



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 1TSR / pdb_00001tsr
Title : P53 CORE DOMAIN IN COMPLEX WITH DNA
Authors : Cho, Y.; Gorina, S.; Jeffrey, P.; Pavletich, N.
Deposited on : 1995-07-28
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

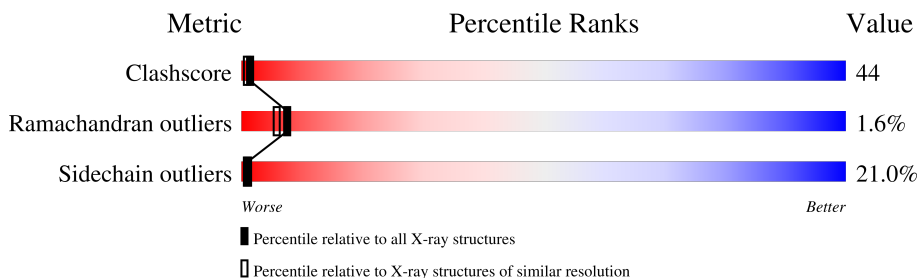
1 Overall quality at a glance

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% 43% 48%
2	F	21	10% 57% 33%
3	A	219	49% 30% 9% • 11%
3	B	219	33% 42% 12% • 11%
3	C	219	26% 41% 19% • 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	23	Total 23	O 23	0	0
5	F	14	Total 14	O 14	0	0
5	A	198	Total 198	O 198	0	0
5	B	71	Total 71	O 71	0	0
5	C	78	Total 78	O 78	0	0

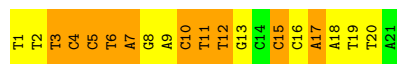
3 Residue-property plots

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.

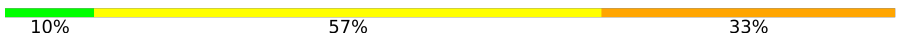
Note EDS was not executed.

- 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: 



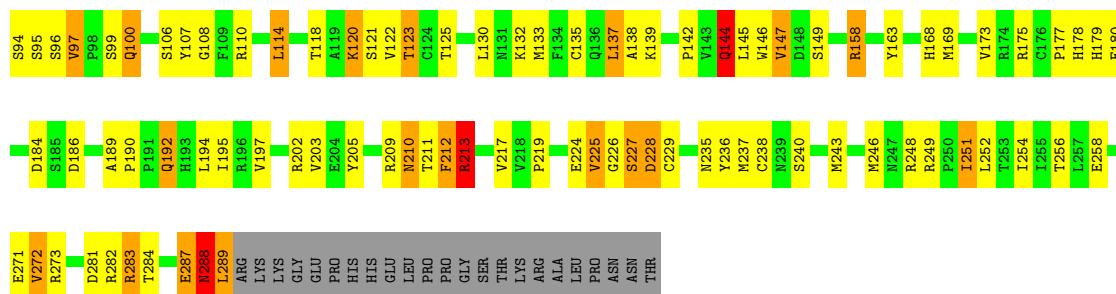
- Molecule 2: DNA (5'-D(*AP*TP*AP*AP*TP*TP*GP*GP*GP*CP*AP*AP*GP*TP*CP*TP*A P*GP*GP*AP*A)-3')

Chain F: 

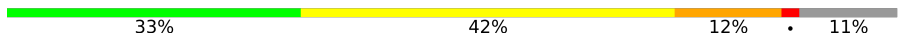


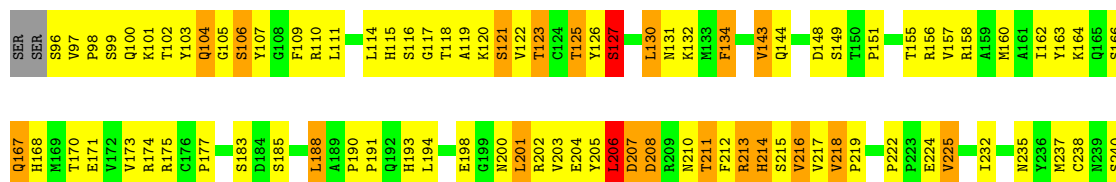
- Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

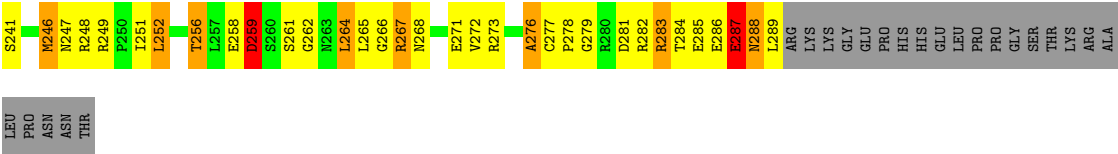
Chain A: 



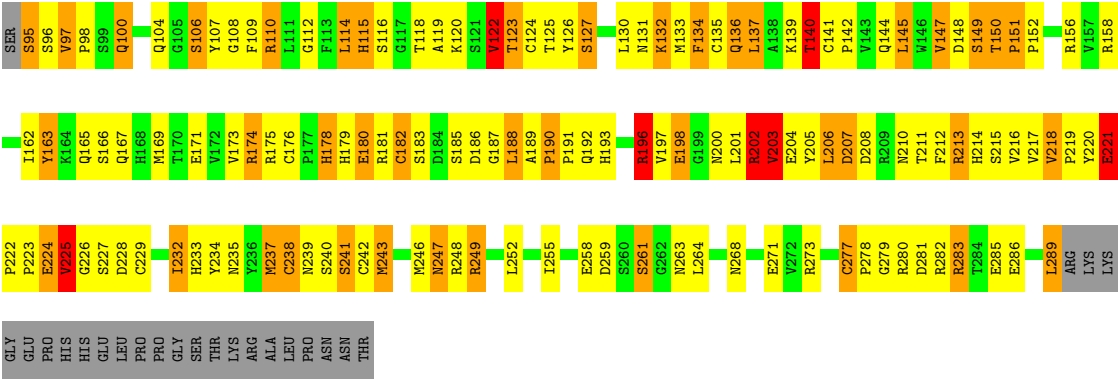
- Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

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	117.50 Å 67.90 Å 108.80 Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	85.7 (6.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.205 , (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	0.50	0/468	1.39	12/719 (1.7%)
2	F	0.52	0/490	1.44	10/756 (1.3%)
3	A	0.99	1/1570 (0.1%)	1.58	21/2129 (1.0%)
3	B	0.99	0/1557	1.79	31/2112 (1.5%)
3	C	0.97	0/1563	1.82	30/2118 (1.4%)
All	All	0.92	1/5648 (0.0%)	1.68	104/7834 (1.3%)

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
3	C	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	210	ASN	C-N	6.95	1.44	1.33

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	95	SER	N-CA-C	-19.80	55.57	111.00
3	C	95	SER	CA-C-O	17.21	150.06	120.80
3	B	218	VAL	N-CA-CB	-10.12	104.85	111.83
3	B	116	SER	N-CA-C	10.10	124.11	111.69
3	B	214	HIS	CA-CB-CG	9.81	123.61	113.80
3	B	104	GLN	N-CA-C	-9.68	90.17	110.80
3	C	212	PHE	CA-CB-CG	-8.91	104.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	117	GLY	N-CA-C	-8.62	103.25	112.04
3	C	237	MET	N-CA-C	8.31	122.84	112.87
3	C	178	HIS	CA-CB-CG	-8.29	105.51	113.80
3	B	222	PRO	N-CA-CB	8.11	107.73	103.19
2	F	14	DT	P-O5'-C5'	-8.07	107.89	120.00
1	E	15	DC	P-O3'-C3'	8.07	132.30	120.20
3	C	247	ASN	N-CA-C	8.01	122.19	111.30
3	C	220	TYR	N-CA-CB	7.83	121.65	109.83
2	F	18	DG	P-O3'-C3'	7.68	131.72	120.20
3	C	169	MET	N-CA-C	7.61	120.24	111.11
3	B	259	ASP	N-CA-CB	7.50	122.46	110.46
3	A	237	MET	N-CA-C	7.48	121.25	112.72
2	F	7	DG	P-O3'-C3'	7.38	131.27	120.20
3	C	148	ASP	CA-CB-CG	-7.29	105.31	112.60
2	F	16	DT	P-O3'-C3'	7.10	130.85	120.20
1	E	3	DT	P-O3'-C3'	7.06	130.78	120.20
3	C	151	PRO	CA-C-N	7.05	124.81	119.66
3	C	151	PRO	C-N-CA	7.05	124.81	119.66
2	F	18	DG	C4'-C3'-O3'	6.89	120.33	110.00
3	A	97	VAL	N-CA-CB	-6.88	104.30	111.87
3	A	186	ASP	N-CA-C	-6.84	104.81	113.02
3	C	247	ASN	N-CA-CB	6.81	121.36	111.62
3	B	237	MET	N-CA-C	6.73	121.34	113.20
3	C	221	GLU	CA-C-N	6.59	124.47	119.66
3	C	221	GLU	C-N-CA	6.59	124.47	119.66
3	B	123	THR	N-CA-C	6.58	118.12	111.07
3	A	288	ASN	CA-CB-CG	6.46	119.06	112.60
3	A	179	HIS	N-CA-C	6.44	117.96	111.07
3	C	106	SER	N-CA-C	6.44	120.71	112.34
3	A	249	ARG	CA-C-N	6.43	126.65	119.90
3	A	249	ARG	C-N-CA	6.43	126.65	119.90
3	B	265	LEU	N-CA-CB	6.31	119.45	110.67
1	E	10	DC	P-O3'-C3'	-6.25	110.83	120.20
2	F	12	DA	P-O3'-C3'	-6.24	110.85	120.20
3	A	235	ASN	CA-CB-CG	6.09	118.69	112.60
3	B	143	VAL	CA-CB-CG1	6.08	120.74	110.40
3	B	206	LEU	N-CA-C	6.06	119.28	109.40
3	A	226	GLY	N-CA-C	-6.05	106.97	115.32
3	A	213	ARG	CG-CD-NE	-6.05	98.69	112.00
3	B	235	ASN	CA-CB-CG	6.01	118.61	112.60
3	B	104	GLN	CA-C-N	-5.98	115.59	122.83
3	B	104	GLN	C-N-CA	-5.98	115.59	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	DA	P-O5'-C5'	5.97	128.96	120.00
3	B	283	ARG	CA-C-N	5.93	129.04	120.79
3	B	283	ARG	C-N-CA	5.93	129.04	120.79
3	C	277	CYS	CA-C-N	5.90	127.21	119.84
3	C	277	CYS	C-N-CA	5.90	127.21	119.84
3	B	115	HIS	CA-CB-CG	-5.86	107.94	113.80
1	E	3	DT	O4'-C1'-N1	5.84	117.16	108.40
3	B	276	ALA	N-CA-C	-5.84	100.16	109.96
3	A	213	ARG	CD-NE-CZ	5.81	132.54	124.40
1	E	11	DT	P-O5'-C5'	5.81	128.71	120.00
3	A	144	GLN	N-CA-C	5.79	118.68	109.24
3	A	123	THR	N-CA-CB	-5.76	102.06	110.53
3	C	243	MET	CA-C-N	-5.76	113.04	122.20
3	C	243	MET	C-N-CA	-5.76	113.04	122.20
1	E	5	DC	P-O3'-C3'	5.73	128.79	120.20
3	A	212	PHE	CA-CB-CG	5.69	119.49	113.80
3	A	243	MET	CA-C-N	-5.68	113.59	122.51
3	A	243	MET	C-N-CA	-5.68	113.59	122.51
3	C	196	ARG	N-CA-CB	5.66	121.39	111.55
3	B	287	GLU	N-CA-C	-5.64	105.22	111.71
3	C	203	VAL	CB-CA-C	-5.63	103.97	111.13
1	E	17	DA	P-O3'-C3'	5.61	128.61	120.20
3	C	163	TYR	N-CA-CB	5.60	118.23	110.17
3	C	122	VAL	N-CA-CB	5.56	118.28	111.60
3	A	283	ARG	CA-C-N	5.46	127.85	120.65
3	A	283	ARG	C-N-CA	5.46	127.85	120.65
3	B	143	VAL	CA-CB-CG2	5.45	119.67	110.40
3	C	224	GLU	N-CA-C	5.43	118.45	110.30
3	B	206	LEU	N-CA-CB	5.41	120.24	110.83
3	B	134	PHE	CA-CB-CG	5.40	119.20	113.80
2	F	19	DG	C1'-O4'-C4'	-5.36	101.66	109.70
3	C	140	THR	N-CA-C	5.36	117.48	108.96
3	B	127	SER	CA-C-N	5.32	125.39	119.32
3	B	127	SER	C-N-CA	5.32	125.39	119.32
3	B	211	THR	N-CA-C	-5.32	107.80	114.56
3	A	195	ILE	N-CA-C	5.30	115.59	108.17
3	C	152	PRO	O-C-N	5.26	123.73	121.31
3	B	100	GLN	N-CA-C	-5.21	103.79	111.81
3	B	252	LEU	CB-CA-C	-5.18	99.47	109.37
3	C	213	ARG	N-CA-CB	5.17	117.57	109.97
3	A	158	ARG	N-CA-CB	-5.15	101.88	110.83
3	A	190	PRO	N-CA-CB	5.12	108.05	103.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	19	DG	C5'-C4'-O4'	5.12	117.07	109.40
2	F	19	DG	C5'-C4'-C3'	5.09	122.53	114.90
3	B	208	ASP	N-CA-CB	5.09	117.63	109.28
3	B	218	VAL	CA-C-N	-5.09	114.71	119.85
3	B	218	VAL	C-N-CA	-5.09	114.71	119.85
3	C	190	PRO	CA-C-N	5.08	125.37	119.47
3	C	190	PRO	C-N-CA	5.08	125.37	119.47
1	E	12	DT	P-O3'-C3'	5.07	127.80	120.20
3	C	202	ARG	N-CA-C	5.04	119.01	113.21
1	E	6	DT	C5'-C4'-C3'	-5.03	107.36	114.90
1	E	3	DT	C4'-C3'-O3'	5.02	117.53	110.00
2	F	13	DG	P-O3'-C3'	5.01	127.71	120.20
1	E	4	DC	N1-C1'-C2'	5.00	121.00	113.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
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	48	0
2	F	435	0	238	39	0
3	A	1535	0	1490	71	0
3	B	1522	0	1477	132	0
3	C	1529	0	1484	176	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	15	0
5	B	71	0	0	8	0
5	C	78	0	0	14	1
5	E	23	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	14	0	0	4	0
All	All	5828	0	4930	453	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 44.

All (453) 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:C:95:SER:O	3:C:96:SER:HA	1.52	1.09
3:B:166:SER:HB2	3:C:114:LEU:HD21	1.29	1.08
2:F:13:DG:H2''	2:F:14:DT:H5''	1.41	1.02
3:C:119:ALA:HB3	3:C:122:VAL:HG13	1.43	0.98
1:E:4:DC:H2'	1:E:5:DC:C6	2.01	0.95
3:B:264:LEU:HD11	3:B:267:ARG:HG3	1.50	0.93
3:B:163:TYR:CE1	3:B:173:VAL:HG22	2.03	0.92
1:E:8:DG:H1	2:F:15:DC:H42	0.93	0.92
3:B:162:ILE:HD11	3:B:252:LEU:HD12	1.52	0.89
3:C:280:ARG:HG2	3:C:283:ARG:NH1	1.88	0.88
3:C:197:VAL:HG12	3:C:234:TYR:CD1	2.09	0.87
3:A:209:ARG:HG3	3:A:209:ARG:HH11	1.39	0.87
2:F:10:DC:H2''	2:F:11:DA:C8	2.09	0.87
3:C:175:ARG:HH12	3:C:183:SER:HB2	1.38	0.86
3:A:133:MET:HE1	3:A:236:TYR:CE1	2.10	0.86
3:C:95:SER:N	3:C:211:THR:HG21	1.91	0.86
3:C:132:LYS:HD3	3:C:271:GLU:HG2	1.59	0.85
3:B:166:SER:CB	3:C:114:LEU:HD21	2.06	0.84
1:E:8:DG:H1	2:F:15:DC:N4	1.76	0.84
3:B:273:ARG:NH1	3:B:281:ASP:OD2	2.10	0.83
3:C:224:GLU:O	3:C:227:SER:N	2.12	0.81
3:A:246:MET:SD	3:A:251:ILE:HD13	2.21	0.81
3:C:132:LYS:CD	3:C:271:GLU:HG2	2.12	0.80
3:C:136:GLN:OE1	3:C:278:PRO:HD2	1.81	0.80
3:C:120:LYS:HG2	3:C:277:CYS:HB3	1.64	0.79
1:E:1:DT:H1'	5:C:347:HOH:O	1.81	0.79
3:B:101:LYS:HB3	3:B:267:ARG:NH2	1.97	0.79
3:C:175:ARG:HH22	3:C:183:SER:HB2	1.48	0.79
1:E:17:DA:H2'	5:E:346:HOH:O	1.82	0.79
3:B:240:SER:O	3:B:246:MET:HB3	1.82	0.79
3:C:175:ARG:NH1	3:C:183:SER:HB2	1.98	0.78
3:C:186:ASP:O	3:C:188:LEU:HD22	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:DA:H2''	2:F:18:DG:OP2	1.81	0.78
3:C:95:SER:C	3:C:96:SER:HA	2.08	0.78
3:C:283:ARG:HH11	3:C:283:ARG:HB3	1.48	0.78
3:A:133:MET:HE1	3:A:236:TYR:HE1	1.49	0.78
3:B:104:GLN:NE2	3:B:110:ARG:HD3	1.98	0.78
3:C:186:ASP:O	3:C:188:LEU:N	2.16	0.78
3:C:130:LEU:HD13	3:C:286:GLU:HG3	1.65	0.77
3:B:119:ALA:O	3:B:279:GLY:HA3	1.84	0.77
2:F:6:DT:H2''	2:F:7:DG:O5'	1.85	0.77
2:F:8:DG:H1'	2:F:9:DG:H5'	1.66	0.77
3:C:104:GLN:HG2	3:C:109:PHE:O	1.85	0.77
3:C:196:ARG:HB3	3:C:205:TYR:OH	1.85	0.77
1:E:4:DC:H2'	1:E:5:DC:H6	1.51	0.76
3:B:121:SER:HA	3:B:277:CYS:HA	1.67	0.76
3:C:110:ARG:HH11	3:C:110:ARG:HB2	1.51	0.75
3:C:140:THR:OG1	3:C:198:GLU:OE2	2.05	0.75
3:C:188:LEU:HD22	3:C:188:LEU:H	1.51	0.75
3:B:207:ASP:OD1	3:B:214:HIS:ND1	2.20	0.74
3:C:127:SER:OG	3:C:130:LEU:HB2	1.87	0.74
1:E:2:DT:H3	2:F:21:DA:H61	1.35	0.74
3:C:196:ARG:HD3	3:C:237:MET:HE2	1.68	0.74
3:A:192:GLN:HG2	5:A:363:HOH:O	1.86	0.74
2:F:20:DA:OP1	2:F:20:DA:H3'	1.88	0.73
3:A:114:LEU:HD22	3:A:142:PRO:HG2	1.71	0.73
3:C:119:ALA:O	3:C:122:VAL:HG22	1.89	0.73
3:B:127:SER:HB3	3:B:130:LEU:HB2	1.71	0.72
3:C:158:ARG:HH21	3:C:217:VAL:HG21	1.53	0.72
3:C:119:ALA:HB3	3:C:122:VAL:CG1	2.19	0.72
3:C:95:SER:C	3:C:96:SER:N	2.48	0.71
2:F:13:DG:C2'	2:F:14:DT:H5''	2.18	0.71
3:C:156:ARG:HD2	3:C:217:VAL:HG12	1.72	0.71
3:C:175:ARG:NH2	3:C:183:SER:HB2	2.06	0.71
1:E:6:DT:H2'	1:E:7:DA:C8	2.27	0.70
3:C:156:ARG:HD2	3:C:217:VAL:CG1	2.21	0.70
1:E:4:DC:H2'	1:E:5:DC:O4'	1.91	0.69
3:C:197:VAL:HG12	3:C:234:TYR:CE1	2.27	0.69
2:F:19:DG:H2''	2:F:20:DA:OP2	1.92	0.69
2:F:20:DA:H1'	2:F:21:DA:O4'	1.92	0.69
3:C:206:LEU:CD1	3:C:207:ASP:H	2.05	0.69
3:B:126:TYR:OH	3:B:131:ASN:ND2	2.25	0.69
3:B:204:GLU:HG2	3:B:205:TYR:N	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:108:GLY:O	3:A:110:ARG:NH1	2.26	0.69
3:B:276:ALA:O	3:B:277:CYS:HB2	1.92	0.69
3:B:287:GLU:HG2	3:B:288:ASN:N	1.99	0.69
2:F:21:DA:H2''	5:F:172:HOH:O	1.92	0.68
3:C:130:LEU:HD21	3:C:285:GLU:HB3	1.74	0.68
2:F:20:DA:H2''	2:F:21:DA:OP2	1.90	0.68
3:C:156:ARG:NE	3:C:217:VAL:HG11	2.07	0.68
3:C:188:LEU:N	3:C:188:LEU:HD13	2.08	0.68
3:A:100:GLN:HG3	5:A:382:HOH:O	1.93	0.68
3:B:156:ARG:NH2	3:B:258:GLU:OE2	2.26	0.68
1:E:5:DC:H3'	1:E:6:DT:H71	1.75	0.68
3:A:107:TYR:O	3:A:147:VAL:HG22	1.94	0.68
3:A:122:VAL:HG11	3:A:125:THR:HB	1.77	0.67
3:C:132:LYS:HD3	3:C:271:GLU:CG	2.23	0.67
3:A:118:THR:HG21	3:A:282:ARG:HG2	1.77	0.67
3:C:118:THR:HG21	3:C:283:ARG:HB2	1.76	0.67
3:C:175:ARG:HH12	3:C:183:SER:CB	2.07	0.67
1:E:10:DC:H2'	1:E:11:DT:H72	1.76	0.67
3:C:95:SER:O	3:C:96:SER:CA	2.38	0.67
3:B:167:GLN:CD	3:B:167:GLN:H	2.01	0.67
3:C:118:THR:HB	3:C:279:GLY:O	1.94	0.67
3:C:126:TYR:OH	3:C:131:ASN:ND2	2.26	0.67
3:A:192:GLN:OE1	5:A:448:HOH:O	2.13	0.66
2:F:18:DG:OP2	2:F:18:DG:H3'	1.95	0.66
3:B:168:HIS:CD2	3:B:249:ARG:HH11	2.12	0.66
3:C:186:ASP:OD2	3:C:196:ARG:NH2	2.28	0.66
3:A:175:ARG:NH2	3:A:184:ASP:OD2	2.28	0.66
3:A:224:GLU:O	3:A:227:SER:HB2	1.96	0.66
3:B:127:SER:OG	3:B:282:ARG:NE	2.25	0.66
3:C:286:GLU:HA	3:C:289:LEU:HD22	1.77	0.66
2:F:15:DC:H5	5:F:81:HOH:O	1.78	0.66
3:B:157:VAL:O	3:B:217:VAL:HG23	1.96	0.66
1:E:10:DC:H2'	1:E:11:DT:C7	2.26	0.66
3:A:118:THR:CG2	3:A:282:ARG:HG2	2.26	0.66
3:B:214:HIS:HD2	5:B:357:HOH:O	1.79	0.65
3:B:118:THR:O	3:B:283:ARG:NH2	2.29	0.65
3:B:167:GLN:N	3:B:167:GLN:OE1	2.30	0.65
3:B:202:ARG:NH1	3:B:219:PRO:HG2	2.12	0.65
3:C:158:ARG:HH21	3:C:217:VAL:CG2	2.10	0.65
3:C:98:PRO:O	3:C:100:GLN:NE2	2.29	0.65
1:E:18:DA:H2''	1:E:19:DT:OP2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:120:LYS:HE2	5:A:347:HOH:O	1.97	0.64
1:E:5:DC:H2'	1:E:6:DT:C6	2.33	0.64
3:A:209:ARG:HG3	3:A:209:ARG:NH1	2.12	0.64
2:F:18:DG:H3'	2:F:18:DG:P	2.38	0.64
3:C:95:SER:C	3:C:96:SER:CA	2.70	0.64
3:A:288:ASN:O	3:A:289:LEU:HB2	1.95	0.64
3:C:280:ARG:HG2	3:C:283:ARG:HH12	1.62	0.64
3:A:282:ARG:NH2	5:A:443:HOH:O	2.28	0.64
3:B:101:LYS:O	3:B:267:ARG:NH2	2.31	0.64
3:B:205:TYR:CE2	3:B:216:VAL:HG13	2.33	0.63
3:B:283:ARG:O	3:B:286:GLU:HB2	1.98	0.63
3:B:101:LYS:CA	3:B:267:ARG:HH21	2.12	0.63
3:C:186:ASP:O	3:C:186:ASP:OD1	2.16	0.63
3:B:202:ARG:HD3	5:B:366:HOH:O	1.97	0.63
3:B:267:ARG:C	3:B:268:ASN:HD22	2.07	0.63
3:C:224:GLU:O	3:C:226:GLY:N	2.32	0.62
3:C:273:ARG:NH1	3:C:285:GLU:OE1	2.31	0.62
1:E:6:DT:H2'	1:E:7:DA:O4'	1.99	0.62
3:B:251:ILE:HD11	3:B:272:VAL:HG11	1.80	0.62
3:C:145:LEU:HD21	3:C:232:ILE:HD11	1.81	0.62
3:C:246:MET:O	3:C:249:ARG:HB2	2.00	0.62
3:A:146:TRP:CH2	3:A:228:ASP:HB2	2.33	0.62
3:C:241:SER:HB3	5:C:336:HOH:O	1.98	0.62
3:C:156:ARG:CZ	3:C:217:VAL:HG11	2.29	0.61
3:C:141:CYS:HB2	3:C:234:TYR:O	2.00	0.61
3:A:137:LEU:HD23	3:A:138:ALA:N	2.15	0.61
3:B:177:PRO:HB2	5:B:355:HOH:O	2.01	0.61
3:A:189:ALA:HB2	3:A:205:TYR:CZ	2.36	0.61
3:B:105:GLY:O	3:B:107:TYR:N	2.34	0.61
3:B:132:LYS:HE3	3:B:271:GLU:OE2	2.01	0.61
3:C:196:ARG:NH1	3:C:235:ASN:OD1	2.34	0.61
3:C:100:GLN:HG3	5:C:350:HOH:O	2.01	0.60
3:A:192:GLN:HB3	5:A:315:HOH:O	2.01	0.60
3:C:175:ARG:HG3	3:C:192:GLN:O	2.01	0.60
3:A:202:ARG:CZ	3:A:219:PRO:HG2	2.32	0.60
2:F:5:DT:H2''	2:F:6:DT:O5'	2.02	0.60
3:B:122:VAL:O	3:B:278:PRO:HG2	2.02	0.60
3:C:188:LEU:O	3:C:190:PRO:HD3	2.02	0.60
3:C:239:ASN:C	3:C:241:SER:H	2.09	0.60
3:B:183:SER:HB3	3:B:191:PRO:HB3	1.83	0.60
3:C:175:ARG:CZ	3:C:183:SER:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ARG:HH22	3:C:183:SER:CB	2.14	0.59
1:E:9:DA:H4'	1:E:10:DC:OP1	2.02	0.59
3:A:144:GLN:HG2	3:A:229:CYS:SG	2.42	0.59
1:E:10:DC:H2''	1:E:11:DT:O5'	2.01	0.59
3:A:209:ARG:HH11	3:A:210:ASN:ND2	2.01	0.59
3:C:118:THR:CB	3:C:283:ARG:HB2	2.32	0.59
3:C:130:LEU:CD2	3:C:285:GLU:HB3	2.32	0.59
3:A:133:MET:HE3	3:A:135:CYS:SG	2.43	0.59
3:A:147:VAL:HG13	3:A:149:SER:O	2.02	0.59
1:E:7:DA:H2''	1:E:8:DG:O5'	2.03	0.59
1:E:19:DT:OP2	1:E:19:DT:H2'	2.02	0.59
3:B:240:SER:HA	3:B:246:MET:HG2	1.85	0.59
3:C:134:PHE:CE1	3:C:282:ARG:HB2	2.37	0.59
3:A:120:LYS:HG3	5:A:493:HOH:O	2.03	0.58
3:B:101:LYS:N	3:B:267:ARG:HH21	2.01	0.58
3:C:197:VAL:CG2	3:C:203:VAL:HG13	2.33	0.58
3:C:217:VAL:HG12	3:C:218:VAL:N	2.18	0.58
3:A:209:ARG:NH1	3:A:210:ASN:ND2	2.52	0.58
2:F:7:DG:H2''	2:F:8:DG:OP2	2.03	0.58
3:C:283:ARG:HH11	3:C:283:ARG:CB	2.16	0.58
3:B:101:LYS:HB3	3:B:267:ARG:HH21	1.68	0.58
5:E:481:HOH:O	3:B:241:SER:HB3	2.04	0.57
3:A:211:THR:OG1	3:A:213:ARG:HB2	2.03	0.57
3:C:112:GLY:N	3:C:144:GLN:O	2.37	0.57
3:B:118:THR:O	3:B:118:THR:HG22	2.05	0.57
3:C:206:LEU:HD12	3:C:207:ASP:H	1.69	0.57
3:A:209:ARG:NH1	3:A:210:ASN:HD21	2.02	0.57
3:C:243:MET:HA	3:C:247:ASN:HB3	1.87	0.57
2:F:19:DG:O6	2:F:20:DA:N6	2.38	0.57
3:B:267:ARG:O	3:B:268:ASN:ND2	2.37	0.57
3:C:123:THR:OG1	3:C:139:LYS:HD3	2.05	0.57
3:B:163:TYR:CD1	3:B:173:VAL:HG22	2.40	0.57
3:C:197:VAL:CG1	3:C:234:TYR:CE1	2.88	0.57
3:C:281:ASP:O	3:C:285:GLU:HB2	2.05	0.57
1:E:4:DC:H2'	1:E:5:DC:C1'	2.34	0.56
1:E:6:DT:C2'	1:E:7:DA:O4'	2.53	0.56
3:B:132:LYS:HD3	3:B:134:PHE:CE1	2.41	0.56
3:B:175:ARG:HG2	3:B:238:CYS:SG	2.46	0.56
2:F:19:DG:C6	2:F:20:DA:C6	2.94	0.56
3:A:163:TYR:CE1	3:A:251:ILE:HD11	2.41	0.56
3:B:251:ILE:HD11	3:B:272:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:DG:H2''	2:F:14:DT:C5'	2.25	0.56
3:A:94:SER:N	3:B:198:GLU:OE2	2.39	0.56
3:B:132:LYS:HG3	3:B:271:GLU:HG2	1.88	0.55
3:B:211:THR:C	3:B:213:ARG:H	2.13	0.55
3:A:100:GLN:HB2	3:A:254:ILE:HD12	1.88	0.55
3:B:208:ASP:O	3:B:212:PHE:HA	2.05	0.55
3:B:208:ASP:O	3:B:212:PHE:N	2.39	0.55
3:C:132:LYS:HD2	3:C:271:GLU:HG2	1.87	0.55
3:B:132:LYS:CG	3:B:271:GLU:HG2	2.37	0.55
3:A:122:VAL:HG13	5:A:470:HOH:O	2.07	0.55
3:A:175:ARG:HH22	3:A:184:ASP:CG	2.15	0.55
3:B:107:TYR:CE1	3:B:151:PRO:HA	2.41	0.55
5:F:490:HOH:O	3:B:120:LYS:HD2	2.07	0.55
3:A:168:HIS:HD2	5:A:476:HOH:O	1.89	0.55
3:C:200:ASN:ND2	3:C:218:VAL:HG22	2.22	0.55
3:B:101:LYS:H	3:B:267:ARG:HH21	1.53	0.54
1:E:4:DC:C6	1:E:5:DC:C5	2.95	0.54
3:A:149:SER:HA	5:A:482:HOH:O	2.06	0.54
1:E:19:DT:C2'	1:E:20:DT:H72	2.38	0.54
3:C:218:VAL:HG13	3:C:219:PRO:N	2.22	0.54
3:A:132:LYS:HE2	3:A:273:ARG:HB2	1.89	0.54
3:B:188:LEU:HD13	3:B:203:VAL:HG12	1.89	0.54
3:C:147:VAL:HG13	3:C:149:SER:O	2.07	0.54
3:A:213:ARG:NH2	5:A:430:HOH:O	2.25	0.54
3:C:176:CYS:SG	3:C:179:HIS:HB2	2.46	0.54
1:E:19:DT:H2''	1:E:20:DT:C7	2.37	0.54
3:C:243:MET:O	3:C:243:MET:HG3	2.07	0.54
3:C:224:GLU:N	3:C:227:SER:HB2	2.23	0.54
1:E:7:DA:H2'	1:E:8:DG:C8	2.43	0.54
3:B:96:SER:O	3:B:97:VAL:HG23	2.08	0.54
3:B:188:LEU:HD13	3:B:203:VAL:CG1	2.38	0.54
1:E:15:DC:H2''	1:E:16:DC:C5'	2.38	0.53
3:B:105:GLY:C	3:B:107:TYR:H	2.16	0.53
3:C:239:ASN:C	3:C:241:SER:N	2.65	0.53
3:B:168:HIS:CD2	3:B:249:ARG:NH1	2.76	0.53
3:C:118:THR:CG2	3:C:283:ARG:HB2	2.38	0.53
2:F:8:DG:O6	3:B:120:LYS:NZ	2.41	0.53
3:B:114:LEU:HD23	3:B:114:LEU:N	2.23	0.53
3:C:197:VAL:HG22	3:C:203:VAL:CG1	2.38	0.53
3:B:171:GLU:CD	3:B:249:ARG:HH22	2.15	0.53
3:C:123:THR:O	3:C:135:CYS:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:DC:C2'	1:E:5:DC:O4'	2.57	0.53
3:B:213:ARG:NH2	5:B:380:HOH:O	2.41	0.53
1:E:10:DC:H2'	1:E:11:DT:C5	2.43	0.53
2:F:18:DG:OP2	2:F:18:DG:C3'	2.56	0.53
3:B:118:THR:CG2	3:B:283:ARG:HG3	2.38	0.53
3:C:202:ARG:NH1	3:C:219:PRO:HG2	2.24	0.53
3:C:175:ARG:HB3	3:C:238:CYS:SG	2.49	0.53
3:B:104:GLN:HE22	3:B:110:ARG:HD3	1.75	0.52
3:C:176:CYS:O	3:C:180:GLU:HB2	2.10	0.52
3:C:206:LEU:HD13	3:C:207:ASP:H	1.73	0.52
3:A:133:MET:CE	3:A:236:TYR:CE1	2.89	0.52
3:C:150:THR:O	3:C:150:THR:HG22	2.09	0.52
3:B:120:LYS:O	3:B:121:SER:HB2	2.10	0.52
3:B:130:LEU:HB3	3:B:132:LYS:HB2	1.91	0.52
2:F:20:DA:OP2	2:F:20:DA:H2'	2.10	0.52
3:B:200:ASN:C	3:B:202:ARG:H	2.17	0.52
3:C:175:ARG:HD2	3:C:193:HIS:O	2.10	0.52
1:E:6:DT:O5'	1:E:7:DA:OP2	2.28	0.51
3:B:132:LYS:NZ	3:B:285:GLU:OE1	2.42	0.51
3:B:105:GLY:C	3:B:107:TYR:N	2.68	0.51
3:C:197:VAL:HG22	3:C:203:VAL:HG11	1.92	0.51
3:B:127:SER:O	3:B:131:ASN:N	2.44	0.51
3:C:175:ARG:HD3	3:C:191:PRO:O	2.10	0.51
3:C:100:GLN:CG	5:C:350:HOH:O	2.59	0.51
3:C:130:LEU:CD1	3:C:286:GLU:HG3	2.38	0.51
3:C:178:HIS:C	3:C:178:HIS:CD2	2.82	0.51
3:A:158:ARG:HH11	3:A:258:GLU:CD	2.19	0.51
3:C:163:TYR:CE2	3:C:173:VAL:HG22	2.45	0.51
2:F:18:DG:H4'	2:F:19:DG:OP1	2.11	0.51
3:A:209:ARG:HH11	3:A:209:ARG:CG	2.17	0.51
3:B:251:ILE:CD1	3:B:272:VAL:CG1	2.89	0.51
3:C:119:ALA:CB	3:C:122:VAL:HG13	2.28	0.50
3:B:203:VAL:CG2	3:B:216:VAL:HG12	2.41	0.50
2:F:16:DT:H2'	2:F:17:DA:C8	2.47	0.50
3:C:108:GLY:O	3:C:110:ARG:NH1	2.45	0.50
1:E:5:DC:C4	1:E:6:DT:H73	2.46	0.50
3:B:101:LYS:CB	3:B:267:ARG:HH21	2.24	0.50
3:B:118:THR:HG21	3:B:283:ARG:HG3	1.92	0.50
3:A:209:ARG:NH1	3:A:209:ARG:CG	2.75	0.50
3:B:101:LYS:HB3	3:B:267:ARG:HH22	1.76	0.50
3:B:251:ILE:HG13	3:B:272:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:TYR:CE1	3:C:151:PRO:HA	2.46	0.50
1:E:12:DT:H2''	1:E:13:DG:C8	2.46	0.50
3:B:211:THR:OG1	3:B:213:ARG:HB2	2.11	0.50
3:C:156:ARG:CD	3:C:217:VAL:HG11	2.40	0.50
1:E:5:DC:C2	1:E:6:DT:C7	2.94	0.50
3:B:251:ILE:HG13	3:B:272:VAL:HG12	1.94	0.50
3:B:272:VAL:HG22	3:B:273:ARG:N	2.27	0.50
2:F:3:DA:H2''	2:F:4:DA:OP2	2.11	0.49
3:A:158:ARG:NH1	3:A:258:GLU:OE1	2.45	0.49
3:C:156:ARG:HD2	3:C:217:VAL:HG11	1.94	0.49
3:C:174:ARG:HE	3:C:192:GLN:NE2	2.11	0.49
3:B:273:ARG:HH12	3:B:281:ASP:CG	2.18	0.49
3:C:233:HIS:ND1	5:C:381:HOH:O	2.35	0.49
3:C:132:LYS:HE2	3:C:285:GLU:OE2	2.13	0.49
3:C:163:TYR:HB3	5:C:379:HOH:O	2.13	0.49
3:C:193:HIS:HE1	3:C:206:LEU:O	1.95	0.49
3:C:277:CYS:N	3:C:278:PRO:CD	2.75	0.48
3:A:273:ARG:NH1	3:A:281:ASP:CG	2.72	0.48
3:C:182:CYS:SG	3:C:183:SER:N	2.86	0.48
1:E:10:DC:H2'	1:E:11:DT:C6	2.49	0.48
3:B:132:LYS:HD3	3:B:134:PHE:CZ	2.49	0.48
3:B:246:MET:HG2	5:B:377:HOH:O	2.13	0.48
3:C:218:VAL:CG1	3:C:219:PRO:N	2.77	0.48
3:A:224:GLU:O	3:A:227:SER:CB	2.62	0.48
3:C:123:THR:O	3:C:278:PRO:HG2	2.14	0.48
3:A:100:GLN:HB2	3:A:254:ILE:CD1	2.43	0.47
3:C:200:ASN:HD21	3:C:219:PRO:HD2	1.78	0.47
3:C:118:THR:HG22	3:C:282:ARG:HD3	1.97	0.47
3:C:225:VAL:HG12	3:C:226:GLY:N	2.28	0.47
3:C:174:ARG:HE	3:C:192:GLN:CD	2.22	0.47
3:C:174:ARG:NE	3:C:192:GLN:NE2	2.62	0.47
3:A:163:TYR:CE2	3:A:173:VAL:HG22	2.49	0.47
3:C:130:LEU:HD11	3:C:289:LEU:CD2	2.45	0.47
1:E:5:DC:H2'	1:E:5:DC:O2	2.14	0.47
3:B:193:HIS:CE1	3:B:214:HIS:HB3	2.49	0.47
3:B:205:TYR:CD2	3:B:216:VAL:HG13	2.49	0.47
3:C:123:THR:HG22	3:C:124:CYS:N	2.29	0.47
3:C:181:ARG:NH1	5:C:322:HOH:O	2.47	0.47
3:C:192:GLN:OE1	3:C:214:HIS:CE1	2.68	0.47
3:C:237:MET:HE2	5:C:342:HOH:O	2.14	0.47
2:F:20:DA:H1'	2:F:21:DA:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:256:THR:HG21	5:A:397:HOH:O	2.15	0.47
3:B:127:SER:OG	3:B:282:ARG:HG3	2.14	0.47
3:B:259:ASP:C	3:B:261:SER:N	2.72	0.47
3:C:123:THR:CG2	3:C:124:CYS:N	2.78	0.47
3:C:145:LEU:CD2	3:C:232:ILE:HD11	2.45	0.47
1:E:17:DA:C2	2:F:7:DG:C2	3.03	0.47
3:C:208:ASP:HB3	3:C:211:THR:OG1	2.15	0.47
1:E:4:DC:C2'	1:E:5:DC:C6	2.87	0.46
3:C:193:HIS:CE1	3:C:206:LEU:O	2.69	0.46
3:C:261:SER:HB2	3:C:263:ASN:OD1	2.14	0.46
3:C:130:LEU:HD11	3:C:289:LEU:HD22	1.98	0.46
2:F:6:DT:H2'	2:F:7:DG:C8	2.50	0.46
2:F:8:DG:C1'	2:F:9:DG:H5'	2.40	0.46
2:F:19:DG:C6	2:F:20:DA:N6	2.84	0.46
3:B:158:ARG:NH1	3:B:215:SER:OG	2.48	0.46
1:E:5:DC:C2	1:E:6:DT:C5	3.04	0.46
3:B:103:TYR:O	3:B:266:GLY:HA2	2.16	0.46
3:C:223:PRO:HB3	3:C:229:CYS:C	2.41	0.46
3:C:200:ASN:OD1	3:C:202:ARG:N	2.45	0.45
3:C:186:ASP:C	3:C:188:LEU:H	2.23	0.45
3:A:175:ARG:HG2	3:A:238:CYS:HB2	1.98	0.45
3:A:212:PHE:CE2	3:B:185:SER:HB2	2.52	0.45
3:B:188:LEU:O	3:B:190:PRO:HD3	2.16	0.45
3:B:208:ASP:O	3:B:212:PHE:CA	2.64	0.45
3:B:125:THR:HG22	3:B:134:PHE:HB2	1.98	0.45
3:B:155:THR:HA	3:B:258:GLU:O	2.16	0.45
3:A:158:ARG:NH2	5:A:435:HOH:O	2.31	0.45
3:A:273:ARG:NH1	3:A:281:ASP:OD2	2.48	0.45
3:B:210:ASN:O	3:C:201:LEU:HD11	2.17	0.45
3:C:137:LEU:HB2	3:C:239:ASN:ND2	2.31	0.45
3:C:268:ASN:HB3	5:C:360:HOH:O	2.15	0.45
3:A:224:GLU:CD	3:A:224:GLU:H	2.24	0.45
3:C:137:LEU:HD12	3:C:239:ASN:N	2.30	0.45
3:B:259:ASP:C	3:B:261:SER:H	2.24	0.45
3:C:132:LYS:HD3	3:C:271:GLU:CD	2.42	0.45
3:C:147:VAL:HG11	3:C:151:PRO:HD3	1.99	0.45
1:E:9:DA:C2	1:E:10:DC:C2	3.04	0.45
3:B:132:LYS:HE2	3:B:273:ARG:HB2	1.98	0.45
3:B:200:ASN:O	3:B:202:ARG:N	2.50	0.45
3:C:175:ARG:NH2	3:C:183:SER:CB	2.78	0.45
3:A:114:LEU:HD22	3:A:142:PRO:CG	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:171:GLU:OE1	3:B:249:ARG:NH1	2.41	0.44
3:C:243:MET:O	3:C:243:MET:CG	2.65	0.44
3:B:101:LYS:H	3:B:267:ARG:NH2	2.15	0.44
3:C:174:ARG:HD2	5:C:328:HOH:O	2.17	0.44
1:E:19:DT:H2''	1:E:20:DT:C6	2.52	0.44
3:A:273:ARG:NH1	5:A:507:HOH:O	2.50	0.44
3:C:134:PHE:CD1	3:C:134:PHE:N	2.84	0.44
3:C:142:PRO:HG3	5:C:381:HOH:O	2.17	0.44
3:C:186:ASP:OD2	3:C:196:ARG:CZ	2.65	0.44
3:B:200:ASN:C	3:B:202:ARG:N	2.76	0.44
3:C:125:THR:OG1	3:C:282:ARG:NH1	2.51	0.44
3:C:197:VAL:CG2	3:C:203:VAL:CG1	2.95	0.44
3:A:209:ARG:HH11	3:A:210:ASN:HD21	1.64	0.44
3:C:197:VAL:HG13	3:C:216:VAL:HG21	1.99	0.43
3:C:217:VAL:HG12	3:C:218:VAL:H	1.82	0.43
3:A:132:LYS:HE3	3:A:271:GLU:OE2	2.18	0.43
3:B:132:LYS:HG3	3:B:271:GLU:CG	2.48	0.43
3:B:164:LYS:HD2	3:B:271:GLU:OE1	2.17	0.43
3:B:272:VAL:O	3:B:272:VAL:HG13	2.17	0.43
3:A:284:THR:O	3:A:287:GLU:HB3	2.17	0.43
3:B:210:ASN:HB3	3:C:201:LEU:HD21	2.00	0.43
3:B:224:GLU:O	3:B:225:VAL:C	2.61	0.43
3:C:127:SER:O	3:C:131:ASN:N	2.50	0.43
3:B:174:ARG:HA	5:B:357:HOH:O	2.17	0.43
3:C:259:ASP:C	3:C:259:ASP:OD1	2.61	0.43
3:A:240:SER:O	3:A:248:ARG:N	2.31	0.43
1:E:5:DC:C3'	1:E:6:DT:H71	2.45	0.43
1:E:15:DC:H2''	1:E:16:DC:O5'	2.18	0.43
3:C:165:GLN:HB3	5:C:389:HOH:O	2.19	0.43
2:F:20:DA:H2'	2:F:20:DA:P	2.58	0.43
3:A:169:MET:HE1	5:A:431:HOH:O	2.19	0.43
3:B:114:LEU:CD2	3:B:144:GLN:NE2	2.82	0.43
3:C:132:LYS:HG3	3:C:133:MET:N	2.33	0.43
3:C:203:VAL:HG12	3:C:216:VAL:HG23	2.01	0.43
1:E:6:DT:P	1:E:6:DT:H3'	2.56	0.43
3:C:115:HIS:CD2	3:C:115:HIS:N	2.87	0.43
3:B:207:ASP:CG	3:B:214:HIS:HD1	2.27	0.42
2:F:19:DG:H1'	2:F:20:DA:O5'	2.19	0.42
3:A:197:VAL:HB	3:A:203:VAL:HG21	2.01	0.42
3:B:118:THR:HG21	3:B:283:ARG:CG	2.49	0.42
3:C:106:SER:N	5:C:368:HOH:O	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:ASP:C	3:C:188:LEU:N	2.76	0.42
1:E:5:DC:N1	1:E:6:DT:H71	2.34	0.42
3:A:137:LEU:HD23	3:A:138:ALA:H	1.84	0.42
3:C:145:LEU:HD22	3:C:232:ILE:CG1	2.49	0.42
3:C:171:GLU:OE1	3:C:249:ARG:NH2	2.53	0.42
3:C:175:ARG:NH1	3:C:183:SER:CB	2.72	0.42
3:B:247:ASN:O	3:B:248:ARG:HB2	2.18	0.42
3:C:221:GLU:HA	3:C:222:PRO:HD2	1.68	0.42
3:B:120:LYS:O	3:B:121:SER:CB	2.67	0.42
3:B:201:LEU:HA	3:B:201:LEU:HD23	1.81	0.42
3:B:259:ASP:O	3:B:262:GLY:N	2.47	0.42
3:C:134:PHE:CZ	3:C:282:ARG:HA	2.55	0.42
3:C:149:SER:O	3:C:151:PRO:HD3	2.20	0.42
1:E:12:DT:OP2	3:B:273:ARG:NH2	2.53	0.41
3:C:123:THR:O	3:C:278:PRO:CG	2.68	0.41
3:B:284:THR:C	3:B:286:GLU:H	2.28	0.41
3:C:224:GLU:HB3	3:C:227:SER:OG	2.20	0.41
3:A:177:PRO:HA	3:A:180:GLU:HG2	2.01	0.41
3:C:97:VAL:O	3:C:97:VAL:CG2	2.68	0.41
1:E:15:DC:H2''	1:E:16:DC:H5'	2.00	0.41
2:F:14:DT:H1'	5:F:57:HOH:O	2.20	0.41
3:B:256:THR:O	3:B:256:THR:HG22	2.20	0.41
3:C:137:LEU:HB2	3:C:239:ASN:HD21	1.85	0.41
2:F:6:DT:H4'	2:F:7:DG:OP1	2.21	0.41
3:B:109:PHE:O	3:B:110:ARG:HG3	2.20	0.41
3:C:280:ARG:HG2	3:C:283:ARG:CZ	2.50	0.41
3:B:286:GLU:O	3:B:289:LEU:N	2.52	0.41
1:E:2:DT:H2''	1:E:3:DT:O4'	2.20	0.41
3:B:162:ILE:CD1	3:B:252:LEU:HD12	2.37	0.41
3:C:203:VAL:CG1	3:C:216:VAL:HG23	2.51	0.41
1:E:5:DC:H2'	1:E:6:DT:H6	1.83	0.41
2:F:16:DT:H2''	2:F:17:DA:O4'	2.20	0.41
3:A:137:LEU:CD2	3:A:138:ALA:N	2.83	0.41
3:B:206:LEU:HD12	3:B:206:LEU:C	2.45	0.41
3:C:147:VAL:CG1	3:C:149:SER:O	2.69	0.41
3:A:133:MET:HE2	3:A:272:VAL:CG1	2.50	0.41
3:A:158:ARG:HD2	3:A:258:GLU:OE2	2.21	0.41
3:B:148:ASP:HB2	5:B:373:HOH:O	2.21	0.41
3:B:174:ARG:HD2	5:B:319:HOH:O	2.20	0.41
3:C:210:ASN:HA	5:C:317:HOH:O	2.20	0.41
2:F:12:DA:H2''	2:F:13:DG:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:137:LEU:CD2	3:A:137:LEU:C	2.94	0.40
3:C:283:ARG:HH11	3:C:283:ARG:CG	2.34	0.40
1:E:1:DT:C2'	1:E:2:DT:OP2	2.69	0.40
3:B:130:LEU:HA	3:B:130:LEU:HD13	1.77	0.40
3:B:157:VAL:O	3:B:217:VAL:HA	2.21	0.40
3:B:166:SER:HB2	3:C:114:LEU:CD2	2.22	0.40
3:B:285:GLU:HG2	3:B:285:GLU:O	2.20	0.40
3:C:189:ALA:HA	3:C:190:PRO:HD2	1.86	0.40
3:A:177:PRO:O	3:A:178:HIS:C	2.65	0.40
3:B:267:ARG:C	3:B:268:ASN:ND2	2.76	0.40
3:B:273:ARG:NH1	3:B:281:ASP:CG	2.74	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:351:HOH:O	5:C:351:HOH:O[2_657]	1.93	0.27

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%)	172 (90%)	16 (8%)	4 (2%)	5	3
3	C	192/219 (88%)	166 (86%)	22 (12%)	4 (2%)	5	3
All	All	578/657 (88%)	527 (91%)	42 (7%)	9 (2%)	7	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	225	VAL

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

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	176/196 (90%)	146 (83%)	30 (17%)	2	2
3	B	173/196 (88%)	144 (83%)	29 (17%)	2	2
3	C	175/196 (89%)	124 (71%)	51 (29%)	0	0
All	All	524/588 (89%)	414 (79%)	110 (21%)	1	1

All (110) 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	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

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Mol	Chain	Res	Type
3	A	145	LEU
3	A	147	VAL
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	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
3	B	123	THR
3	B	125	THR
3	B	127	SER
3	B	130	LEU
3	B	143	VAL
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

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Mol	Chain	Res	Type
3	B	267	ARG
3	B	287	GLU
3	B	288	ASN
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
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

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Mol	Chain	Res	Type
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	283	ARG
3	C	289	LEU

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

Mol	Chain	Res	Type
3	A	131	ASN
3	A	144	GLN
3	A	168	HIS
3	A	192	GLN
3	A	210	ASN
3	A	233	HIS
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	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	247	ASN
3	C	263	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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	95:SER	C	96:SER	N	2.48

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.