3:C:286:GLU:HA	3:C:289:LEU:HD22	1.73	0.70
1:E:1006:DT:H2'	1:E:1007:DA:C8	2.27	0.70
3:C:156:ARG:NE	3:C:217:VAL:HG11	2.06	0.69
2:F:1120:DA:H1'	2:F:1121:DA:O4'	1.92	0.69
3:B:204:GLU:HG2	3:B:205:TYR:N	2.06	0.69
3:C:118:THR:HG21	3:C:283:ARG:HB2	1.74	0.69
2:F:1120:DA:H2''	2:F:1121:DA:OP2	1.91	0.69
3:C:197:VAL:HG12	3:C:234:TYR:CE1	2.28	0.69
3:B:276:ALA:O	3:B:277:CYS:HB2	1.92	0.69
2:F:1119:DG:H2''	2:F:1120:DA:OP2	1.93	0.68
1:E:1004:DC:H2'	1:E:1005:DC:O4'	1.92	0.68
3:B:177:PRO:HB2	5:B:2294:HOH:O	1.93	0.68
3:B:167:GLN:CD	3:B:167:GLN:H	2.00	0.68
3:A:122:VAL:HG11	3:A:125:THR:HB	1.76	0.68
3:A:100:GLN:HG3	5:A:2098:HOH:O	1.93	0.68
3:C:158:ARG:HH21	3:C:217:VAL:CG2	2.07	0.68
3:B:156:ARG:NH2	3:B:258:GLU:OE2	2.27	0.67
3:A:118:THR:CG2	3:A:282:ARG:HG2	2.24	0.67
2:F:1118:DG:OP2	2:F:1118:DG:H3'	1.94	0.67
3:A:224:GLU:O	3:A:227:SER:HB2	1.95	0.67
1:E:1005:DC:H3'	1:E:1006:DT:H71	1.76	0.67
3:B:118:THR:O	3:B:283:ARG:NH2	2.28	0.67
3:A:120:LYS:HE2	5:A:2052:HOH:O	1.94	0.67
3:B:101:LYS:CA	3:B:267:ARG:HH21	2.08	0.67
3:C:126:TYR:OH	3:C:131:ASN:ND2	2.26	0.67
3:A:107:TYR:O	3:A:147:VAL:HG22	1.95	0.67
3:B:126:TYR:OH	3:B:131:ASN:ND2	2.27	0.66
3:B:168:HIS:CD2	3:B:249:ARG:HH11	2.12	0.66
3:C:132:LYS:HD3	3:C:271:GLU:CG	2.24	0.66
1:E:1010:DC:H2'	1:E:1011:DT:H72	1.77	0.66
3:B:157:VAL:O	3:B:217:VAL:HG23	1.95	0.66
3:B:287:GLU:HG2	3:B:288:ASN:N	2.00	0.66
3:A:118:THR:HG21	3:A:282:ARG:HG2	1.78	0.66
3:B:101:LYS:O	3:B:267:ARG:NH2	2.29	0.66
3:C:119:ALA:O	3:C:122:VAL:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ARG:HH12	3:C:183:SER:CB	2.08	0.66
3:B:127:SER:OG	3:B:282:ARG:NE	2.26	0.66
3:A:175:ARG:NH2	3:A:184:ASP:OD2	2.28	0.65
3:A:192:GLN:OE1	5:A:2196:HOH:O	2.13	0.65
3:C:98:PRO:O	3:C:100:GLN:NE2	2.28	0.65
3:C:280:ARG:HG2	3:C:283:ARG:HH12	1.61	0.65
3:B:167:GLN:N	3:B:167:GLN:OE1	2.30	0.65
3:A:209:ARG:HG3	3:A:209:ARG:NH1	2.11	0.65
3:C:118:THR:HB	3:C:279:GLY:O	1.96	0.65
2:F:1118:DG:H3'	2:F:1118:DG:P	2.37	0.64
3:B:202:ARG:NH1	3:B:219:PRO:HG2	2.13	0.64
3:A:267:ARG:NH1	5:A:2213:HOH:O	2.29	0.64
3:C:120:LYS:HG2	3:C:277:CYS:HB3	1.79	0.64
3:C:273:ARG:NH1	3:C:285:GLU:OE1	2.29	0.64
3:B:283:ARG:O	3:B:286:GLU:HB2	1.97	0.64
1:E:1010:DC:H2'	1:E:1011:DT:C7	2.28	0.64
3:A:189:ALA:HB2	3:A:205:TYR:CZ	2.33	0.64
1:E:1018:DA:H2''	1:E:1019:DT:OP2	1.96	0.64
1:E:1005:DC:H2'	1:E:1006:DT:C6	2.33	0.64
3:A:288:ASN:O	3:A:289:LEU:HB2	1.96	0.64
3:A:282:ARG:NH2	5:A:2186:HOH:O	2.27	0.63
3:C:196:ARG:NH1	3:C:235:ASN:OD1	2.31	0.63
3:C:246:MET:O	3:C:249:ARG:HB2	1.98	0.63
2:F:1115:DC:H5	5:F:2075:HOH:O	1.80	0.63
3:B:240:SER:HA	3:B:246:MET:HG2	1.80	0.63
3:B:251:ILE:HD11	3:B:272:VAL:HG11	1.79	0.63
3:B:214:HIS:HD2	5:B:2308:HOH:O	1.81	0.63
3:C:100:GLN:HG3	5:C:2312:HOH:O	1.98	0.63
3:C:224:GLU:O	3:C:226:GLY:N	2.31	0.63
3:B:202:ARG:HD3	5:B:2336:HOH:O	1.98	0.63
1:E:1006:DT:H2'	1:E:1007:DA:O4'	1.99	0.62
3:C:186:ASP:O	3:C:186:ASP:OD1	2.16	0.62
3:A:192:GLN:HB3	5:A:2003:HOH:O	1.99	0.62
3:A:211:THR:HG23	3:A:213:ARG:CB	2.25	0.62
3:B:132:LYS:HE3	3:B:271:GLU:OE2	2.00	0.62
3:B:205:TYR:CE2	3:B:216:VAL:HG13	2.35	0.62
3:C:141:CYS:HB2	3:C:234:TYR:O	2.00	0.62
2:F:1113:DG:H2''	2:F:1114:DT:C5'	2.19	0.62
3:C:175:ARG:CZ	3:C:183:SER:HB2	2.30	0.61
3:A:209:ARG:NH1	3:A:210:ASN:HD21	1.97	0.61
3:B:267:ARG:C	3:B:268:ASN:HD22	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:137:LEU:HD23	3:A:138:ALA:N	2.15	0.61
3:C:132:LYS:HD2	3:C:271:GLU:HG2	1.82	0.61
3:C:206:LEU:HD12	3:C:207:ASP:H	1.65	0.61
3:C:156:ARG:CZ	3:C:217:VAL:HG11	2.30	0.61
2:F:1121:DA:H2''	5:F:2138:HOH:O	2.01	0.61
3:A:209:ARG:NH1	3:A:210:ASN:ND2	2.49	0.61
3:A:211:THR:HG21	3:A:213:ARG:HB2	1.83	0.61
3:A:120:LYS:HG3	5:A:2274:HOH:O	2.00	0.60
3:B:105:GLY:O	3:B:107:TYR:N	2.34	0.60
3:B:132:LYS:CG	3:B:271:GLU:HG2	2.31	0.60
3:C:175:ARG:HH22	3:C:183:SER:CB	2.13	0.60
3:A:202:ARG:CZ	3:A:219:PRO:HG2	2.31	0.60
3:A:209:ARG:HH11	3:A:210:ASN:ND2	2.00	0.60
3:C:239:ASN:C	3:C:241:SER:H	2.09	0.60
3:C:118:THR:CB	3:C:283:ARG:HB2	2.32	0.60
3:C:134:PHE:CE1	3:C:282:ARG:HB2	2.35	0.60
3:C:175:ARG:HG3	3:C:192:GLN:O	2.01	0.60
3:C:145:LEU:HD21	3:C:232:ILE:HD11	1.83	0.60
3:C:217:VAL:HG12	3:C:218:VAL:N	2.17	0.60
3:C:241:SER:HB3	5:C:2219:HOH:O	2.01	0.60
1:E:1010:DC:H2''	1:E:1011:DT:O5'	2.00	0.60
3:C:186:ASP:OD2	3:C:196:ARG:NH2	2.35	0.60
3:C:130:LEU:CD2	3:C:285:GLU:HB3	2.31	0.60
1:E:1007:DA:H2''	1:E:1008:DG:O5'	2.02	0.60
3:A:146:TRP:CH2	3:A:228:ASP:HB2	2.36	0.59
3:B:122:VAL:O	3:B:278:PRO:HG2	2.02	0.59
3:B:118:THR:O	3:B:118:THR:HG22	2.03	0.59
5:E:2375:HOH:O	3:B:241:SER:HB3	2.03	0.59
1:E:1019:DT:OP2	1:E:1019:DT:H2'	2.01	0.59
3:B:132:LYS:HG3	3:B:271:GLU:HG2	1.84	0.59
2:F:1119:DG:O6	2:F:1120:DA:N6	2.36	0.59
3:C:197:VAL:CG2	3:C:203:VAL:HG13	2.33	0.59
1:E:1009:DA:H4'	1:E:1010:DC:OP1	2.03	0.58
3:C:281:ASP:O	3:C:285:GLU:HB2	2.04	0.58
3:C:188:LEU:O	3:C:190:PRO:HD3	2.03	0.58
3:B:183:SER:HB3	3:B:191:PRO:HB3	1.85	0.58
3:A:144:GLN:HG2	3:A:229:CYS:SG	2.43	0.58
3:B:188:LEU:HD13	3:B:203:VAL:CG1	2.34	0.58
3:C:147:VAL:HG13	3:C:149:SER:O	2.03	0.58
3:A:163:TYR:CE1	3:A:251:ILE:HD11	2.39	0.58
3:B:211:THR:C	3:B:213:ARG:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:283:ARG:HH11	3:C:283:ARG:CB	2.16	0.58
3:B:101:LYS:N	3:B:267:ARG:HH21	2.02	0.58
3:B:267:ARG:O	3:B:268:ASN:ND2	2.36	0.58
3:B:132:LYS:HD3	3:B:134:PHE:CE1	2.39	0.57
2:F:1107:DG:H2''	2:F:1108:DG:OP2	2.04	0.57
3:B:101:LYS:HB3	3:B:267:ARG:HH21	1.70	0.57
3:B:118:THR:CG2	3:B:283:ARG:HG3	2.33	0.57
3:B:118:THR:HG21	3:B:283:ARG:HG3	1.85	0.57
3:C:112:GLY:N	3:C:144:GLN:O	2.37	0.57
3:C:197:VAL:CG1	3:C:234:TYR:CE1	2.88	0.57
3:A:133:MET:HE3	3:A:135:CYS:SG	2.44	0.57
3:A:147:VAL:HG13	3:A:149:SER:O	2.03	0.57
3:B:171:GLU:CD	3:B:249:ARG:HH22	2.11	0.57
2:F:1105:DT:H2''	2:F:1106:DT:O5'	2.05	0.57
5:F:2384:HOH:O	3:B:120:LYS:HD2	2.05	0.57
3:C:176:CYS:SG	3:C:179:HIS:HB2	2.44	0.56
3:C:243:MET:HA	3:C:247:ASN:HB3	1.87	0.56
3:C:119:ALA:CB	3:C:122:VAL:HG13	2.28	0.56
3:B:188:LEU:HD13	3:B:203:VAL:HG12	1.86	0.56
3:B:208:ASP:O	3:B:212:PHE:HA	2.04	0.56
1:E:1006:DT:C2'	1:E:1007:DA:O4'	2.54	0.56
2:F:1108:DG:O6	3:B:120:LYS:NZ	2.38	0.56
3:A:94:SER:N	3:B:198:GLU:OE2	2.39	0.56
3:A:149:SER:HA	5:A:2253:HOH:O	2.04	0.56
2:F:1120:DA:OP2	2:F:1120:DA:H2'	2.05	0.56
1:E:1007:DA:H2'	1:E:1008:DG:C8	2.41	0.56
3:A:175:ARG:HH22	3:A:184:ASP:CG	2.14	0.56
2:F:1119:DG:C6	2:F:1120:DA:C6	2.95	0.55
3:C:123:THR:OG1	3:C:139:LYS:HD3	2.07	0.55
1:E:1019:DT:H2''	1:E:1020:DT:C7	2.36	0.55
3:B:175:ARG:HG2	3:B:238:CYS:SG	2.47	0.55
3:B:208:ASP:O	3:B:212:PHE:N	2.39	0.55
3:B:251:ILE:HD11	3:B:272:VAL:CG1	2.36	0.55
1:E:1015:DC:H2''	1:E:1016:DC:C5'	2.36	0.55
3:B:166:SER:HB2	3:C:114:LEU:CD2	2.21	0.55
3:C:200:ASN:ND2	3:C:218:VAL:HG22	2.22	0.55
1:E:1019:DT:C2'	1:E:1020:DT:H72	2.38	0.54
3:B:168:HIS:CD2	3:B:249:ARG:NH1	2.75	0.54
3:A:211:THR:HG21	5:A:2039:HOH:O	2.06	0.54
3:C:218:VAL:HG13	3:C:219:PRO:N	2.22	0.54
3:B:96:SER:O	3:B:97:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1004:DC:C6	1:E:1005:DC:C5	2.95	0.54
1:E:1012:DT:H2''	1:E:1013:DG:C8	2.42	0.54
1:E:1004:DC:H2'	1:E:1005:DC:C1'	2.36	0.54
3:C:118:THR:CG2	3:C:283:ARG:HB2	2.36	0.54
3:C:239:ASN:C	3:C:241:SER:N	2.65	0.54
3:B:105:GLY:C	3:B:107:TYR:H	2.16	0.54
3:A:100:GLN:HB2	3:A:254:ILE:HD12	1.89	0.53
2:F:1118:DG:OP2	2:F:1118:DG:C3'	2.55	0.53
3:B:107:TYR:CE1	3:B:151:PRO:HA	2.43	0.53
3:B:130:LEU:HB3	3:B:132:LYS:HB2	1.90	0.53
3:B:211:THR:OG1	3:B:213:ARG:HB2	2.07	0.53
3:A:132:LYS:HE2	3:A:273:ARG:HB2	1.90	0.53
3:C:156:ARG:HD2	3:C:217:VAL:HG11	1.90	0.53
3:C:156:ARG:CD	3:C:217:VAL:HG11	2.37	0.53
3:C:197:VAL:HG22	3:C:203:VAL:CG1	2.38	0.53
3:A:208:ASP:CB	3:A:211:THR:HG22	2.38	0.53
3:C:175:ARG:HD2	3:C:193:HIS:O	2.08	0.53
3:C:224:GLU:N	3:C:227:SER:HB2	2.24	0.53
1:E:1005:DC:C4	1:E:1006:DT:H73	2.44	0.53
1:E:1005:DC:C2	1:E:1006:DT:C7	2.91	0.53
1:E:1004:DC:C2'	1:E:1005:DC:O4'	2.58	0.52
3:A:213:ARG:NH2	5:A:2169:HOH:O	2.27	0.52
3:B:251:ILE:HG13	3:B:272:VAL:HG12	1.91	0.52
3:B:251:ILE:HG13	3:B:272:VAL:CG1	2.39	0.52
3:C:123:THR:O	3:C:135:CYS:HA	2.08	0.52
3:C:123:THR:O	3:C:278:PRO:HG2	2.09	0.52
3:C:130:LEU:CD1	3:C:286:GLU:HG3	2.37	0.52
3:B:101:LYS:H	3:B:267:ARG:HH21	1.57	0.52
3:A:209:ARG:HH11	3:A:209:ARG:CG	2.16	0.52
3:C:175:ARG:HD3	3:C:191:PRO:O	2.10	0.52
3:A:133:MET:CE	3:A:236:TYR:CE1	2.89	0.52
3:C:176:CYS:O	3:C:180:GLU:HB2	2.10	0.52
3:B:104:GLN:HE22	3:B:110:ARG:HD3	1.67	0.52
3:C:178:HIS:C	3:C:178:HIS:CD2	2.82	0.52
3:B:203:VAL:CG2	3:B:216:VAL:HG12	2.40	0.52
3:B:163:TYR:CD1	3:B:173:VAL:HG22	2.46	0.51
3:C:150:THR:O	3:C:150:THR:HG22	2.10	0.51
3:A:168:HIS:HD2	5:A:2243:HOH:O	1.93	0.51
3:B:188:LEU:O	3:B:190:PRO:HD3	2.10	0.51
3:B:105:GLY:C	3:B:107:TYR:N	2.69	0.51
3:A:122:VAL:HG13	5:A:2233:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:ARG:NH1	3:C:219:PRO:HG2	2.26	0.51
3:C:193:HIS:HE1	3:C:206:LEU:O	1.93	0.51
3:B:272:VAL:HG22	3:B:273:ARG:N	2.26	0.51
3:A:158:ARG:HH11	3:A:258:GLU:CD	2.19	0.51
3:A:209:ARG:NH1	3:A:209:ARG:CG	2.74	0.51
2:F:1118:DG:H4'	2:F:1119:DG:OP1	2.11	0.51
3:B:101:LYS:CB	3:B:267:ARG:HH21	2.23	0.51
3:B:251:ILE:CD1	3:B:272:VAL:CG1	2.89	0.51
1:E:1006:DT:O5'	1:E:1007:DA:OP2	2.29	0.50
3:B:200:ASN:C	3:B:202:ARG:H	2.19	0.50
3:C:100:GLN:CG	5:C:2312:HOH:O	2.59	0.50
3:C:200:ASN:HD21	3:C:219:PRO:HD2	1.74	0.50
3:B:127:SER:O	3:B:131:ASN:N	2.44	0.50
1:E:1010:DC:H2'	1:E:1011:DT:C5	2.45	0.50
3:C:107:TYR:CE1	3:C:151:PRO:HA	2.46	0.50
3:C:132:LYS:HE2	3:C:285:GLU:OE2	2.12	0.50
3:B:120:LYS:O	3:B:121:SER:HB2	2.12	0.50
3:B:174:ARG:HD2	5:B:2036:HOH:O	2.11	0.50
2:F:1120:DA:H1'	2:F:1121:DA:C8	2.46	0.50
3:B:132:LYS:HD3	3:B:134:PHE:CZ	2.47	0.50
3:C:197:VAL:HG22	3:C:203:VAL:HG11	1.94	0.50
3:B:132:LYS:NZ	3:B:285:GLU:OE1	2.44	0.49
3:C:224:GLU:HB3	3:C:227:SER:OG	2.12	0.49
3:A:158:ARG:NH1	3:A:258:GLU:OE1	2.45	0.49
3:A:273:ARG:NH1	3:A:281:ASP:CG	2.71	0.49
3:B:101:LYS:HB3	3:B:267:ARG:HH22	1.74	0.49
2:F:1116:DT:H2'	2:F:1117:DA:C8	2.48	0.49
3:C:123:THR:HG22	3:C:124:CYS:N	2.27	0.49
3:C:206:LEU:HD13	3:C:207:ASP:H	1.76	0.49
2:F:1106:DT:H4'	2:F:1107:DG:OP1	2.13	0.49
3:C:132:LYS:HD3	3:C:271:GLU:CD	2.38	0.49
3:C:233:HIS:ND1	5:C:2354:HOH:O	2.35	0.49
3:C:196:ARG:HB3	3:C:205:TYR:HH	1.76	0.49
2:F:1103:DA:H2''	2:F:1104:DA:OP2	2.12	0.49
3:B:114:LEU:HD23	3:B:114:LEU:N	2.27	0.49
3:C:108:GLY:O	3:C:110:ARG:NH1	2.46	0.48
3:C:175:ARG:HB3	3:C:238:CYS:SG	2.53	0.48
3:C:218:VAL:CG1	3:C:219:PRO:N	2.76	0.48
1:E:1005:DC:C2	1:E:1006:DT:C5	3.01	0.48
3:C:123:THR:CG2	3:C:124:CYS:N	2.76	0.48
3:C:163:TYR:HB3	5:C:2352:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:277:CYS:N	3:C:278:PRO:CD	2.75	0.48
2:F:1119:DG:C6	2:F:1120:DA:N6	2.82	0.48
1:E:1004:DC:C2'	1:E:1005:DC:C6	2.86	0.48
1:E:1005:DC:H2'	1:E:1005:DC:O2	2.13	0.48
3:B:213:ARG:NH2	5:B:2377:HOH:O	2.45	0.48
1:E:1006:DT:P	1:E:1006:DT:H3'	2.54	0.48
2:F:1106:DT:H2'	2:F:1107:DG:C8	2.48	0.47
3:B:155:THR:HA	3:B:258:GLU:O	2.14	0.47
3:C:182:CYS:SG	3:C:183:SER:N	2.87	0.47
3:C:145:LEU:CD2	3:C:232:ILE:HD11	2.44	0.47
3:C:192:GLN:OE1	3:C:214:HIS:CE1	2.67	0.47
3:A:211:THR:HG23	3:A:213:ARG:N	2.20	0.47
3:A:224:GLU:O	3:A:227:SER:CB	2.63	0.47
3:C:163:TYR:CE2	3:C:173:VAL:HG22	2.49	0.47
3:C:223:PRO:HB3	3:C:229:CYS:C	2.39	0.47
1:E:1010:DC:H2'	1:E:1011:DT:C6	2.50	0.47
3:B:103:TYR:O	3:B:266:GLY:HA2	2.15	0.47
3:B:109:PHE:O	3:B:110:ARG:HG3	2.14	0.47
3:C:130:LEU:HD11	3:C:289:LEU:CD2	2.45	0.47
3:C:208:ASP:HB3	3:C:211:THR:OG1	2.15	0.47
3:C:137:LEU:HB2	3:C:239:ASN:ND2	2.29	0.47
1:E:1017:DA:C2	2:F:1107:DG:C2	3.02	0.47
3:B:125:THR:HG22	3:B:134:PHE:HB2	1.96	0.47
3:B:259:ASP:C	3:B:261:SER:N	2.72	0.47
3:C:193:HIS:CE1	3:C:206:LEU:O	2.68	0.46
3:A:256:THR:HG21	5:A:2119:HOH:O	2.16	0.46
3:B:208:ASP:O	3:B:212:PHE:CA	2.63	0.46
1:E:1004:DC:N3	2:F:1119:DG:N1	2.57	0.46
3:A:100:GLN:HB2	3:A:254:ILE:CD1	2.45	0.46
3:A:114:LEU:HD22	3:A:142:PRO:CG	2.44	0.46
3:A:224:GLU:CD	3:A:224:GLU:H	2.23	0.46
3:B:132:LYS:HE2	3:B:273:ARG:HB2	1.96	0.46
3:B:174:ARG:HA	5:B:2308:HOH:O	2.15	0.46
3:C:134:PHE:CD1	3:C:134:PHE:N	2.82	0.46
3:C:174:ARG:HE	3:C:192:GLN:NE2	2.14	0.46
3:B:205:TYR:CD2	3:B:216:VAL:HG13	2.51	0.46
3:A:273:ARG:NH1	3:A:281:ASP:OD2	2.48	0.46
3:C:165:GLN:HB3	5:C:2362:HOH:O	2.15	0.46
3:C:175:ARG:NH2	3:C:183:SER:CB	2.77	0.46
3:C:225:VAL:HG12	3:C:226:GLY:N	2.31	0.46
3:C:174:ARG:NE	3:C:192:GLN:NE2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ARG:HE	3:C:192:GLN:CD	2.24	0.45
3:C:181:ARG:NH1	5:C:2117:HOH:O	2.48	0.45
3:B:158:ARG:NH1	3:B:215:SER:OG	2.49	0.45
3:B:171:GLU:OE1	3:B:249:ARG:NH1	2.39	0.45
3:A:163:TYR:CE2	3:A:173:VAL:HG22	2.51	0.45
3:B:132:LYS:HG3	3:B:271:GLU:CG	2.46	0.45
1:E:1019:DT:H2''	1:E:1020:DT:C6	2.51	0.45
3:A:137:LEU:HD23	3:A:138:ALA:H	1.81	0.45
3:A:158:ARG:NH2	5:A:2174:HOH:O	2.31	0.45
3:C:186:ASP:C	3:C:188:LEU:H	2.24	0.45
3:C:200:ASN:OD1	3:C:202:ARG:N	2.46	0.45
3:B:118:THR:HG21	3:B:283:ARG:CG	2.47	0.45
3:C:174:ARG:HD2	5:C:2180:HOH:O	2.17	0.45
1:E:1005:DC:N1	1:E:1006:DT:H71	2.32	0.44
3:B:193:HIS:CE1	3:B:214:HIS:HB3	2.52	0.44
3:B:246:MET:HG2	5:B:2373:HOH:O	2.17	0.44
3:C:189:ALA:HA	3:C:190:PRO:HD2	1.83	0.44
3:C:284:THR:O	3:C:287:GLU:N	2.45	0.44
3:C:137:LEU:HD12	3:C:239:ASN:N	2.31	0.44
3:A:169:MET:HE1	5:A:2170:HOH:O	2.18	0.44
3:A:284:THR:O	3:A:287:GLU:HB3	2.16	0.44
3:C:221:GLU:HA	3:C:222:PRO:HD2	1.67	0.44
3:C:147:VAL:HG11	3:C:151:PRO:HD3	2.00	0.44
3:C:237:MET:HE2	5:C:2272:HOH:O	2.16	0.44
3:C:197:VAL:HG13	3:C:216:VAL:HG21	1.99	0.44
3:C:206:LEU:CD1	3:C:207:ASP:N	2.79	0.44
1:E:1015:DC:H2''	1:E:1016:DC:O5'	2.17	0.44
3:A:175:ARG:HG2	3:A:238:CYS:HB2	2.00	0.44
3:A:211:THR:C	3:A:213:ARG:H	2.25	0.44
3:B:114:LEU:CD2	3:B:144:GLN:NE2	2.81	0.44
3:B:207:ASP:CG	3:B:214:HIS:HD1	2.26	0.44
3:C:127:SER:O	3:C:131:ASN:N	2.50	0.44
3:C:186:ASP:OD2	3:C:196:ARG:CZ	2.65	0.44
2:F:1120:DA:H2'	2:F:1120:DA:P	2.58	0.43
3:B:224:GLU:O	3:B:225:VAL:C	2.60	0.43
3:B:256:THR:O	3:B:256:THR:HG22	2.18	0.43
3:B:272:VAL:O	3:B:272:VAL:HG13	2.17	0.43
3:A:137:LEU:CD2	3:A:138:ALA:N	2.81	0.43
3:C:137:LEU:HD12	3:C:238:CYS:C	2.43	0.43
3:C:171:GLU:OE1	3:C:249:ARG:NH2	2.52	0.43
3:C:197:VAL:CG2	3:C:203:VAL:CG1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:240:SER:O	3:A:248:ARG:N	2.31	0.43
3:B:200:ASN:C	3:B:202:ARG:N	2.76	0.43
3:C:259:ASP:C	3:C:259:ASP:OD1	2.61	0.43
3:C:261:SER:HB2	3:C:263:ASN:OD1	2.18	0.43
3:C:145:LEU:HD22	3:C:232:ILE:CG1	2.48	0.43
3:C:268:ASN:HB3	5:C:2325:HOH:O	2.17	0.43
1:E:1009:DA:C2	1:E:1010:DC:C2	3.06	0.43
3:B:210:ASN:O	3:C:201:LEU:HD11	2.19	0.43
3:C:123:THR:O	3:C:278:PRO:CG	2.66	0.43
3:B:200:ASN:O	3:B:202:ARG:N	2.51	0.43
2:F:1108:DG:C1'	2:F:1109:DG:H5'	2.43	0.43
3:B:103:TYR:CD2	3:B:264:LEU:HD21	2.53	0.43
3:C:115:HIS:CD2	3:C:115:HIS:N	2.87	0.43
3:C:203:VAL:HG12	3:C:216:VAL:HG23	2.01	0.43
3:C:217:VAL:HG12	3:C:218:VAL:H	1.82	0.43
3:C:134:PHE:CZ	3:C:282:ARG:HA	2.54	0.43
1:E:1015:DC:H2''	1:E:1016:DC:H5'	1.99	0.42
3:B:259:ASP:O	3:B:262:GLY:N	2.46	0.42
3:C:147:VAL:CG1	3:C:149:SER:O	2.67	0.42
1:E:1005:DC:C3'	1:E:1006:DT:H71	2.45	0.42
3:B:101:LYS:C	3:B:267:ARG:HH21	2.26	0.42
3:C:132:LYS:HG3	3:C:133:MET:N	2.32	0.42
3:A:197:VAL:HB	3:A:203:VAL:HG21	2.01	0.42
3:C:206:LEU:HD12	3:C:207:ASP:N	2.33	0.42
3:B:254:ILE:HD13	3:B:254:ILE:HG21	1.83	0.42
2:F:1119:DG:H1'	2:F:1120:DA:O5'	2.20	0.42
3:B:132:LYS:HG2	3:B:271:GLU:HG2	2.02	0.42
3:C:137:LEU:HB2	3:C:239:ASN:HD21	1.84	0.42
3:C:280:ARG:HG2	3:C:283:ARG:CZ	2.49	0.42
2:F:1108:DG:N7	3:B:120:LYS:NZ	2.64	0.42
3:B:259:ASP:C	3:B:261:SER:H	2.27	0.42
3:B:201:LEU:HA	3:B:201:LEU:HD23	1.82	0.42
3:A:177:PRO:HA	3:A:180:GLU:HG2	2.01	0.42
3:B:284:THR:C	3:B:286:GLU:H	2.28	0.42
3:C:186:ASP:C	3:C:188:LEU:N	2.77	0.42
3:C:240:SER:HA	3:C:246:MET:HE3	2.02	0.42
3:B:247:ASN:O	3:B:248:ARG:HB2	2.19	0.42
3:B:130:LEU:HA	3:B:130:LEU:HD13	1.75	0.42
3:C:130:LEU:HD11	3:C:289:LEU:HD22	2.02	0.42
1:E:1005:DC:H2'	1:E:1006:DT:H6	1.82	0.41
3:B:120:LYS:O	3:B:121:SER:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:173:VAL:CG1	3:B:246:MET:HE1	2.50	0.41
1:E:1016:DC:H2''	1:E:1017:DA:OP2	2.20	0.41
3:B:127:SER:OG	3:B:282:ARG:HG3	2.19	0.41
3:B:285:GLU:HG2	3:B:285:GLU:O	2.20	0.41
3:B:157:VAL:O	3:B:217:VAL:HA	2.20	0.41
1:E:1012:DT:OP2	3:B:273:ARG:NH2	2.54	0.41
3:A:132:LYS:HE3	3:A:271:GLU:OE2	2.20	0.41
3:A:137:LEU:CD2	3:A:137:LEU:C	2.94	0.41
3:B:264:LEU:CD1	3:B:267:ARG:HG3	2.34	0.41
3:C:142:PRO:HG3	5:C:2354:HOH:O	2.20	0.41
3:C:197:VAL:HG12	3:C:234:TYR:HD1	1.78	0.41
1:E:1006:DT:H3'	1:E:1006:DT:OP2	2.21	0.41
3:B:101:LYS:H	3:B:267:ARG:NH2	2.17	0.41
3:B:286:GLU:O	3:B:289:LEU:N	2.52	0.41
3:C:106:SER:N	5:C:2339:HOH:O	2.27	0.41
1:E:1001:DT:C2'	1:E:1002:DT:OP2	2.68	0.41
3:A:208:ASP:HB3	3:A:211:THR:CG2	2.45	0.41
3:C:283:ARG:HH11	3:C:283:ARG:CG	2.34	0.40
3:A:177:PRO:O	3:A:178:HIS:C	2.65	0.40
3:A:212:PHE:CE2	3:B:185:SER:HB2	2.56	0.40
3:B:165:GLN:O	3:B:169:MET:HG3	2.21	0.40
1:E:1002:DT:H2''	1:E:1003:DT:O4'	2.21	0.40
3:C:106:SER:O	5:C:2338:HOH:O	2.22	0.40
3:C:118:THR:HG21	3:C:283:ARG:CB	2.48	0.40
3:C:203:VAL:CG1	3:C:216:VAL:HG23	2.52	0.40
3:B:251:ILE:CG1	3:B:272:VAL:CG1	3.00	0.40
2:F:1116:DT:H2''	2:F:1117:DA:O4'	2.21	0.40
3:B:114:LEU:HD21	3:B:144:GLN:HE21	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2313:HOH:O	5:C:2313:HOH:O[2_657]	1.91	0.29

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	194/219 (89%)	189 (97%)	4 (2%)	1 (0%)	24	27
3	B	192/219 (88%)	171 (89%)	17 (9%)	4 (2%)	5	3
3	C	193/219 (88%)	167 (86%)	22 (11%)	4 (2%)	5	3
All	All	579/657 (88%)	527 (91%)	43 (7%)	9 (2%)	7	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	225	VAL
3	C	187	GLY
3	C	225	VAL
3	B	106	SER
3	B	201	LEU
3	C	182	CYS
3	C	242	CYS
3	B	121	SER
3	B	98	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	176/196 (90%)	143 (81%)	33 (19%)	1	1
3	B	173/196 (88%)	145 (84%)	28 (16%)	2	2
3	C	175/196 (89%)	121 (69%)	54 (31%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	524/588 (89%)	409 (78%)	115 (22%)	1 1

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	95	SER
3	A	96	SER
3	A	97	VAL
3	A	99	SER
3	A	100	GLN
3	A	101	LYS
3	A	106	SER
3	A	114	LEU
3	A	120	LYS
3	A	121	SER
3	A	123	THR
3	A	130	LEU
3	A	137	LEU
3	A	139	LYS
3	A	144	GLN
3	A	145	LEU
3	A	147	VAL
3	A	169	MET
3	A	192	GLN
3	A	194	LEU
3	A	213	ARG
3	A	217	VAL
3	A	225	VAL
3	A	227	SER
3	A	228	ASP
3	A	251	ILE
3	A	252	LEU
3	A	272	VAL
3	A	282	ARG
3	A	283	ARG
3	A	287	GLU
3	A	288	ASN
3	A	289	LEU
3	B	99	SER
3	B	102	THR
3	B	106	SER
3	B	111	LEU

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Mol	Chain	Res	Type
3	B	123	THR
3	B	125	THR
3	B	127	SER
3	B	130	LEU
3	B	149	SER
3	B	160	MET
3	B	167	GLN
3	B	170	THR
3	B	188	LEU
3	B	194	LEU
3	B	206	LEU
3	B	207	ASP
3	B	213	ARG
3	B	216	VAL
3	B	218	VAL
3	B	225	VAL
3	B	232	ILE
3	B	246	MET
3	B	256	THR
3	B	259	ASP
3	B	264	LEU
3	B	267	ARG
3	B	287	GLU
3	B	288	ASN
3	C	95	SER
3	C	97	VAL
3	C	100	GLN
3	C	110	ARG
3	C	114	LEU
3	C	115	HIS
3	C	116	SER
3	C	122	VAL
3	C	123	THR
3	C	127	SER
3	C	132	LYS
3	C	134	PHE
3	C	136	GLN
3	C	137	LEU
3	C	140	THR
3	C	145	LEU
3	C	147	VAL
3	C	149	SER

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Mol	Chain	Res	Type
3	C	150	THR
3	C	162	ILE
3	C	166	SER
3	C	167	GLN
3	C	174	ARG
3	C	180	GLU
3	C	185	SER
3	C	188	LEU
3	C	196	ARG
3	C	198	GLU
3	C	202	ARG
3	C	203	VAL
3	C	204	GLU
3	C	206	LEU
3	C	207	ASP
3	C	213	ARG
3	C	215	SER
3	C	218	VAL
3	C	221	GLU
3	C	225	VAL
3	C	228	ASP
3	C	232	ILE
3	C	238	CYS
3	C	240	SER
3	C	241	SER
3	C	248	ARG
3	C	249	ARG
3	C	252	LEU
3	C	255	ILE
3	C	258	GLU
3	C	261	SER
3	C	264	LEU
3	C	269	SER
3	C	283	ARG
3	C	286	GLU
3	C	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	131	ASN
3	A	144	GLN

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Mol	Chain	Res	Type
3	A	168	HIS
3	A	192	GLN
3	A	210	ASN
3	A	235	ASN
3	A	247	ASN
3	A	288	ASN
3	B	100	GLN
3	B	104	GLN
3	B	131	ASN
3	B	168	HIS
3	B	178	HIS
3	B	210	ASN
3	B	233	HIS
3	B	268	ASN
3	B	288	ASN
3	C	115	HIS
3	C	131	ASN
3	C	178	HIS
3	C	193	HIS
3	C	214	HIS
3	C	239	ASN
3	C	247	ASN
3	C	263	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.