Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 08:17 AM EST

PDB ID	:	1TUP
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 (i) 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 (i)) were used in the production of this report:

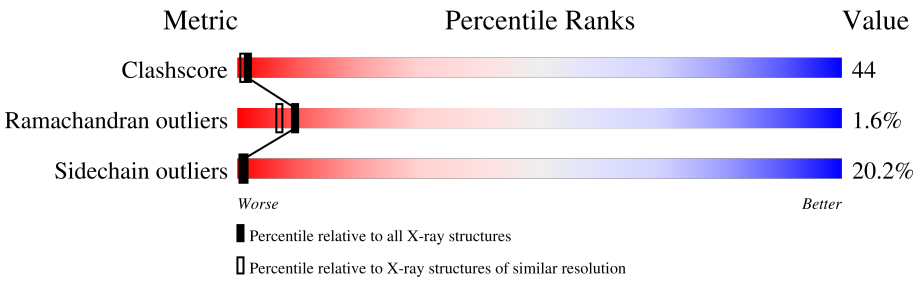
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	21	10% 29% 62%
2	F	21	48% 52%
3	A	219	49% 29% 11% • 11%
3	B	219	34% 41% 12% • 11%
3	C	219	26% 41% 18% • 11%

2 Entry composition (i)

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
			Total	C	N	O	P			
1	E	21	420	204	69	127	20	0	0	0

- 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
			Total	C	N	O	P			
2	F	21	435	208	86	121	20	0	0	0

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

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

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

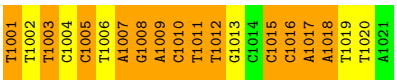
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: DNA (5'-D(*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: 10% 29% 62%

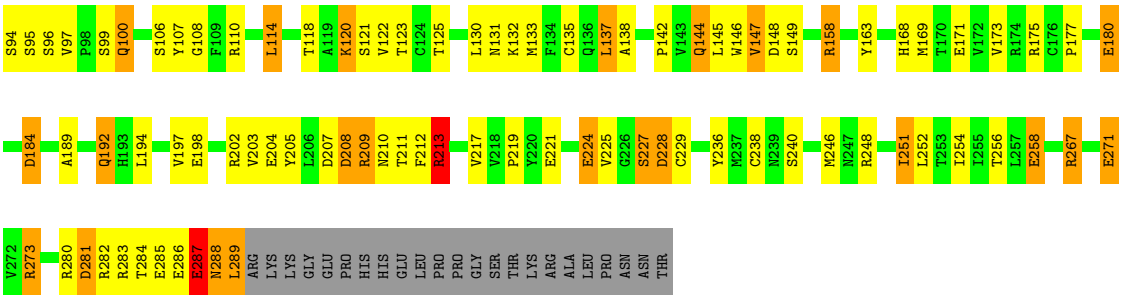


• Molecule 2: DNA (5'-D(*AP*TP*AP*AP*TP*TP*GP*GP*GP*CP*AP*AP*GP*TP*CP*TP *A P*GP*GP*AP*A)-3')

Chain F: 48% 52%

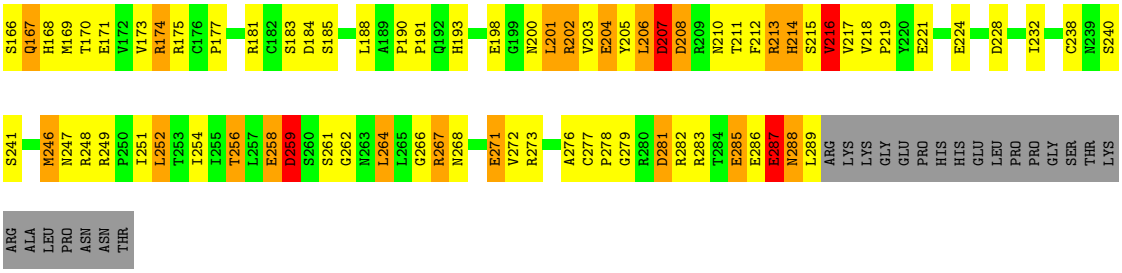
• Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

Chain A: 49% 29% 11% • 11%



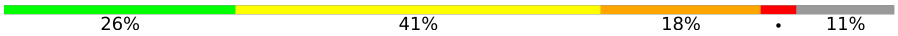
• Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

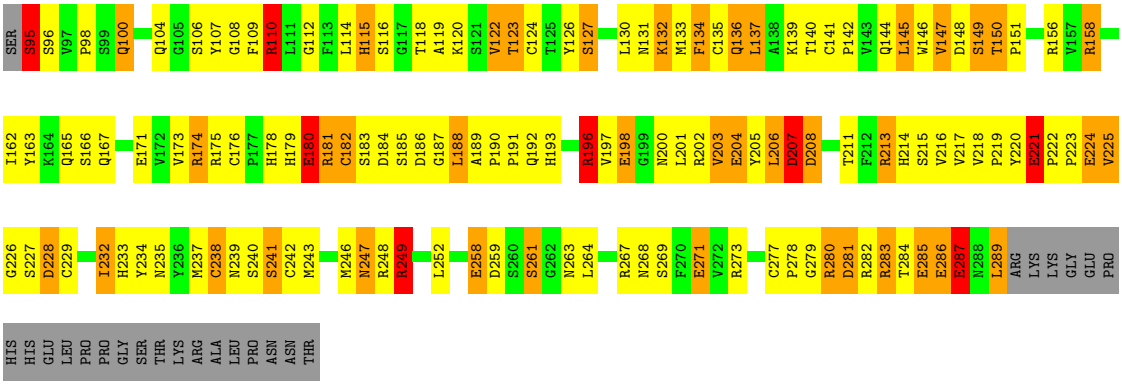
Chain B: 34% 41% 12% • 11%



• Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

Chain C:





4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.05	0/468	1.84	17/719 (2.4%)
2	F	1.13	1/490 (0.2%)	1.93	21/756 (2.8%)
3	A	0.86	11/1570 (0.7%)	1.38	20/2129 (0.9%)
3	B	0.87	7/1557 (0.4%)	1.44	23/2112 (1.1%)
3	C	0.86	9/1564 (0.6%)	1.51	30/2121 (1.4%)
All	All	0.90	28/5649 (0.5%)	1.54	111/7837 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	1	0
3	C	1	0
All	All	2	0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	271	GLU	CD-OE1	6.37	1.32	1.25
3	C	204	GLU	CD-OE2	6.30	1.32	1.25
3	C	287	GLU	CD-OE2	6.27	1.32	1.25
3	A	224	GLU	CD-OE2	6.06	1.32	1.25
3	B	287	GLU	CD-OE2	6.03	1.32	1.25
3	A	180	GLU	CD-OE1	6.02	1.32	1.25
3	B	221	GLU	CD-OE2	5.94	1.32	1.25
3	B	285	GLU	CD-OE2	5.86	1.32	1.25
3	C	224	GLU	CD-OE2	5.85	1.32	1.25
3	B	224	GLU	CD-OE1	5.82	1.32	1.25
3	A	287	GLU	CD-OE1	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	180	GLU	CD-OE1	5.67	1.31	1.25
3	B	204	GLU	CD-OE1	5.66	1.31	1.25
3	C	286	GLU	CD-OE2	5.63	1.31	1.25
2	F	1110	DC	C3'-O3'	-5.62	1.36	1.44
3	A	258	GLU	CD-OE2	5.54	1.31	1.25
3	C	285	GLU	CD-OE1	5.49	1.31	1.25
3	A	286	GLU	CD-OE2	5.46	1.31	1.25
3	A	198	GLU	CD-OE2	5.34	1.31	1.25
3	A	171	GLU	CD-OE1	5.29	1.31	1.25
3	B	258	GLU	CD-OE1	5.23	1.31	1.25
3	C	271	GLU	CD-OE2	5.21	1.31	1.25
3	A	221	GLU	CD-OE2	5.17	1.31	1.25
3	C	258	GLU	CD-OE1	5.15	1.31	1.25
3	C	221	GLU	CD-OE2	5.13	1.31	1.25
3	B	271	GLU	CD-OE1	5.08	1.31	1.25
3	A	204	GLU	CD-OE2	5.06	1.31	1.25
3	A	285	GLU	CD-OE2	5.06	1.31	1.25

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1003	DT	O4'-C1'-N1	13.37	117.36	108.00
1	E	1015	DC	P-O3'-C3'	10.91	132.79	119.70
3	C	267	ARG	NE-CZ-NH1	10.88	125.74	120.30
3	A	158	ARG	NE-CZ-NH2	-10.08	115.26	120.30
2	F	1107	DG	P-O3'-C3'	9.96	131.65	119.70
2	F	1121	DA	O4'-C1'-N9	9.85	114.89	108.00
2	F	1118	DG	P-O3'-C3'	9.82	131.49	119.70
2	F	1116	DT	P-O3'-C3'	9.57	131.19	119.70
3	A	213	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	E	1003	DT	O4'-C4'-C3'	-9.18	100.49	106.00
1	E	1003	DT	P-O3'-C3'	9.13	130.66	119.70
3	C	96	SER	N-CA-CB	8.96	123.94	110.50
2	F	1102	DT	O4'-C4'-C3'	-8.74	100.76	106.00
3	A	158	ARG	NE-CZ-NH1	8.72	124.66	120.30
3	C	267	ARG	NE-CZ-NH2	-8.69	115.95	120.30
3	C	110	ARG	NE-CZ-NH1	8.66	124.63	120.30
2	F	1119	DG	C1'-O4'-C4'	-8.30	101.80	110.10
2	F	1119	DG	O4'-C1'-N9	7.74	113.42	108.00
1	E	1010	DC	P-O3'-C3'	-7.72	110.43	119.70
1	E	1005	DC	P-O3'-C3'	7.71	128.96	119.70
1	E	1017	DA	P-O3'-C3'	7.70	128.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	104	GLN	N-CA-C	-7.68	90.27	111.00
3	A	148	ASP	CB-CG-OD1	-7.63	111.43	118.30
2	F	1118	DG	O4'-C1'-N9	7.62	113.33	108.00
2	F	1114	DT	P-O5'-C5'	-7.58	108.77	120.90
1	E	1012	DT	P-O3'-C3'	7.34	128.51	119.70
3	C	158	ARG	NE-CZ-NH1	7.23	123.91	120.30
2	F	1112	DA	P-O3'-C3'	-7.14	111.13	119.70
3	C	110	ARG	NE-CZ-NH2	-7.12	116.74	120.30
3	A	213	ARG	NE-CZ-NH1	7.11	123.85	120.30
3	C	213	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	F	1113	DG	P-O3'-C3'	7.03	128.14	119.70
3	A	273	ARG	NE-CZ-NH2	-7.03	116.79	120.30
3	B	207	ASP	CB-CG-OD1	-6.94	112.06	118.30
3	B	184	ASP	CB-CG-OD1	6.86	124.47	118.30
3	C	196	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	F	1119	DG	O4'-C1'-C2'	-6.84	100.42	105.90
3	C	158	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	F	1102	DT	C1'-O4'-C4'	-6.74	103.36	110.10
3	A	267	ARG	NE-CZ-NH1	6.68	123.64	120.30
3	C	184	ASP	CB-CG-OD1	-6.65	112.31	118.30
2	F	1113	DG	C1'-O4'-C4'	-6.64	103.46	110.10
3	B	259	ASP	N-CA-CB	6.60	122.47	110.60
1	E	1009	DA	O4'-C1'-N9	6.56	112.59	108.00
3	B	148	ASP	CB-CG-OD2	-6.55	112.40	118.30
3	A	280	ARG	NE-CZ-NH1	6.55	123.57	120.30
3	A	281	ASP	CB-CG-OD1	-6.54	112.41	118.30
3	B	184	ASP	CB-CG-OD2	-6.50	112.45	118.30
3	A	184	ASP	CB-CG-OD2	-6.44	112.50	118.30
3	B	202	ARG	NE-CZ-NH1	6.42	123.51	120.30
3	B	156	ARG	NE-CZ-NH2	-6.38	117.11	120.30
3	A	273	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	C	228	ASP	CB-CG-OD1	-6.34	112.59	118.30
2	F	1102	DT	O4'-C1'-N1	6.34	112.44	108.00
3	C	207	ASP	CB-CG-OD2	-6.33	112.60	118.30
3	C	207	ASP	CB-CG-OD1	6.26	123.93	118.30
3	A	213	ARG	CG-CD-NE	-6.24	98.69	111.80
3	A	213	ARG	CD-NE-CZ	6.21	132.29	123.60
3	B	259	ASP	CB-CG-OD1	6.19	123.87	118.30
3	A	207	ASP	CB-CG-OD2	-6.19	112.73	118.30
3	C	220	TYR	N-CA-CB	6.12	121.62	110.60
3	C	247	ASN	N-CA-CB	6.11	121.60	110.60
2	F	1119	DG	P-O3'-C3'	6.06	126.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1117	DA	O4'-C1'-N9	6.03	112.22	108.00
3	C	196	ARG	N-CA-CB	6.02	121.43	110.60
3	C	281	ASP	CB-CG-OD2	-6.01	112.89	118.30
3	A	281	ASP	CB-CG-OD2	6.01	123.71	118.30
3	C	208	ASP	CB-CG-OD1	-6.01	112.89	118.30
3	B	207	ASP	CB-CG-OD2	5.91	123.62	118.30
3	C	249	ARG	NE-CZ-NH1	5.88	123.24	120.30
3	B	214	HIS	CA-CB-CG	5.86	123.56	113.60
1	E	1015	DC	O4'-C1'-N1	-5.86	103.90	108.00
1	E	1018	DA	P-O3'-C3'	5.81	126.67	119.70
3	B	252	LEU	CB-CA-C	-5.70	99.36	110.20
3	B	228	ASP	CB-CG-OD2	-5.70	113.17	118.30
3	B	216	VAL	CA-CB-CG2	5.68	119.42	110.90
3	B	216	VAL	CG1-CB-CG2	5.64	119.93	110.90
3	C	281	ASP	CB-CG-OD1	5.60	123.34	118.30
3	C	267	ARG	CD-NE-CZ	5.59	131.43	123.60
3	A	207	ASP	CB-CG-OD1	5.57	123.31	118.30
3	C	259	ASP	CB-CG-OD1	-5.55	113.31	118.30
3	C	184	ASP	CB-CG-OD2	5.49	123.24	118.30
3	A	208	ASP	CB-CG-OD2	5.48	123.23	118.30
3	A	184	ASP	CB-CG-OD1	5.47	123.22	118.30
1	E	1001	DT	O4'-C4'-C3'	-5.46	102.32	104.50
3	B	259	ASP	CB-CG-OD2	-5.44	113.40	118.30
2	F	1105	DT	P-O3'-C3'	5.43	126.21	119.70
3	A	208	ASP	CB-CG-OD1	-5.40	113.44	118.30
3	C	228	ASP	CB-CG-OD2	5.38	123.14	118.30
3	C	148	ASP	CB-CG-OD2	-5.38	113.46	118.30
3	A	148	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	1016	DC	P-O5'-C5'	-5.31	112.41	120.90
1	E	1011	DT	P-O5'-C5'	5.27	129.34	120.90
3	C	208	ASP	CB-CG-OD2	5.27	123.05	118.30
3	B	208	ASP	CB-CG-OD2	5.25	123.03	118.30
2	F	1109	DG	P-O5'-C5'	-5.22	112.55	120.90
3	C	196	ARG	NE-CZ-NH2	-5.17	117.72	120.30
3	C	95	SER	C-N-CA	-5.14	108.86	121.70
3	B	148	ASP	CB-CG-OD1	5.11	122.90	118.30
1	E	1008	DG	N3-C4-N9	5.11	129.06	126.00
3	B	116	SER	N-CA-C	5.09	124.73	111.00
3	C	213	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	E	1003	DT	C1'-O4'-C4'	-5.08	105.02	110.10
1	E	1007	DA	P-O5'-C5'	5.06	129.00	120.90
3	B	181	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	281	ASP	CB-CG-OD1	-5.05	113.75	118.30
3	B	228	ASP	CB-CG-OD1	5.04	122.84	118.30
2	F	1101	DA	C1'-O4'-C4'	-5.04	105.06	110.10
2	F	1117	DA	O4'-C1'-C2'	-5.01	101.89	105.90
3	B	206	LEU	N-CA-CB	5.01	120.42	110.40
3	C	184	ASP	N-CA-CB	5.00	119.60	110.60

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 (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	E	420	0	241	51	0
2	F	435	0	238	40	0
3	A	1535	0	1490	74	0
3	B	1522	0	1477	129	0
3	C	1529	0	1485	169	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	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	448	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 (448) 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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:133:MET:HE1	3:A:236:TYR:CE1	2.21	0.75
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:287:GLU:HG2	3:B:288:ASN:N	2.00	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:A:118:THR:HG21	3:A:282:ARG:HG2	1.78	0.66
3:A:133:MET:HE1	3:A:236:TYR:HE1	1.59	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
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:A:133:MET:HE3	3:A:135:CYS:SG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:GLN:CD	3:B:167:GLN:H	2.00	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:147:VAL:HG13	3:A:149:SER:O	2.03	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:267:ARG:C	3:B:268:ASN:HD22	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:239:ASN:C	3:C:241:SER:H	2.09	0.55
3:B:166:SER:HB2	3:C:114:LEU:CD2	2.21	0.55
3:A:133:MET:CE	3:A:236:TYR:CE1	2.89	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
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: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:B:211:THR:C	3:B:213:ARG:H	2.11	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:171:GLU:CD	3:B:249:ARG:HH22	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:122:VAL:HG13	5:A:2233:HOH:O	2.11	0.51
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:A:175:ARG:HH22	3:A:184:ASP:CG	2.14	0.51
3:B:272:VAL:HG22	3:B:273:ARG:N	2.26	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: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:C:178:HIS:C	3:C:178:HIS:CD2	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:105:GLY:C	3:B:107:TYR:H	2.16	0.49
3:C:233:HIS:ND1	5:C:2354:HOH:O	2.35	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
3:C:239:ASN:C	3:C:241:SER:N	2.65	0.48
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:237:MET:HE2	5:C:2272:HOH:O	2.13	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
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:133:MET:HG2	3:C:134:PHE:N	2.29	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: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:105:GLY:C	3:B:107:TYR:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:ARG:HH11	3:A:258:GLU:CD	2.19	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: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:N	3:C:134:PHE:CD1	2.82	0.46
3:C:174:ARG:HE	3:C:192:GLN:NE2	2.14	0.46
3:B:200:ASN:C	3:B:202:ARG:H	2.19	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
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:B:173:VAL:CG1	3:B:246:MET:HE1	2.47	0.45
3:A:158:ARG:NH2	5:A:2174:HOH:O	2.31	0.45
3:A:273:ARG:NH1	3:A:281:ASP:CG	2.71	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: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:132:LYS:HD3	3:C:271:GLU:CD	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:114:LEU:CD2	3:B:144:GLN:NE2	2.81	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: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: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
3:A:240:SER:O	3:A:248:ARG:N	2.31	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:C:132:LYS:HG3	3:C:133:MET:N	2.32	0.42
3:C:223:PRO:HB3	3:C:229:CYS:C	2.39	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:201:LEU:HA	3:B:201:LEU:HD23	1.82	0.42
3:B:259:ASP:C	3:B:261:SER:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:MET:O	3:C:243:MET:CG	2.67	0.42
3:A:177:PRO:HA	3:A:180:GLU:HG2	2.01	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
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:A:224:GLU:CD	3:A:224:GLU:H	2.23	0.41
3:B:157:VAL:O	3:B:217:VAL:HA	2.20	0.41
3:C:243:MET:O	3:C:243:MET:HG3	2.18	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: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:C:174:ARG:HE	3:C:192:GLN:CD	2.24	0.41
3:A:208:ASP:HB3	3:A:211:THR:CG2	2.45	0.41
3:B:137:LEU:O	3:B:138:ALA:HB3	2.21	0.41
3:C:196:ARG:HD3	3:C:237:MET:CE	2.51	0.41
3:C:283:ARG:HH11	3:C:283:ARG:CG	2.34	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
3:C:186:ASP:C	3:C:188:LEU:H	2.24	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%)	29 31
3	B	192/219 (88%)	171 (89%)	17 (9%)	4 (2%)	7 4
3	C	193/219 (88%)	167 (86%)	22 (11%)	4 (2%)	7 4
All	All	579/657 (88%)	527 (91%)	43 (7%)	9 (2%)	9 7

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%)	146 (83%)	30 (17%)	2 1
3	B	173/196 (88%)	147 (85%)	26 (15%)	3 2
3	C	175/196 (89%)	125 (71%)	50 (29%)	0 0
All	All	524/588 (89%)	418 (80%)	106 (20%)	1 1

All (106) 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	131	ASN
3	A	137	LEU
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	209	ARG
3	A	213	ARG
3	A	217	VAL
3	A	227	SER
3	A	228	ASP
3	A	251	ILE
3	A	252	LEU
3	A	283	ARG
3	A	287	GLU
3	A	288	ASN
3	A	289	LEU
3	B	99	SER
3	B	100	GLN
3	B	102	THR
3	B	106	SER

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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	174	ARG
3	B	206	LEU
3	B	207	ASP
3	B	213	ARG
3	B	216	VAL
3	B	218	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	100	GLN
3	C	110	ARG
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	145	LEU
3	C	146	TRP
3	C	147	VAL
3	C	149	SER
3	C	150	THR
3	C	162	ILE
3	C	166	SER
3	C	167	GLN

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Mol	Chain	Res	Type
3	C	174	ARG
3	C	180	GLU
3	C	181	ARG
3	C	185	SER
3	C	188	LEU
3	C	196	ARG
3	C	198	GLU
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	221	GLU
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	258	GLU
3	C	261	SER
3	C	264	LEU
3	C	269	SER
3	C	280	ARG
3	C	283	ARG
3	C	287	GLU
3	C	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	288	ASN
3	B	100	GLN
3	B	104	GLN

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Mol	Chain	Res	Type
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

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 monosaccharides 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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.