



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:04 AM UTC

PDB ID : 6KQF / pdb_00006kqf
Title : Thermus thermophilus initial transcription complex comprising sigma A and 5'-OH RNA of 5 nt
Authors : Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on : 2019-08-17
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

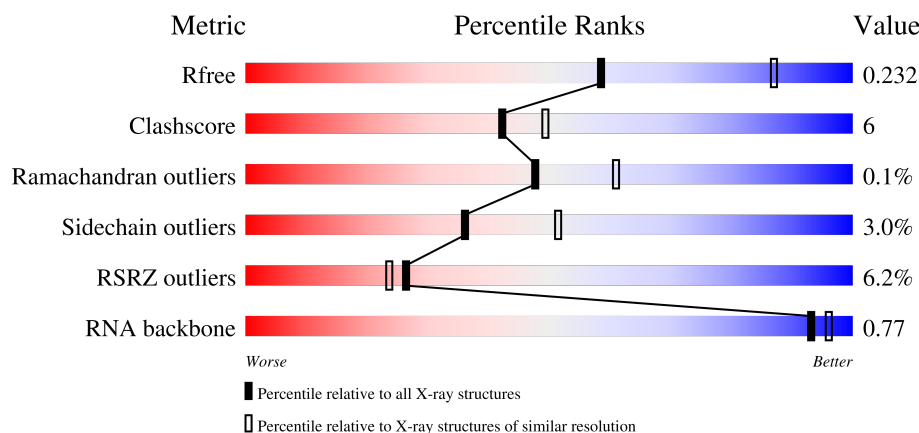
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	3% 61% 11% 27%
1	B	315	4% 57% 13% 29%
2	C	1119	3% 82% 16%
3	D	1524	8% 81% 15%

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Mol	Chain	Length	Quality of chain
4	E	99	4% 84% 11% 5%
5	F	443	7% 67% 11% 22%
6	G	21	10% 29% 52% 19%
7	H	27	4% 37% 52% 11%
8	I	5	60% 40%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29358 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1814	1158	316	338	2			
1	B	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	3	0
			8786	5559	1567	1636	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	3	0
			11759	7458	2070	2195	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2803	1767	508	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			350	166	68	100	16			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*
GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G*)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-R(*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	5	Total	C	N	O	P	0	0	0
			102	47	18	33	4			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

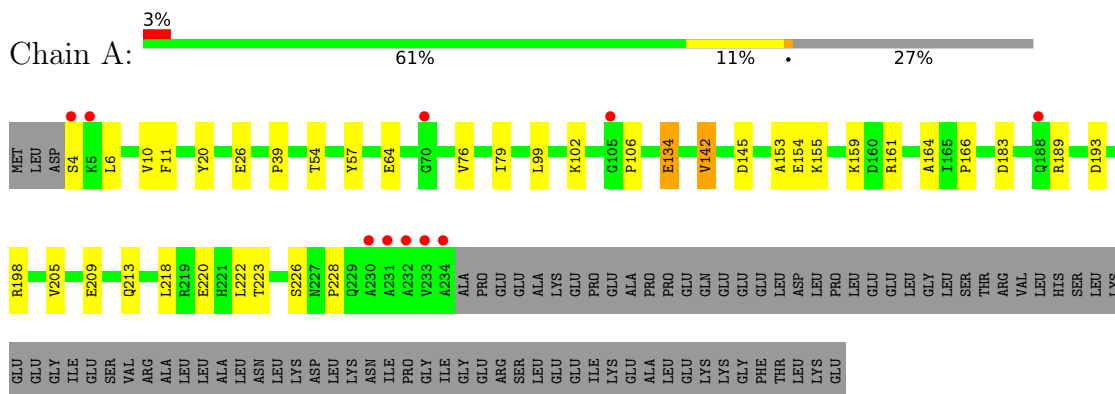
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	38	Total O 38 38	0	0
11	B	25	Total O 25 25	0	0
11	C	246	Total O 246 246	0	0
11	D	310	Total O 310 310	0	0
11	E	30	Total O 30 30	0	0
11	F	46	Total O 46 46	0	0
11	G	16	Total O 16 16	0	0
11	H	8	Total O 8 8	0	0
11	I	5	Total O 5 5	0	0

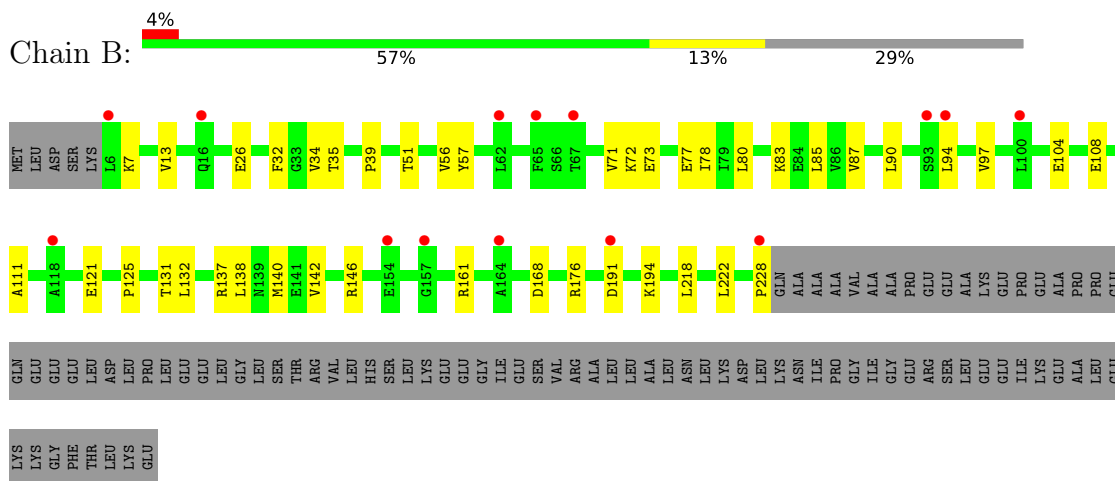
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

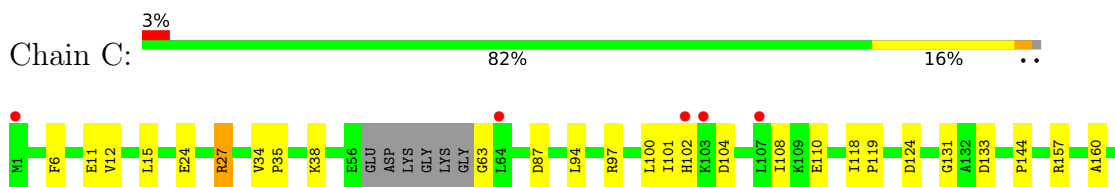
- Molecule 1: DNA-directed RNA polymerase subunit alpha

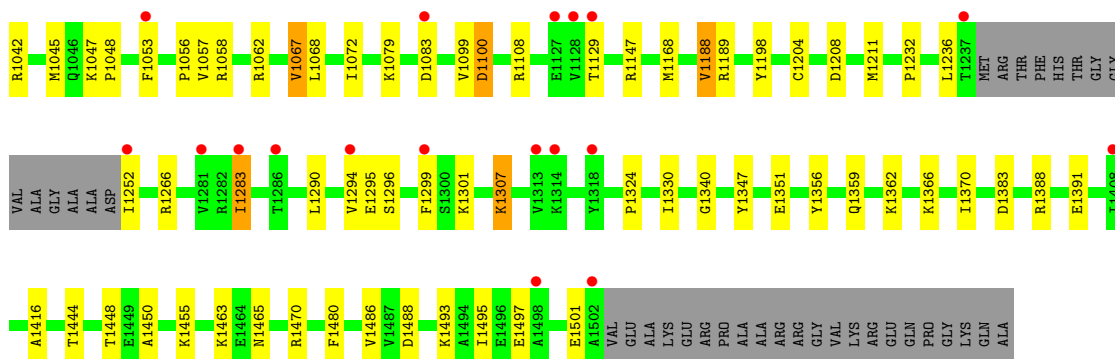


- Molecule 1: DNA-directed RNA polymerase subunit alpha

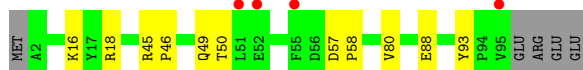
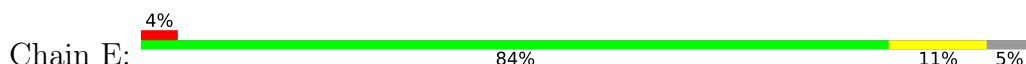


- Molecule 2: DNA-directed RNA polymerase subunit beta

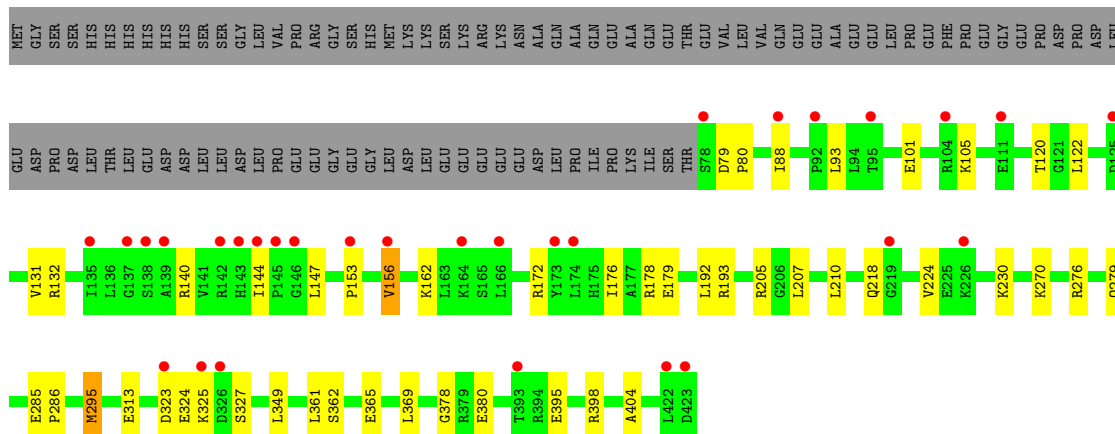




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA

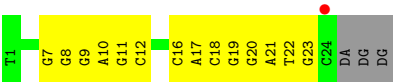


- Molecule 6: DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G*)-3')





● Molecule 8: RNA (5'-R(*CP*UP*CP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.64Å 103.64Å 296.19Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	48.85 – 2.45 48.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.85-2.45) 99.8 (48.85-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.199 , 0.230 0.201 , 0.232	Depositor DCC
R_{free} test set	10041 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.014 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29358	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	A	0.30	0/1849	0.77	0/2515
1	B	0.28	0/1790	0.76	0/2435
2	C	0.35	2/8963 (0.0%)	0.76	7/12122 (0.1%)
3	D	0.32	0/11975	0.76	5/16189 (0.0%)
4	E	0.32	0/775	0.71	0/1045
5	F	0.33	0/2848	0.74	1/3833 (0.0%)
6	G	0.24	0/393	0.57	0/606
7	H	0.18	0/556	0.57	0/858
8	I	0.17	0/113	0.32	0/174
All	All	0.33	2/29262 (0.0%)	0.75	13/39777 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1056	LYS	C-O	-7.06	1.15	1.24
2	C	904	PRO	C-O	-6.66	1.15	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	633	VAL	N-CA-C	12.56	123.43	110.62
2	C	1059	ASP	N-CA-C	-6.47	97.97	108.52
3	D	1340	GLY	CA-C-N	6.37	125.60	118.97
3	D	1340	GLY	C-N-CA	6.37	125.60	118.97
2	C	1058	ASP	N-CA-C	6.29	122.30	113.56
2	C	422	ARG	N-CA-C	-5.91	105.25	112.88
3	D	433	GLY	N-CA-C	5.56	118.64	110.80
2	C	1057	SER	N-CA-C	5.31	118.09	108.69
3	D	108	VAL	N-CA-C	5.30	113.95	109.02
2	C	269	LEU	N-CA-C	-5.21	103.16	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	327	SER	N-CA-C	5.10	116.94	109.24
2	C	217	LEU	N-CA-C	-5.06	105.77	111.28
2	C	215	GLY	N-CA-C	5.03	125.09	113.18

There are no chirality outliers.

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	A	1814	0	1869	27	0
1	B	1758	0	1808	25	0
2	C	8786	0	8891	114	0
3	D	11759	0	12002	154	0
4	E	761	0	778	6	0
5	F	2803	0	2871	30	0
6	G	350	0	192	20	0
7	H	495	0	272	27	0
8	I	102	0	55	4	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	A	38	0	0	0	0
11	B	25	0	0	0	0
11	C	246	0	0	3	0
11	D	310	0	0	10	0
11	E	30	0	0	0	0
11	F	46	0	0	0	0
11	G	16	0	0	1	0
11	H	8	0	0	1	0
11	I	5	0	0	0	0
All	All	29358	0	28738	360	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (360) 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)
7:H:21:DA:H2''	7:H:22:DT:H5''	1.34	1.06
6:G:19:DG:H2''	6:G:20:DG:H5'	1.40	1.04
6:G:15:DT:H2'	6:G:16:DC:C6	1.94	1.00
7:H:21:DA:H2''	7:H:22:DT:C5'	1.93	0.99
6:G:19:DG:C2'	6:G:20:DG:H5'	2.03	0.89
7:H:21:DA:C2'	7:H:22:DT:H5''	2.05	0.87
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.63	0.78
6:G:18:DA:N7	11:G:101:HOH:O	2.21	0.73
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.72	0.71
2:C:628:PHE:H	2:C:638:ASP:HB3	1.56	0.70
3:D:87:ARG:NH2	11:D:2103:HOH:O	2.24	0.70
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.73	0.70
7:H:10:DA:H2'	7:H:11:DG:C8	2.27	0.69
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.26	0.68
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.74	0.68
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.75	0.67
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.26	0.67
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.75	0.67
3:D:65:ARG:NH1	5:F:378:GLY:O	2.27	0.66
7:H:20:DG:H2'	7:H:21:DA:C8	2.31	0.66
2:C:617:ASP:OD1	2:C:617:ASP:N	2.29	0.65
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.65
3:D:661:MET:SD	11:D:2364:HOH:O	2.54	0.65
2:C:216:GLU:O	2:C:216:GLU:HG3	1.96	0.65
2:C:758:ARG:HH21	2:C:788:THR:HB	1.62	0.65
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.30	0.64
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.80	0.64
2:C:428:ARG:NH2	2:C:447:ALA:O	2.30	0.64
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.31	0.64
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.31	0.64
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.31	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.80	0.63
2:C:631:SER:HB3	2:C:637:LEU:HD13	1.80	0.63
2:C:215:GLY:O	2:C:216:GLU:HB3	1.99	0.63
3:D:109:PRO:HB3	7:H:21:DA:H5''	1.81	0.62
3:D:894:LYS:H	3:D:894:LYS:HD3	1.64	0.62
3:D:530:VAL:HG12	3:D:531:ASP:H	1.64	0.62
7:H:12:DC:O5'	7:H:12:DC:H6	1.81	0.62
6:G:9:DC:O2	7:H:19:DG:N2	2.23	0.62
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.82	0.62
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.79	0.62
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.82	0.62
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.81	0.61
2:C:226:VAL:HA	2:C:229:MET:HE2	1.82	0.61
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.83	0.61
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.81	0.60
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.83	0.60
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.83	0.60
7:H:20:DG:H2'	7:H:21:DA:O4'	2.01	0.60
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.34	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.59
6:G:18:DA:H2'	6:G:19:DG:C8	2.37	0.59
2:C:805:ARG:O	2:C:807[A]:ARG:NH2	2.34	0.59
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.85	0.58
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.86	0.58
3:D:546:ARG:NH2	11:D:2107:HOH:O	2.29	0.58
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.87	0.57
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.87	0.57
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.86	0.57
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.87	0.57
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.86	0.57
6:G:5:DC:H1'	6:G:6:DA:OP2	2.04	0.57
7:H:21:DA:C1'	7:H:22:DT:H5''	2.34	0.57
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.86	0.57
6:G:15:DT:C4	6:G:16:DC:N4	2.73	0.56
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.88	0.56
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	1.87	0.56
1:B:94:LEU:O	1:B:146:ARG:NH2	2.39	0.56
3:D:657:LEU:HG	3:D:661:MET:HE2	1.85	0.56
3:D:966:GLU:O	3:D:969:ARG:HG2	2.06	0.56
3:D:1470:ARG:NH1	11:D:2113:HOH:O	2.39	0.56
3:D:162:ARG:O	3:D:414:ARG:NH1	2.36	0.55
6:G:8:DC:N3	7:H:20:DG:N2	2.51	0.55
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.87	0.55
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.89	0.55
6:G:16:DC:H2'	6:G:17:DG:C8	2.42	0.55
1:A:4:SER:O	1:A:189:ARG:NH2	2.37	0.55
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.88	0.55
3:D:562:ALA:O	5:F:140:ARG:NH1	2.27	0.55
2:C:715:THR:OG1	2:C:718:GLY:O	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.89	0.54
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.34	0.54
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.43	0.54
3:D:553:ARG:NH2	11:D:2118:HOH:O	2.40	0.54
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.90	0.54
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.90	0.54
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.88	0.54
2:C:1057:SER:HB2	3:D:622:ARG:O	2.07	0.54
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.90	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.90	0.53
6:G:8:DC:C4	6:G:9:DC:N4	2.76	0.53
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.90	0.53
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.38	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.53
7:H:19:DG:H2''	7:H:20:DG:O5'	2.08	0.53
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.39	0.53
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.90	0.53
3:D:1450:ALA:HA	3:D:1455:LYS:HE3	1.90	0.53
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.91	0.53
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.90	0.52
2:C:405:ARG:NH2	11:C:1212:HOH:O	2.41	0.52
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.91	0.52
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.41	0.52
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.90	0.52
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.90	0.52
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.92	0.52
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.90	0.52
3:D:411:THR:O	5:F:178:ARG:NH1	2.43	0.52
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.91	0.52
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.92	0.51
2:C:971:LYS:NZ	11:C:1215:HOH:O	2.42	0.51
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.46	0.51
6:G:10:DG:N2	7:H:18:DC:O2	2.43	0.51
7:H:22:DT:H2''	7:H:23:DG:C8	2.45	0.51
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.93	0.51
1:A:209:GLU:O	1:A:213:GLN:HG2	2.10	0.51
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.92	0.51
2:C:923:GLU:OE2	2:C:964:LYS:NZ	2.42	0.51
7:H:16:DC:H2''	7:H:17:DA:C8	2.46	0.51
2:C:133:ASP:HB3	2:C:395:LYS:HD2	1.92	0.51
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:224:GLU:CD	2:C:224:GLU:H	2.19	0.51
2:C:905:ILE:HG13	2:C:905:ILE:O	2.11	0.51
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.26	0.51
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.92	0.51
2:C:846:LYS:NZ	8:I:5:A:OP1	2.38	0.51
2:C:94:LEU:HD22	2:C:118:ILE:HD11	1.93	0.50
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.44	0.50
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.42	0.50
2:C:911:GLU:O	2:C:915:LYS:HG2	2.12	0.50
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.94	0.50
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.92	0.50
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.41	0.50
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.93	0.50
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.93	0.50
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.94	0.50
1:B:51:THR:OG1	1:B:87:VAL:O	2.29	0.50
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.93	0.50
6:G:8:DC:C2	7:H:20:DG:N2	2.79	0.50
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.47	0.49
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.45	0.49
3:D:704:ARG:CD	3:D:738:ALA:HB2	2.41	0.49
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.94	0.49
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.27	0.49
3:D:704:ARG:HD3	3:D:736:PHE:O	2.12	0.49
5:F:276:ARG:O	5:F:279:GLN:HG3	2.12	0.49
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.95	0.49
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.95	0.49
3:D:1232:PRO:HG2	3:D:1356:TYR:HE1	1.77	0.49
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.46	0.49
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.94	0.49
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.94	0.49
5:F:323:ASP:OD1	5:F:325:LYS:N	2.45	0.49
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.48	0.49
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.95	0.49
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.94	0.49
2:C:420:ARG:C	2:C:422:ARG:H	2.20	0.49
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.94	0.49
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.94	0.49
2:C:223:ASP:OD1	2:C:225:SER:OG	2.30	0.48
2:C:427:VAL:HG23	2:C:428:ARG:HG3	1.95	0.48
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.44	0.48
3:D:834:THR:OG1	3:D:835:SER:N	2.45	0.48
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.94	0.48
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.31	0.48
3:D:534:ARG:NH2	5:F:313:GLU:O	2.46	0.48
5:F:93:LEU:HD21	5:F:193:ARG:HD2	1.95	0.48
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.95	0.48
2:C:816:LYS:HG3	2:C:819:VAL:HG21	1.95	0.48
3:D:621:LYS:NZ	11:D:2130:HOH:O	2.46	0.48
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.47	0.48
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.95	0.48
2:C:724:ARG:NH2	2:C:734:LEU:O	2.47	0.48
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.13	0.48
3:D:1444:THR:O	3:D:1448:THR:HG23	2.13	0.48
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.79	0.48
3:D:226:PRO:HG2	3:D:245:LEU:HD11	1.96	0.47
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.95	0.47
3:D:487:ALA:O	3:D:491:LYS:HG2	2.14	0.47
7:H:17:DA:N9	7:H:18:DC:C5	2.83	0.47
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.42	0.47
2:C:537:LYS:NZ	11:C:1224:HOH:O	2.47	0.47
2:C:764:GLU:H	2:C:764:GLU:HG3	1.42	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.78	0.47
3:D:637:LEU:HD11	3:D:727:GLN:HB3	1.96	0.47
3:D:975:GLU:O	3:D:979:GLU:HG2	2.14	0.47
3:D:794:GLN:HB3	11:D:2101:HOH:O	2.15	0.47
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.96	0.47
2:C:203:ASP:OD1	2:C:204:GLN:N	2.48	0.47
2:C:572:ILE:HG13	2:C:573:ARG:HG3	1.96	0.47
3:D:231:VAL:O	3:D:236:TYR:OH	2.32	0.47
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.30	0.47
6:G:16:DC:H2'	6:G:17:DG:H8	1.79	0.46
7:H:20:DG:C2'	7:H:21:DA:C8	2.96	0.46
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.50	0.46
3:D:1266:ARG:NE	7:H:18:DC:OP1	2.49	0.46
1:B:191:ASP:OD1	1:B:191:ASP:N	2.41	0.46
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.98	0.46
2:C:101:ILE:HG12	2:C:108:ILE:HG12	1.98	0.46
3:D:1211:MET:HE1	4:E:16:LYS:HD2	1.97	0.46
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.16	0.46
7:H:21:DA:C2'	7:H:22:DT:C5'	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.96	0.46
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.82	0.46
5:F:172:ARG:O	5:F:176:ILE:HG12	2.15	0.46
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.98	0.46
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.98	0.46
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.97	0.46
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.98	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.98	0.45
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.49	0.45
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.97	0.45
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.49	0.45
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.97	0.45
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.98	0.45
2:C:436:GLY:HA2	2:C:538:GLN:O	2.17	0.45
2:C:616:GLU:OE1	2:C:648:ARG:NH1	2.49	0.45
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.45
3:D:1362:LYS:HD3	11:D:2349:HOH:O	2.16	0.45
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.17	0.45
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.98	0.45
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.98	0.45
3:D:178:LEU:HG	3:D:192:ALA:HA	1.97	0.45
7:H:9:DG:C2	7:H:10:DA:C2	3.04	0.45
3:D:729:HIS:O	3:D:732:VAL:HG22	2.17	0.45
5:F:362:SER:OG	5:F:365:GLU:HG2	2.17	0.45
1:A:220:GLU:O	1:A:223:THR:HB	2.17	0.45
3:D:658:LEU:HA	3:D:661:MET:HE3	1.99	0.45
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.98	0.45
2:C:218:VAL:HG22	2:C:222:MET:HE2	2.00	0.44
2:C:1068:GLU:OE2	2:C:1072:LYS:NZ	2.50	0.44
3:D:1307:LYS:H	3:D:1307:LYS:HG3	1.53	0.44
7:H:11:DG:OP2	11:H:101:HOH:O	2.21	0.44
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.17	0.44
7:H:20:DG:H2''	7:H:21:DA:C5'	2.47	0.44
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.52	0.44
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.52	0.44
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.52	0.44
2:C:394:PHE:CE2	6:G:20:DG:H5''	2.52	0.44
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.99	0.44
6:G:15:DT:H2'	6:G:16:DC:H6	1.69	0.44
5:F:105:LYS:HD3	5:F:179:GLU:HG2	1.99	0.44
7:H:17:DA:C5	7:H:18:DC:N4	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.00	0.44
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.53	0.44
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.51	0.44
3:D:142:LEU:HB2	3:D:161:LEU:HD21	1.99	0.44
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.99	0.43
6:G:15:DT:O2	8:I:5:A:C2	2.72	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.18	0.43
2:C:300:ASP:OD1	2:C:301:GLU:N	2.52	0.43
2:C:343:GLN:HG3	2:C:385:PHE:HB2	2.00	0.43
3:D:1045[B]:MET:HE3	3:D:1045[B]:MET:HB2	1.83	0.43
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.54	0.43
3:D:374:GLU:HG2	3:D:375:GLU:HG3	2.00	0.43
3:D:901:GLN:NE2	11:D:2128:HOH:O	2.45	0.43
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.87	0.43
2:C:15:LEU:HD11	2:C:583:LEU:HD11	2.00	0.43
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.99	0.43
2:C:177:GLU:HG3	2:C:178:PRO:HD2	2.00	0.43
3:D:185:VAL:N	3:D:201:GLY:O	2.51	0.43
3:D:1463:LYS:HB3	3:D:1463:LYS:HE2	1.81	0.43
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.18	0.43
5:F:270:LYS:HE2	5:F:295:MET:HE1	2.00	0.43
1:B:32:PHE:HA	1:B:35:THR:HB	2.01	0.43
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.18	0.43
3:D:1283:ILE:H	3:D:1283:ILE:HG13	1.59	0.43
1:A:10:VAL:HG12	1:A:26:GLU:O	2.19	0.43
2:C:872:ASN:ND2	3:D:784:ASP:OD2	2.44	0.43
2:C:1057:SER:CB	3:D:622:ARG:O	2.67	0.43
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	2.01	0.43
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.43
2:C:584:GLU:OE2	2:C:584:GLU:N	2.49	0.42
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	2.01	0.42
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.87	0.42
5:F:279:GLN:HB3	5:F:286:PRO:HD3	2.01	0.42
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.54	0.42
3:D:38:LYS:HA	3:D:38:LYS:HD3	1.92	0.42
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.52	0.42
2:C:850:ALA:HB1	3:D:633:VAL:HG12	2.00	0.42
3:D:1047:LYS:HG2	3:D:1053[A]:PHE:CE2	2.55	0.42
1:A:153:ALA:HB1	1:A:166:PRO:HB2	2.02	0.42
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.83	0.42
5:F:193:ARG:NH1	7:H:7:DG:N7	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:15:DT:O2	8:I:5:A:H2	2.03	0.42
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.02	0.42
2:C:419:THR:HG23	2:C:422:ARG:HG3	2.00	0.42
2:C:540:PHE:HB3	2:C:544:THR:HB	2.02	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.77	0.42
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.79	0.42
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.46	0.42
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.55	0.42
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.02	0.42
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.84	0.42
2:C:765:SER:O	2:C:767:PRO:HD3	2.19	0.42
2:C:905:ILE:O	2:C:906:PHE:HB2	2.20	0.42
3:D:959:GLU:H	3:D:959:GLU:CD	2.25	0.42
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.42
3:D:428:LYS:HB3	3:D:428:LYS:HE2	1.87	0.42
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.45	0.42
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.93	0.42
7:H:22:DT:H4'	7:H:23:DG:OP1	2.19	0.42
1:B:80:LEU:HD21	3:D:842:VAL:HG12	2.01	0.41
1:B:108:GLU:HG2	1:B:131:THR:HG22	2.02	0.41
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.86	0.41
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.55	0.41
3:D:669:ASN:ND2	3:D:672:ALA:H	2.18	0.41
2:C:102[A]:HIS:CE1	2:C:104:ASP:HB2	2.55	0.41
2:C:420:ARG:HE	2:C:420:ARG:HB2	1.62	0.41
3:D:433:GLY:HA2	3:D:449:SER:H	1.85	0.41
3:D:475:LYS:O	3:D:479:GLU:HG2	2.21	0.41
1:A:11:PHE:O	1:B:228:PRO:HA	2.20	0.41
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.02	0.41
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.87	0.41
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.41
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.03	0.41
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.90	0.41
2:C:1081:VAL:HA	2:C:1082:PRO:HD2	1.90	0.41
6:G:19:DG:H1	8:I:1:C:H42	1.67	0.41
1:A:226:SER:O	1:A:228:PRO:HD3	2.21	0.41
3:D:316:GLN:NE2	11:D:2148:HOH:O	2.52	0.41
2:C:119:PRO:HG2	2:C:386:PHE:CD2	2.56	0.41
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.56	0.41
1:A:154:GLU:CD	1:A:154:GLU:H	2.27	0.41
3:D:161:LEU:HB3	3:D:452:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:951:ILE:HG13	3:D:1062:ARG:HD2	2.02	0.41
5:F:295:MET:HA	5:F:295:MET:HE2	2.02	0.41
1:B:85:LEU:HG	1:B:87:VAL:HG23	2.03	0.41
2:C:847:GLY:HA2	3:D:741:ASP:HA	2.01	0.41
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.31	0.41
3:D:353:VAL:HG22	3:D:368:VAL:HG22	2.03	0.41
3:D:397:LYS:O	3:D:448:GLU:HG2	2.20	0.41
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.55	0.41
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.45	0.41
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.54	0.41
5:F:79:ASP:OD2	7:H:8:DG:N1	2.38	0.41
3:D:90:MET:SD	3:D:521:PRO:HD3	2.62	0.40
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.56	0.40
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.48	0.40
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.03	0.40
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.57	0.40
3:D:452:ILE:H	3:D:452:ILE:HG13	1.65	0.40
6:G:15:DT:C2'	6:G:16:DC:O4'	2.69	0.40
2:C:63:GLY:N	2:C:367:LEU:HD12	2.35	0.40
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.92	0.40
2:C:771:GLU:O	2:C:775:ARG:HB2	2.22	0.40
2:C:954:THR:HA	2:C:955:PRO:HD3	1.92	0.40
3:D:155:ASP:OD2	3:D:159:ARG:NH1	2.53	0.40
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.85	0.40
2:C:34:VAL:HA	2:C:35:PRO:HD2	1.92	0.40
2:C:360:LEU:HD12	2:C:360:LEU:HA	1.86	0.40
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.57	0.40
2:C:876:VAL:H	2:C:877:PRO:HD2	1.87	0.40
3:D:208:PRO:HA	3:D:390:PRO:HA	2.02	0.40
3:D:1294:VAL:HB	3:D:1301:LYS:HB2	2.03	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.83	0.40
2:C:850:ALA:HB1	3:D:632:VAL:HG13	2.03	0.40
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/315 (73%)	230 (100%)	0	0	100	100
1	B	221/315 (70%)	215 (97%)	6 (3%)	0	100	100
2	C	1111/1119 (99%)	1082 (97%)	28 (2%)	1 (0%)	48	61
3	D	1485/1524 (97%)	1445 (97%)	39 (3%)	1 (0%)	48	61
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3483/3815 (91%)	3400 (98%)	81 (2%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	764	GLU
3	D	563	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	
1	A	201/273 (74%)	197 (98%)	4 (2%)	48	63
1	B	196/273 (72%)	192 (98%)	4 (2%)	48	63
2	C	938/941 (100%)	904 (96%)	34 (4%)	31	45
3	D	1256/1279 (98%)	1222 (97%)	34 (3%)	39	54
4	E	83/88 (94%)	80 (96%)	3 (4%)	31	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	300/388 (77%)	289 (96%)	11 (4%)	30	44
All	All	2974/3242 (92%)	2884 (97%)	90 (3%)	36	51

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	134	GLU
1	A	142	VAL
1	A	205	VAL
1	B	7	LYS
1	B	34	VAL
1	B	72	LYS
1	B	97	VAL
2	C	11	GLU
2	C	27	ARG
2	C	182	VAL
2	C	190	LYS
2	C	200	LEU
2	C	216	GLU
2	C	217	LEU
2	C	224	GLU
2	C	261	ILE
2	C	276	LYS
2	C	284	ARG
2	C	358	ARG
2	C	360	LEU
2	C	384	GLU
2	C	390	GLN
2	C	419	THR
2	C	513	VAL
2	C	583	LEU
2	C	595	LEU
2	C	610	ARG
2	C	617	ASP
2	C	620	LEU
2	C	723	THR
2	C	764	GLU
2	C	775	ARG
2	C	807[A]	ARG
2	C	807[B]	ARG
2	C	815	LEU

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Mol	Chain	Res	Type
2	C	816	LYS
2	C	939	ARG
2	C	952	LEU
2	C	1056	LYS
2	C	1058	ASP
2	C	1078	GLU
3	D	67	ARG
3	D	71	LYS
3	D	74	GLU
3	D	133	ILE
3	D	145	VAL
3	D	149	LYS
3	D	152	LEU
3	D	231	VAL
3	D	275	GLU
3	D	276	ASP
3	D	354	VAL
3	D	415	VAL
3	D	427	VAL
3	D	452	ILE
3	D	530	VAL
3	D	687	VAL
3	D	754	PHE
3	D	810	GLU
3	D	864	VAL
3	D	894	LYS
3	D	956	ILE
3	D	986	ARG
3	D	1067	VAL
3	D	1083	ASP
3	D	1100	ASP
3	D	1129	THR
3	D	1188	VAL
3	D	1252	ILE
3	D	1283	ILE
3	D	1290	LEU
3	D	1295	GLU
3	D	1307	LYS
3	D	1486	VAL
3	D	1501	GLU
4	E	49	GLN
4	E	50	THR

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Mol	Chain	Res	Type
4	E	93	TYR
5	F	88	ILE
5	F	156	VAL
5	F	162	LYS
5	F	205	ARG
5	F	218	GLN
5	F	224	VAL
5	F	295	MET
5	F	324	GLU
5	F	349	LEU
5	F	369	LEU
5	F	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	ASN
2	C	117	HIS
2	C	434	HIS
2	C	543	ASN
2	C	663	ASN
2	C	860	HIS
2	C	991	GLN
2	C	1026	GLN
3	D	66	GLN
3	D	669	ASN
3	D	696	HIS
3	D	901	GLN
3	D	994	GLN
3	D	1172	HIS
3	D	1184	GLN
3	D	1334	GLN
5	F	83	GLN
5	F	218	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	4/5 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 6 ligands modelled in this entry, 6 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	0.26	10 (4%)	40	39	39, 58, 85, 127	1 (0%)
1	B	223/315 (70%)	0.62	14 (6%)	26	23	44, 69, 96, 111	0
2	C	1112/1119 (99%)	0.15	36 (3%)	50	51	27, 50, 105, 130	3 (0%)
3	D	1486/1524 (97%)	0.49	124 (8%)	17	15	26, 58, 115, 137	4 (0%)
4	E	94/99 (94%)	0.09	4 (4%)	40	39	32, 50, 86, 106	0
5	F	346/443 (78%)	0.76	30 (8%)	16	14	38, 67, 107, 131	0
6	G	17/21 (80%)	1.12	2 (11%)	9	8	55, 69, 156, 162	0
7	H	24/27 (88%)	0.67	1 (4%)	40	40	68, 93, 155, 175	0
8	I	5/5 (100%)	0.56	0	100	100	46, 48, 62, 74	0
All	All	3538/3868 (91%)	0.40	221 (6%)	26	24	26, 58, 112, 175	8 (0%)

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1252	ILE	5.3
3	D	420	VAL	5.0
5	F	139	ALA	4.9
5	F	78	SER	4.9
2	C	64	LEU	4.9
2	C	1057	SER	4.8
3	D	184	GLU	4.6
3	D	144	GLY	4.4
3	D	415	VAL	4.4
3	D	1502	ALA	4.4
1	A	232	ALA	4.3
1	A	233	VAL	4.2
3	D	409	VAL	4.1
3	D	203	ALA	4.1
1	B	191	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	157	GLY	4.1
3	D	161	LEU	4.0
5	F	146	GLY	3.7
3	D	142	LEU	3.7
4	E	95	VAL	3.7
3	D	1129	THR	3.6
2	C	102[A]	HIS	3.6
3	D	396	VAL	3.6
3	D	1128	VAL	3.6
3	D	182	GLY	3.5
1	B	228	PRO	3.5
3	D	447	VAL	3.4
3	D	147	VAL	3.4
3	D	175	VAL	3.3
3	D	140	ALA	3.3
3	D	402	PRO	3.3
3	D	310	LEU	3.3
2	C	812	GLY	3.3
3	D	1283	ILE	3.3
5	F	326	ASP	3.3
3	D	207	PHE	3.2
1	A	234	ALA	3.2
4	E	55	PHE	3.2
2	C	419	THR	3.2
5	F	142	ARG	3.2
3	D	434	ARG	3.1
3	D	1313	VAL	3.1
3	D	416	ALA	3.1
1	B	62	LEU	3.1
3	D	812	ALA	3.1
3	D	440	VAL	3.1
4	E	51	LEU	3.0
3	D	417	PRO	3.0
3	D	431	VAL	3.0
5	F	422	LEU	3.0
3	D	446	VAL	2.9
1	B	67	THR	2.9
3	D	170	PRO	2.9
5	F	325	LYS	2.9
6	G	4	DG	2.9
3	D	531	ASP	2.9
2	C	191	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
7	H	24	DC	2.9
3	D	444	VAL	2.9
3	D	1237	THR	2.9
2	C	362	GLY	2.9
5	F	153	PRO	2.8
3	D	269	PHE	2.8
3	D	429	SER	2.8
3	D	454	ALA	2.8
3	D	470	LEU	2.8
3	D	393	ILE	2.8
2	C	361	MET	2.8
5	F	95	THR	2.8
3	D	180	LYS	2.8
3	D	665	GLY	2.7
3	D	432	TYR	2.7
5	F	138	SER	2.7
3	D	202	VAL	2.7
5	F	174	LEU	2.7
3	D	258	VAL	2.7
3	D	355	VAL	2.7
1	B	100	LEU	2.7
3	D	421	LEU	2.7
3	D	290	PRO	2.7
1	A	4	SER	2.7
3	D	407	VAL	2.7
3	D	400	VAL	2.7
3	D	241	ILE	2.6
3	D	1314	LYS	2.6
3	D	633	VAL	2.6
2	C	213	ALA	2.6
3	D	193	PRO	2.6
5	F	145	PRO	2.6
2	C	236	ILE	2.6
3	D	133	ILE	2.6
2	C	107	LEU	2.6
3	D	242	LEU	2.6
3	D	401	TYR	2.6
3	D	172	PRO	2.5
3	D	452	ILE	2.5
5	F	144	ILE	2.5
3	D	196	VAL	2.5
3	D	829	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	530	VAL	2.5
3	D	201	GLY	2.5
3	D	564	GLU	2.5
3	D	259	VAL	2.5
3	D	137	PRO	2.4
3	D	139	GLY	2.4
3	D	418	GLY	2.4
3	D	430	ASP	2.4
3	D	211	VAL	2.4
3	D	1294	VAL	2.4
3	D	1286	THR	2.4
3	D	173	PRO	2.4
3	D	556	LYS	2.4
1	A	188	GLN	2.4
3	D	152	LEU	2.4
3	D	316	GLN	2.4
3	D	1318	TYR	2.4
3	D	821	VAL	2.4
3	D	412	GLY	2.4
3	D	141	ILE	2.4
3	D	178	LEU	2.4
2	C	275	TYR	2.4
3	D	427	VAL	2.4
3	D	443	VAL	2.4
3	D	324	ALA	2.4
2	C	360	LEU	2.4
3	D	816	HIS	2.4
1	A	230	ALA	2.4
2	C	103	LYS	2.4
3	D	433	GLY	2.3
3	D	191	LEU	2.3
5	F	323	ASP	2.3
3	D	3	LYS	2.3
1	B	154	GLU	2.3
3	D	445	ARG	2.3
2	C	1	MET	2.3
3	D	179	VAL	2.3
2	C	1091	GLU	2.3
3	D	809	PRO	2.3
1	B	93	SER	2.3
3	D	394	LEU	2.3
3	D	1083	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	226	LYS	2.3
5	F	143	HIS	2.3
5	F	219	GLY	2.3
2	C	764	GLU	2.3
3	D	323	GLU	2.3
3	D	186	VAL	2.3
3	D	435	VAL	2.3
3	D	149	LYS	2.2
5	F	125	ASP	2.2
2	C	420	ARG	2.2
3	D	213	VAL	2.2
5	F	104	ARG	2.2
1	A	5	LYS	2.2
1	A	105	GLY	2.2
2	C	245	GLY	2.2
3	D	148	GLU	2.2
2	C	243	ARG	2.2
2	C	186	VAL	2.2
3	D	359	ALA	2.2
3	D	1498	ALA	2.2
3	D	205	TYR	2.2
3	D	153	LEU	2.2
5	F	423	ASP	2.2
4	E	52	GLU	2.2
2	C	247	PRO	2.2
2	C	811	PRO	2.2
5	F	164	LYS	2.2
3	D	463	GLN	2.2
3	D	245	LEU	2.2
2	C	421	GLU	2.2
5	F	111	GLU	2.2
1	B	65	PHE	2.2
3	D	68	PHE	2.2
1	B	164	ALA	2.1
3	D	295	GLY	2.1
3	D	132	TYR	2.1
3	D	565	ILE	2.1
3	D	1408	ILE	2.1
3	D	437	VAL	2.1
3	D	1281	VAL	2.1
1	B	118	ALA	2.1
2	C	418	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	774	LEU	2.1
3	D	204	LEU	2.1
5	F	137	GLY	2.1
5	F	393	THR	2.1
2	C	244	PRO	2.1
2	C	767	PRO	2.1
3	D	1299	PHE	2.1
5	F	156	VAL	2.1
3	D	369	ALA	2.1
1	B	94	LEU	2.1
2	C	221	LEU	2.1
3	D	532	GLY	2.1
3	D	801	GLY	2.1
2	C	511	GLU	2.1
5	F	92	PRO	2.1
1	B	16	GLN	2.1
1	A	70	GLY	2.1
2	C	388	ARG	2.1
3	D	378	ILE	2.1
2	C	252	LYS	2.1
5	F	173	TYR	2.1
3	D	314	PRO	2.1
3	D	185	VAL	2.0
1	A	231	ALA	2.0
2	C	807[A]	ARG	2.0
3	D	830	ALA	2.0
5	F	166	LEU	2.0
3	D	1127	GLU	2.0
2	C	225	SER	2.0
3	D	449	SER	2.0
3	D	368	VAL	2.0
3	D	1053[A]	PHE	2.0
1	B	6	LEU	2.0
2	C	593	ALA	2.0
2	C	188	LYS	2.0
5	F	88	ILE	2.0
5	F	135	ILE	2.0
6	G	16	DC	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	B	2001	1/1	0.92	0.07	64,64,64,64	0
9	MG	F	2001	1/1	0.93	0.07	52,52,52,52	0
9	MG	D	2004	1/1	0.97	0.09	74,74,74,74	0
9	MG	D	2003	1/1	0.99	0.03	37,37,37,37	0
10	ZN	D	2001	1/1	1.00	0.03	36,36,36,36	0
10	ZN	D	2002	1/1	1.00	0.02	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.