



# Full wwPDB X-ray Structure Validation Report

Oct 1, 2014 – 11:05 PM EDT

PDB ID : 4Q4Z  
Title : Thermus thermophilus RNA polymerase de novo transcription initiation complex  
Authors : Murakami, K.S.  
Deposited on : 2014-04-15  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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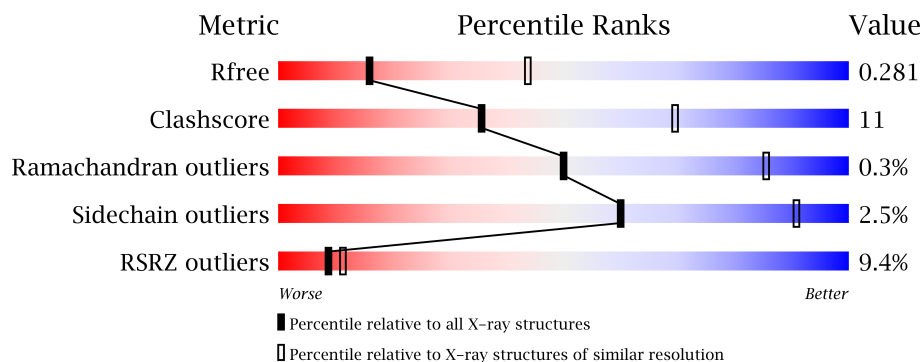
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	
5	F	423	
6	G	22	
7	H	27	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	MG	D	2003	-	X
10	MG	D	2004	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28755 atoms, of which 0 are hydrogen and 0 are deuterium.

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	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	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	0	0
			8774	5550	1565	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1494	Total	C	N	O	S	0	1	0
			11808	7484	2083	2205	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
			2807	1770	509	524	4			

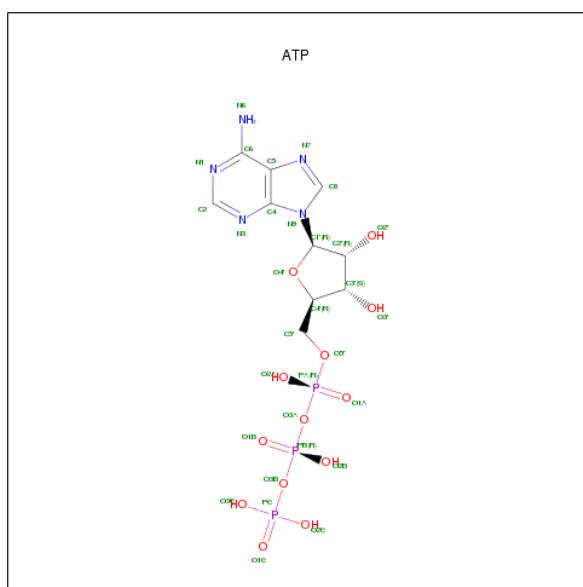
- Molecule 6 is a DNA chain called DNA (5'-D(\*CP\*CP\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*AP\*GP\*CP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	18	Total	C	N	O	P	0	0	0
			370	175	68	109	18			

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

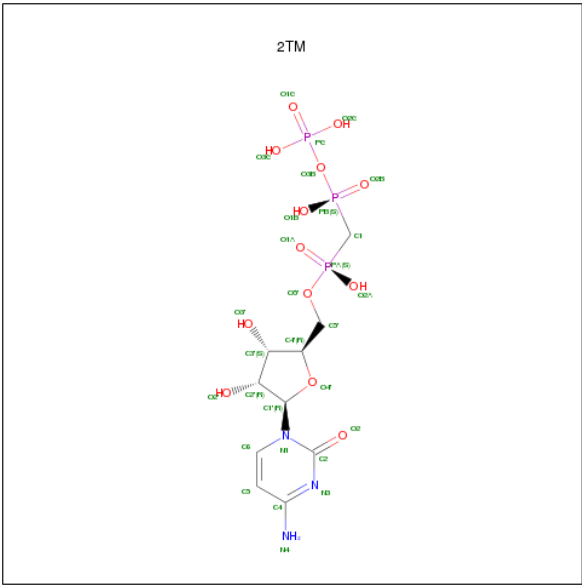
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	3	Total	Mg	0	0
			3	3		

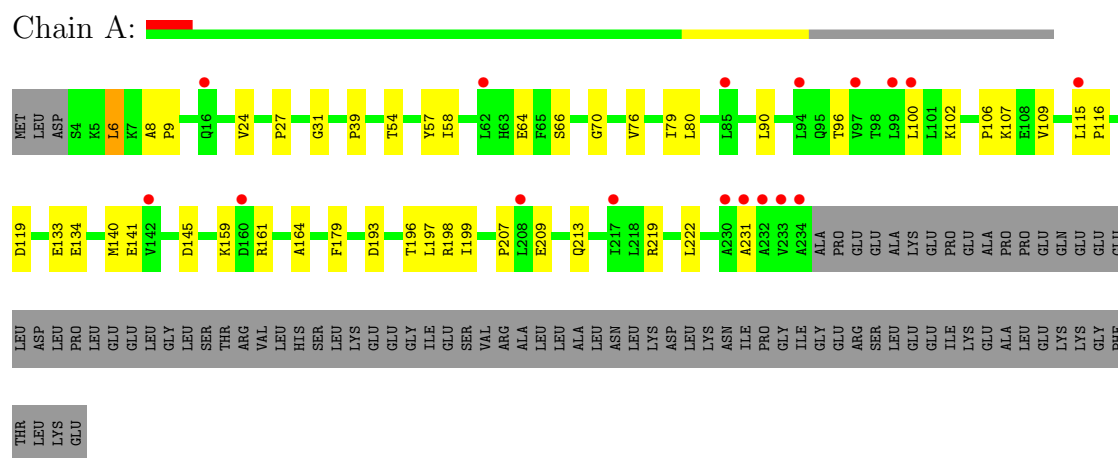
- Molecule 11 is 5'-O-[(S)-HYDROXY{[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]METHYL}PHOSPHORYL]CYTIDINE (three-letter code: 2TM) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



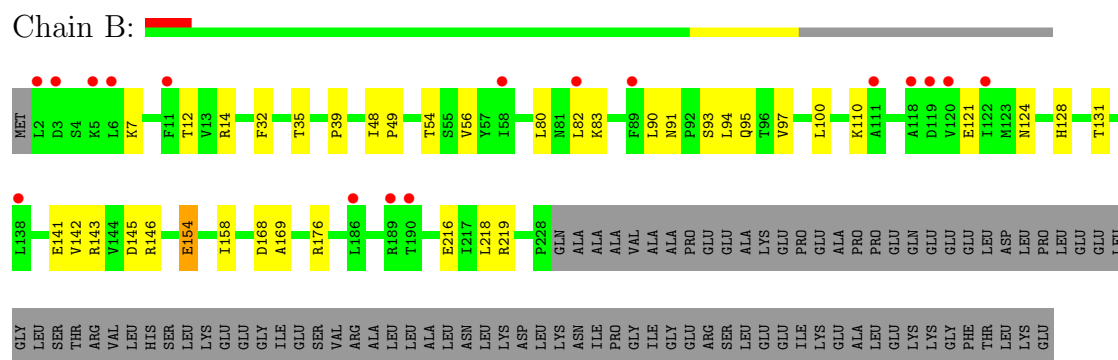
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

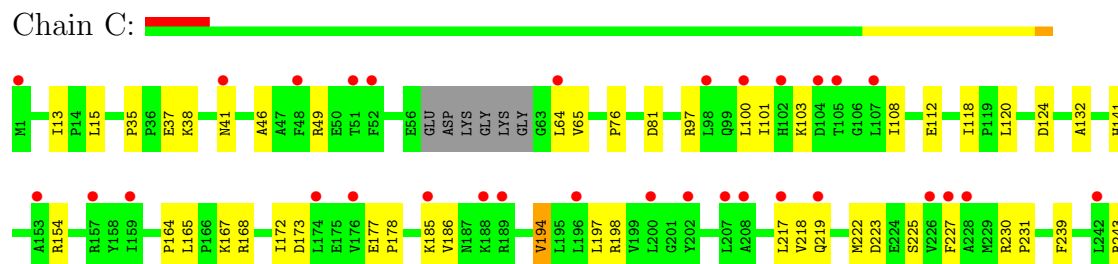
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

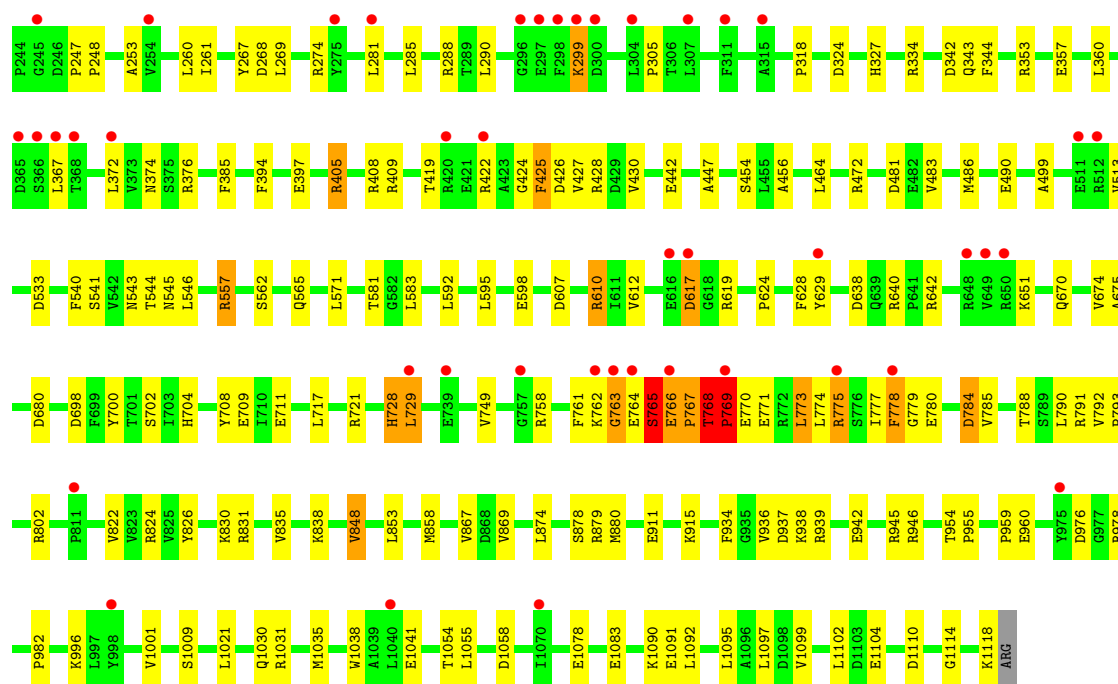


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



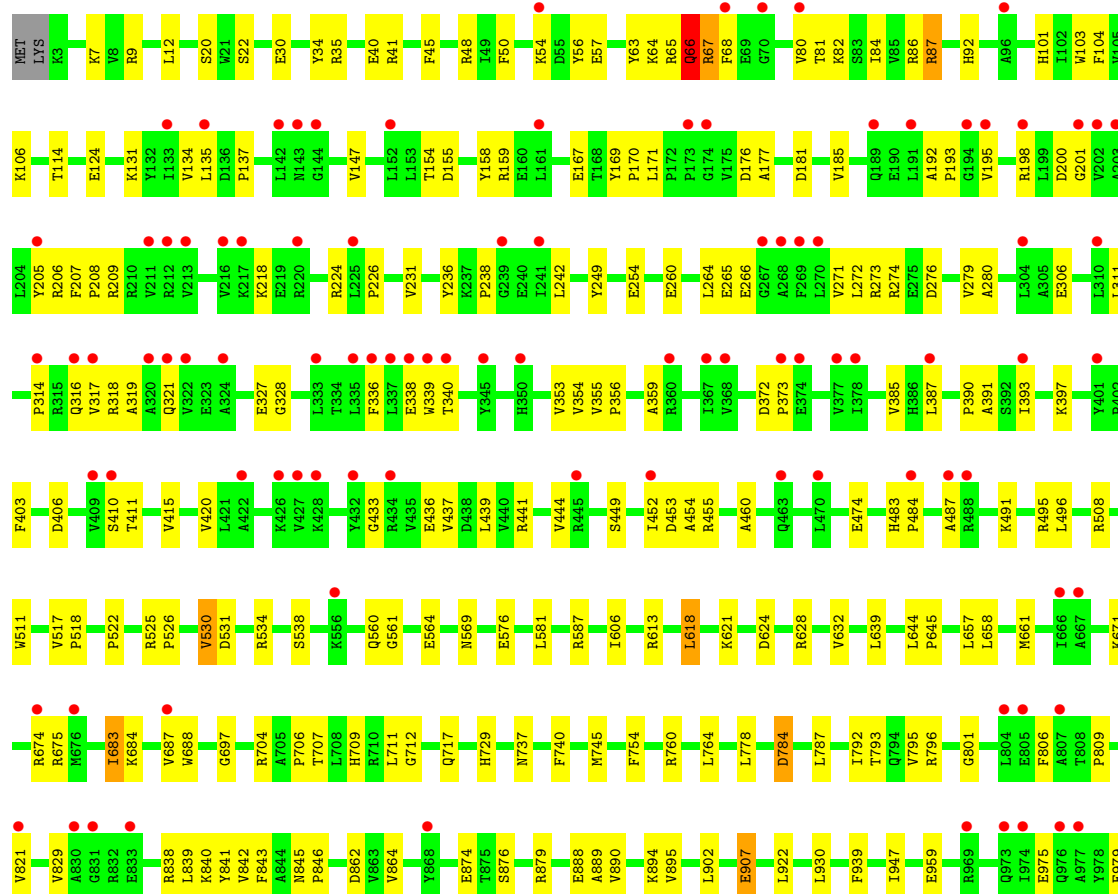
#### • Molecule 2: DNA-directed RNA polymerase subunit beta



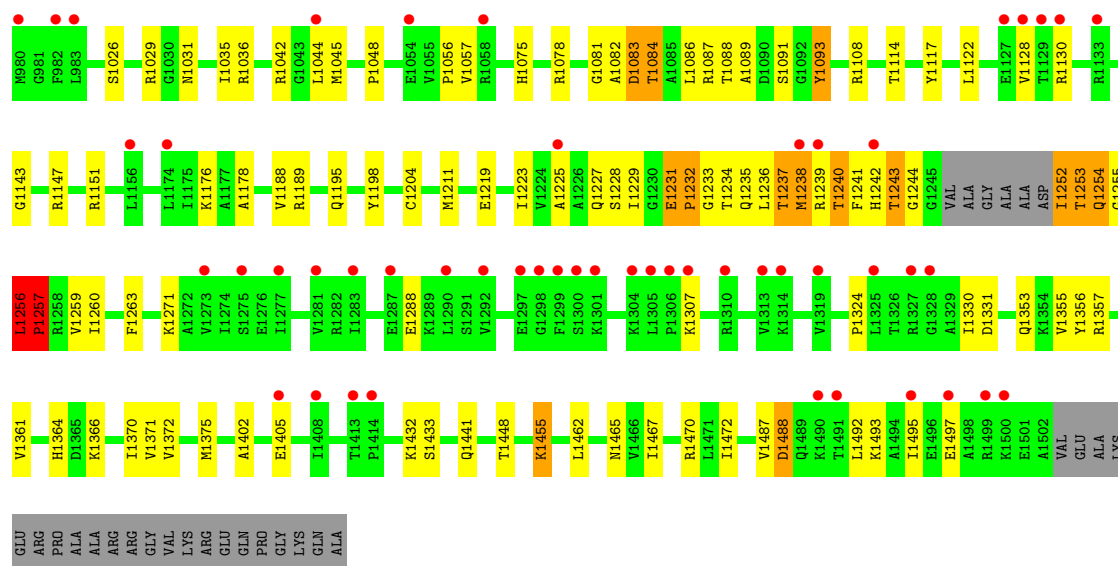


• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

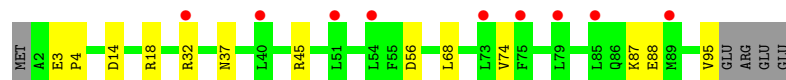






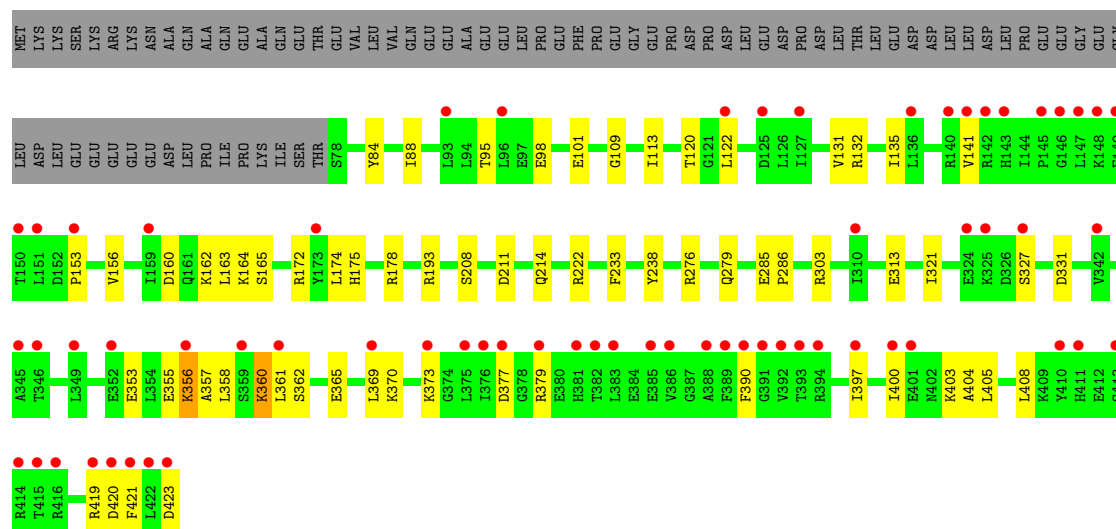
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



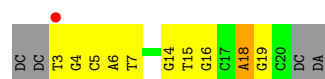
- Molecule 5: RNA polymerase sigma factor SigA

Chain F:



- Molecule 6: DNA (5'-D(\*CP\*CP\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*AP\*GP\*CP\*CP\*A)-3')

Chain G:



- Molecule 7: DNA (25-MER)

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.49Å 102.16Å 294.72Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	29.78 – 2.90 43.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	89.5 (29.78-2.90) 84.3 (43.54-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9.1692)	Depositor
R, $R_{free}$	0.256 , 0.275 0.264 , 0.281	Depositor DCC
$R_{free}$ test set	1619 reflections (1.57%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 0.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	3 of 111819 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	28755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2TM, MG, ZN, ATP

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	0.24	0/1841	0.46	0/2504
1	B	0.22	0/1821	0.44	0/2476
2	C	0.31	1/8941 (0.0%)	0.50	6/12092 (0.0%)
3	D	0.35	1/12019 (0.0%)	0.50	4/16248 (0.0%)
4	E	0.24	0/775	0.41	0/1045
5	F	0.23	0/2852	0.40	0/3837
6	G	0.72	2/414 (0.5%)	1.16	3/637 (0.5%)
7	H	0.57	0/580	1.13	3/895 (0.3%)
All	All	0.33	4/29243 (0.0%)	0.52	16/39734 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1093	TYR	CE2-CZ	-6.38	1.30	1.38
6	G	18	DA	O3'-P	-5.67	1.54	1.61
6	G	3	DT	O3'-P	-5.63	1.54	1.61
2	C	769	PRO	N-CD	5.43	1.55	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	761	PHE	O-C-N	-10.43	106.01	122.70
6	G	18	DA	O4'-C1'-N9	9.34	114.54	108.00
3	D	1257	PRO	CA-N-CD	-8.41	99.72	111.50
3	D	1232	PRO	CA-N-CD	-7.58	100.88	111.50
2	C	761	PHE	C-N-CA	7.11	139.47	121.70
2	C	761	PHE	CA-C-N	7.08	132.78	117.20
6	G	18	DA	C4'-C3'-C2'	6.18	108.67	103.10
3	D	1256	LEU	C-N-CD	6.01	141.01	128.40
2	C	766	GLU	C-N-CD	5.84	140.67	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	765	SER	N-CA-C	-5.53	96.06	111.00
3	D	1231	GLU	C-N-CD	5.36	139.65	128.40
6	G	18	DA	O5'-P-OP1	5.31	117.08	110.70
7	H	15	DT	O4'-C1'-N1	5.30	111.71	108.00
2	C	769	PRO	CA-N-CD	-5.24	104.16	111.50
7	H	20	DG	C1'-O4'-C4'	-5.24	104.86	110.10
7	H	12	DC	O4'-C1'-N1	5.20	111.64	108.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1863	38	0
1	B	1789	0	1841	24	0
2	C	8774	0	8877	226	3
3	D	11808	0	12041	258	4
4	E	761	0	778	9	1
5	F	2807	0	2882	101	2
6	G	370	0	202	19	0
7	H	516	0	283	31	1
8	C	31	0	11	2	0
9	D	2	0	0	0	0
10	D	3	0	0	0	0
11	D	29	0	0	0	0
12	A	4	0	0	9	0
12	B	1	0	0	0	0
12	C	22	0	0	29	0
12	D	26	0	0	25	0
12	E	2	0	0	1	0
12	G	1	0	0	0	0
All	All	28755	0	28778	603	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (603) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:773:LEU:CD2	5:F:373:LYS:HG3	1.14	1.60
5:F:358:LEU:HD13	5:F:370:LYS:NZ	1.33	1.41
2:C:773:LEU:CD2	5:F:373:LYS:CG	2.03	1.36
2:C:778:PHE:HE2	5:F:419:ARG:NH2	1.25	1.35
2:C:764:GLU:O	2:C:766:GLU:N	1.62	1.32
5:F:358:LEU:CD1	5:F:370:LYS:CE	2.09	1.30
5:F:358:LEU:CD1	5:F:370:LYS:NZ	1.92	1.30
2:C:768:THR:O	2:C:771:GLU:N	1.65	1.28
5:F:355:GLU:OE1	5:F:358:LEU:HD12	1.21	1.27
5:F:358:LEU:HD11	5:F:370:LYS:CE	1.64	1.26
1:A:107:LYS:HG3	12:A:404:HOH:O	1.23	1.25
2:C:778:PHE:CE2	5:F:419:ARG:NH2	2.08	1.21
2:C:764:GLU:OE1	3:D:54:LYS:HE2	1.37	1.20
2:C:778:PHE:HE2	5:F:419:ARG:CZ	1.55	1.19
3:D:1091:SER:OG	3:D:1234:THR:OG1	1.61	1.17
2:C:996:LYS:HG2	12:C:1321:HOH:O	1.44	1.17
2:C:778:PHE:CE2	5:F:419:ARG:CZ	2.26	1.17
2:C:878:SER:HB3	12:C:1301:HOH:O	1.44	1.16
2:C:773:LEU:HD23	5:F:373:LYS:HG3	1.25	1.15
5:F:358:LEU:CD1	5:F:370:LYS:HZ1	1.50	1.14
12:C:1314:HOH:O	5:F:331:ASP:HA	1.45	1.14
2:C:773:LEU:HD22	5:F:373:LYS:CG	1.69	1.11
5:F:358:LEU:HD11	5:F:370:LYS:HE2	1.21	1.11
2:C:773:LEU:HD23	5:F:373:LYS:CB	1.80	1.10
2:C:773:LEU:HD12	2:C:777:ILE:HD11	1.29	1.10
7:H:21:DA:H2''	7:H:22:DT:H5'	1.30	1.09
6:G:6:DA:N1	7:H:22:DT:N3	2.01	1.08
2:C:717:LEU:CD2	2:C:763:GLY:HA2	1.86	1.06
2:C:773:LEU:HD23	5:F:373:LYS:CG	1.73	1.06
3:D:1056:PRO:HA	12:D:2114:HOH:O	1.54	1.04
1:A:107:LYS:CG	12:A:404:HOH:O	1.83	1.04
1:A:107:LYS:CD	12:A:404:HOH:O	2.01	1.04
3:D:1044:LEU:HA	12:D:2114:HOH:O	1.57	1.04
1:A:107:LYS:HE2	12:A:404:HOH:O	1.54	1.03
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.39	1.01
3:D:538:SER:HB2	12:D:2119:HOH:O	1.60	1.01
3:D:1223:ILE:O	3:D:1227:GLN:HG3	1.60	1.01
2:C:717:LEU:HD21	2:C:763:GLY:HA2	1.44	1.00
2:C:768:THR:O	2:C:770:GLU:N	1.95	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:728:HIS:HB3	5:F:423:ASP:O	1.61	0.98
3:D:65:ARG:CZ	3:D:68:PHE:CE2	2.47	0.97
1:A:107:LYS:CE	12:A:404:HOH:O	2.08	0.97
2:C:543:ASN:HB3	12:C:1316:HOH:O	0.79	0.96
5:F:358:LEU:HD13	5:F:370:LYS:CE	1.82	0.96
6:G:7:DT:H3	7:H:21:DA:N6	1.65	0.95
2:C:777:ILE:HA	5:F:405:LEU:HD11	1.48	0.94
3:D:538:SER:CB	12:D:2119:HOH:O	2.16	0.93
3:D:1235:GLN:HG3	3:D:1239:ARG:HD3	1.50	0.92
3:D:1081:GLY:O	3:D:1084:THR:OG1	1.85	0.92
2:C:1041:GLU:HG2	12:C:1315:HOH:O	1.69	0.91
2:C:764:GLU:OE1	3:D:54:LYS:CE	2.19	0.91
2:C:268:ASP:HA	12:C:1307:HOH:O	1.71	0.90
2:C:768:THR:C	2:C:770:GLU:H	1.75	0.89
2:C:481:ASP:HA	12:C:1322:HOH:O	1.72	0.88
2:C:880:MET:CE	3:D:1242:HIS:CD2	2.55	0.88
5:F:358:LEU:HD13	5:F:370:LYS:HZ1	0.71	0.88
2:C:774:LEU:HA	2:C:777:ILE:CD1	2.02	0.88
3:D:206:ARG:NH2	5:F:101:GLU:OE2	2.06	0.88
3:D:65:ARG:NH2	3:D:68:PHE:CE2	2.41	0.88
5:F:358:LEU:CD1	5:F:370:LYS:HE3	2.04	0.87
3:D:65:ARG:CZ	3:D:68:PHE:HE2	1.87	0.87
3:D:947:ILE:HA	12:D:2120:HOH:O	1.73	0.86
3:D:1225:ALA:O	3:D:1229:ILE:HD12	1.76	0.85
5:F:355:GLU:OE1	5:F:358:LEU:CD1	2.18	0.85
2:C:764:GLU:CD	3:D:54:LYS:HE2	1.96	0.85
3:D:581:LEU:HD21	12:D:2108:HOH:O	1.77	0.84
2:C:768:THR:C	2:C:770:GLU:N	2.27	0.83
2:C:778:PHE:CZ	5:F:419:ARG:CZ	2.61	0.83
2:C:880:MET:HE1	3:D:1242:HIS:CD2	2.14	0.83
5:F:357:ALA:O	5:F:360:LYS:HB2	1.78	0.82
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.62	0.81
2:C:717:LEU:HD23	2:C:763:GLY:HA2	1.61	0.81
7:H:21:DA:C2'	7:H:22:DT:H5'	2.09	0.81
2:C:764:GLU:O	2:C:765:SER:C	2.20	0.80
2:C:472:ARG:HD2	12:C:1322:HOH:O	1.83	0.79
2:C:774:LEU:CA	2:C:777:ILE:HD12	2.11	0.79
3:D:1086:LEU:O	3:D:1089:ALA:HB3	1.82	0.78
7:H:20:DG:H2''	7:H:21:DA:C5'	2.14	0.78
2:C:773:LEU:CD1	2:C:777:ILE:HD11	2.13	0.77
3:D:675:ARG:NH2	5:F:420:ASP:O	2.17	0.77
2:C:762:LYS:HG2	2:C:784:ASP:O	1.85	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:68:PHE:O	3:D:80:VAL:HG23	1.84	0.77
2:C:773:LEU:HD22	5:F:373:LYS:HG3	0.77	0.77
2:C:773:LEU:HD23	5:F:373:LYS:HB2	1.67	0.77
2:C:880:MET:HE2	3:D:1242:HIS:CD2	2.19	0.77
3:D:65:ARG:NH2	3:D:68:PHE:HE2	1.78	0.77
6:G:7:DT:C2	7:H:21:DA:N1	2.53	0.77
2:C:422:ARG:HD2	7:H:15:DT:OP2	1.84	0.76
5:F:355:GLU:CD	5:F:358:LEU:HD12	2.07	0.76
3:D:1082:ALA:O	3:D:1086:LEU:HD13	1.87	0.74
5:F:358:LEU:CD2	5:F:370:LYS:HE3	2.17	0.74
3:D:1432:LYS:HD3	12:D:2122:HOH:O	1.86	0.74
2:C:409:ARG:HH11	2:C:454:SER:HB2	1.53	0.74
2:C:758:ARG:HH21	2:C:788:THR:HB	1.53	0.73
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.73
2:C:1030:GLN:OE1	3:D:628:ARG:NH1	2.20	0.73
6:G:7:DT:O2	7:H:21:DA:N1	2.21	0.73
5:F:361:LEU:HD11	5:F:408:LEU:HG	1.72	0.72
7:H:20:DG:H2"	7:H:21:DA:H5"	1.72	0.72
3:D:1084:THR:O	3:D:1088:THR:OG1	2.07	0.72
2:C:764:GLU:O	2:C:766:GLU:HG3	1.90	0.71
2:C:541:SER:HB2	12:C:1302:HOH:O	1.90	0.71
2:C:167:LYS:HD3	7:H:12:DC:H5	1.55	0.71
2:C:728:HIS:HD2	5:F:423:ASP:HB2	1.54	0.71
3:D:65:ARG:CD	5:F:379:ARG:HB3	2.21	0.71
3:D:63:TYR:HD1	3:D:68:PHE:CE1	2.09	0.70
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.70
6:G:4:DG:H2"	6:G:5:DC:OP2	1.91	0.70
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.25	0.70
3:D:68:PHE:O	3:D:80:VAL:CG2	2.39	0.70
2:C:628:PHE:H	2:C:638:ASP:HB3	1.57	0.69
2:C:717:LEU:CD2	2:C:763:GLY:CA	2.69	0.69
3:D:65:ARG:NH2	3:D:68:PHE:CZ	2.60	0.69
3:D:1255:GLY:O	3:D:1259:VAL:HG23	1.93	0.69
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.73	0.69
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.75	0.68
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.74	0.68
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.75	0.68
2:C:428:ARG:NH2	2:C:447:ALA:O	2.27	0.68
2:C:771:GLU:HB3	2:C:775:ARG:NH2	2.09	0.67
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.67
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.77	0.67
3:D:576:GLU:HB3	12:D:2102:HOH:O	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:21:DA:H2''	7:H:22:DT:C5'	2.18	0.67
2:C:773:LEU:HD12	2:C:777:ILE:CD1	2.17	0.66
3:D:1228:SER:O	3:D:1232:PRO:HD2	1.95	0.66
3:D:1240:THR:O	3:D:1241:PHE:HB2	1.94	0.66
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.28	0.66
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.29	0.66
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.61	0.66
2:C:230:ARG:HD3	2:C:231:PRO:HD2	1.78	0.66
2:C:768:THR:O	2:C:770:GLU:C	2.35	0.66
3:D:526:PRO:HD2	12:D:2119:HOH:O	1.95	0.66
2:C:670:GLN:HE21	2:C:700:TYR:H	1.42	0.65
2:C:784:ASP:N	2:C:784:ASP:OD2	2.29	0.65
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.77	0.65
3:D:1044:LEU:O	3:D:1244:GLY:HA2	1.95	0.65
3:D:433:GLY:HA2	3:D:449:SER:H	1.62	0.65
5:F:357:ALA:HA	5:F:360:LYS:CG	2.27	0.65
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.79	0.65
3:D:411:THR:O	5:F:178:ARG:NH1	2.26	0.65
2:C:778:PHE:HE2	5:F:419:ARG:HH22	1.37	0.65
3:D:947:ILE:HD13	12:D:2120:HOH:O	1.97	0.65
3:D:1231:GLU:OE1	3:D:1232:PRO:HD3	1.97	0.65
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.30	0.64
2:C:717:LEU:HD21	2:C:763:GLY:CA	2.24	0.64
5:F:355:GLU:O	5:F:358:LEU:HB2	1.97	0.64
3:D:1253:THR:OG1	3:D:1254:GLN:N	2.31	0.64
6:G:7:DT:N3	7:H:21:DA:N6	2.28	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.64
3:D:63:TYR:CD1	3:D:68:PHE:CE1	2.85	0.64
2:C:764:GLU:C	2:C:766:GLU:N	2.49	0.64
3:D:1233:GLY:O	3:D:1237:THR:OG1	2.16	0.63
3:D:1252:ILE:HG13	3:D:1252:ILE:O	1.98	0.63
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.79	0.63
3:D:316:GLN:NE2	3:D:340:THR:O	2.31	0.63
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.80	0.63
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.80	0.63
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.31	0.63
5:F:357:ALA:HA	5:F:360:LYS:HG2	1.81	0.63
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.64	0.62
2:C:562:SER:HA	12:C:1316:HOH:O	1.99	0.62
3:D:1083:ASP:OD2	3:D:1253:THR:HG22	2.00	0.62
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.28	0.62
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.81	0.62
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.82	0.61
3:D:534:ARG:NH2	5:F:313:GLU:O	2.33	0.61
3:D:65:ARG:HD3	5:F:379:ARG:HB3	1.81	0.61
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.82	0.61
5:F:358:LEU:HD13	5:F:370:LYS:HE3	1.73	0.61
3:D:671:LYS:NZ	5:F:421:PHE:HA	2.14	0.61
2:C:773:LEU:O	2:C:777:ILE:HG13	2.01	0.61
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.32	0.61
6:G:6:DA:H2''	6:G:7:DT:C5'	2.30	0.61
2:C:763:GLY:C	2:C:765:SER:H	2.04	0.60
2:C:376:ARG:HE	5:F:276:ARG:HG3	1.66	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.60
2:C:274:ARG:HD2	2:C:288:ARG:HG2	1.83	0.60
3:D:1432:LYS:O	3:D:1455:LYS:NZ	2.34	0.60
12:C:1315:HOH:O	3:D:1462:LEU:HB3	2.01	0.60
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.66	0.60
2:C:764:GLU:O	2:C:766:GLU:CA	2.48	0.60
3:D:959:GLU:OE1	3:D:959:GLU:N	2.30	0.60
3:D:846:PRO:HD2	12:D:2115:HOH:O	2.02	0.60
4:E:32:ARG:O	4:E:95:VAL:HG21	2.01	0.60
3:D:1091:SER:OG	3:D:1234:THR:CB	2.48	0.60
3:D:1231:GLU:HB3	3:D:1232:PRO:CD	2.32	0.59
2:C:960:GLU:CB	12:C:1303:HOH:O	2.51	0.59
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.32	0.59
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.68	0.59
2:C:768:THR:O	2:C:770:GLU:CA	2.51	0.59
6:G:7:DT:C4	7:H:21:DA:N6	2.57	0.59
7:H:20:DG:H2''	7:H:21:DA:H5'	1.83	0.59
3:D:65:ARG:NE	3:D:68:PHE:HE2	1.99	0.59
3:D:845:ASN:HB2	12:D:2115:HOH:O	2.01	0.58
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.86	0.58
3:D:1231:GLU:HB3	3:D:1232:PRO:HD2	1.85	0.58
1:B:94:LEU:O	1:B:146:ARG:NH2	2.36	0.57
7:H:20:DG:C2'	7:H:21:DA:H5''	2.33	0.57
2:C:422:ARG:CD	7:H:15:DT:OP2	2.51	0.57
2:C:581:THR:HB	12:C:1312:HOH:O	2.04	0.57
2:C:376:ARG:NE	5:F:276:ARG:HG3	2.19	0.57
2:C:778:PHE:CE2	5:F:419:ARG:NH1	2.71	0.57
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.87	0.57
5:F:358:LEU:CD1	5:F:370:LYS:HZ3	2.12	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.38	0.57
3:D:65:ARG:NE	3:D:68:PHE:CE2	2.71	0.57
3:D:45:PHE:O	3:D:86:ARG:NH2	2.37	0.57
5:F:233:PHE:CD2	7:H:2:DA:H1'	2.40	0.57
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.87	0.57
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.41	0.56
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.87	0.56
2:C:878:SER:CB	12:C:1301:HOH:O	2.24	0.56
3:D:1492:LEU:HD22	4:E:74:VAL:HG21	1.87	0.56
1:A:106:PRO:HD3	1:A:134:GLU:HG2	1.88	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.19	0.56
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.88	0.56
1:A:70:GLY:N	2:C:607:ASP:OD1	2.38	0.56
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.87	0.55
3:D:1045:MET:HE1	3:D:1243:THR:O	2.07	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.88	0.55
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.55
2:C:198:ARG:HE	2:C:227:PHE:HA	1.72	0.55
2:C:728:HIS:CB	5:F:423:ASP:O	2.45	0.55
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.41	0.55
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.88	0.55
2:C:409:ARG:HD2	12:C:1311:HOH:O	2.06	0.55
2:C:419:THR:HG22	2:C:422:ARG:HE	1.71	0.55
1:B:93:SER:O	1:B:95:GLN:NE2	2.39	0.55
3:D:1229:ILE:CG2	3:D:1356:TYR:OH	2.55	0.55
3:D:526:PRO:CD	12:D:2119:HOH:O	2.54	0.55
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.06	0.55
3:D:411:THR:HG23	3:D:436:GLU:HA	1.89	0.55
6:G:6:DA:H2''	6:G:7:DT:H5'	1.87	0.55
3:D:63:TYR:CD1	3:D:68:PHE:HE1	2.25	0.55
1:A:31:GLY:HA2	12:A:403:HOH:O	2.06	0.55
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.88	0.55
2:C:353:ARG:NH1	2:C:357:GLU:OE2	2.40	0.54
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.87	0.54
2:C:629:TYR:HB3	12:C:1319:HOH:O	2.08	0.54
3:D:56:TYR:CE2	3:D:66:GLN:HG3	2.42	0.54
1:A:231:ALA:HB2	1:B:12:THR:HG22	1.89	0.54
2:C:773:LEU:CD1	2:C:777:ILE:CG1	2.85	0.54
3:D:657:LEU:HG	3:D:661:MET:HE2	1.89	0.54
6:G:7:DT:O2	7:H:21:DA:C2	2.59	0.54
2:C:243:ARG:NH1	7:H:9:DG:O6	2.39	0.54
2:C:167:LYS:HD3	7:H:12:DC:C5	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:846:PRO:CD	12:D:2115:HOH:O	2.55	0.54
2:C:778:PHE:CZ	5:F:419:ARG:NE	2.75	0.54
6:G:5:DC:H1'	6:G:6:DA:C8	2.43	0.54
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.08	0.54
2:C:838:LYS:NZ	8:C:1201:ATP:O1A	2.41	0.53
5:F:357:ALA:C	5:F:360:LYS:HB2	2.28	0.53
2:C:64:LEU:HB3	2:C:100:LEU:HD11	1.90	0.53
3:D:697:GLY:HA3	12:E:101:HOH:O	2.09	0.53
3:D:1235:GLN:O	3:D:1239:ARG:HB2	2.09	0.53
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.90	0.53
5:F:358:LEU:HD22	5:F:370:LYS:HE3	1.89	0.53
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.89	0.53
2:C:778:PHE:HZ	5:F:419:ARG:NE	2.07	0.53
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.90	0.53
2:C:835:VAL:HG23	12:C:1308:HOH:O	2.09	0.53
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.90	0.53
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.90	0.53
2:C:598:GLU:O	2:C:651:LYS:NZ	2.35	0.53
3:D:894:LYS:HD2	3:D:894:LYS:H	1.74	0.53
1:A:199:ILE:HB	1:A:207:PRO:HB3	1.91	0.52
2:C:425:PHE:O	2:C:427:VAL:N	2.42	0.52
2:C:557:ARG:HD3	2:C:879:ARG:HB3	1.90	0.52
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.92	0.52
2:C:422:ARG:CG	7:H:15:DT:OP2	2.57	0.52
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.92	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
3:D:658:LEU:HA	3:D:661:MET:HE3	1.92	0.52
3:D:439:LEU:CD1	5:F:172:ARG:HG3	2.40	0.52
3:D:65:ARG:C	3:D:66:GLN:O	2.46	0.52
3:D:684:LYS:O	3:D:687:VAL:HG12	2.09	0.52
2:C:223:ASP:OD1	2:C:225:SER:OG	2.24	0.52
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.90	0.52
6:G:15:DT:H2'	6:G:16:DG:C8	2.44	0.52
3:D:1086:LEU:CD1	3:D:1086:LEU:N	2.72	0.52
2:C:217:LEU:H	2:C:217:LEU:HD12	1.73	0.52
2:C:427:VAL:O	2:C:427:VAL:HG22	2.08	0.52
2:C:541:SER:O	2:C:545:ASN:ND2	2.43	0.52
3:D:1253:THR:O	3:D:1257:PRO:HD2	2.10	0.52
3:D:65:ARG:O	3:D:68:PHE:HB2	2.08	0.52
5:F:355:GLU:HA	5:F:358:LEU:HG	1.91	0.52
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.91	0.52
3:D:1253:THR:O	3:D:1257:PRO:HG2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:439:LEU:HD13	5:F:172:ARG:HG3	1.91	0.52
2:C:717:LEU:HD23	2:C:763:GLY:CA	2.37	0.52
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.10	0.52
3:D:200:ASP:O	3:D:397:LYS:HG2	2.10	0.52
3:D:564:GLU:HG3	12:D:2110:HOH:O	2.09	0.52
2:C:729:LEU:HD11	2:C:791:ARG:HH22	1.75	0.52
3:D:321:GLN:HB2	3:D:336:PHE:HB2	1.92	0.52
12:C:1315:HOH:O	3:D:1462:LEU:HD13	2.10	0.51
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.92	0.51
3:D:231:VAL:O	3:D:236:TYR:OH	2.28	0.51
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.93	0.51
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.25	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.51
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.75	0.51
7:H:24:DC:C2	7:H:25:DA:C5	2.99	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.93	0.51
3:D:1219:GLU:HA	12:D:2117:HOH:O	2.09	0.51
2:C:778:PHE:O	2:C:780:GLU:N	2.44	0.51
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.46	0.51
2:C:624:PRO:CB	12:C:1313:HOH:O	2.58	0.50
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.27	0.50
3:D:209:ARG:HE	3:D:391:ALA:HB2	1.74	0.50
3:D:671:LYS:HZ3	5:F:421:PHE:HA	1.74	0.50
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.93	0.50
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.93	0.50
3:D:1271:LYS:HE2	3:D:1331:ASP:HB2	1.93	0.50
2:C:15:LEU:HD11	2:C:583:LEU:HD11	1.93	0.50
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.92	0.50
3:D:975:GLU:O	3:D:979:GLU:HG2	2.12	0.50
2:C:610:ARG:HD3	2:C:612:VAL:HG23	1.92	0.50
3:D:1488:ASP:N	3:D:1488:ASP:OD1	2.31	0.50
2:C:543:ASN:C	12:C:1316:HOH:O	2.49	0.49
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.13	0.49
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.94	0.49
5:F:160:ASP:O	5:F:164:LYS:HG2	2.12	0.49
2:C:168:ARG:O	2:C:267:TYR:HA	2.13	0.49
1:B:154:GLU:HG3	3:D:840:LYS:HZ1	1.76	0.49
1:A:209:GLU:O	1:A:213:GLN:HG2	2.12	0.49
3:D:274:ARG:NH2	3:D:279:VAL:HG21	2.27	0.49
2:C:430:VAL:HG23	3:D:1078:ARG:HG2	1.95	0.49
2:C:773:LEU:CD1	2:C:777:ILE:CD1	2.86	0.49
3:D:1087:ARG:HB2	3:D:1237:THR:CG2	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.47	0.49
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.48	0.49
5:F:353:GLU:O	5:F:356:LYS:HB2	2.12	0.49
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.95	0.49
2:C:874:LEU:O	3:D:1029:ARG:HG3	2.12	0.49
3:D:155:ASP:OD1	3:D:159:ARG:NH1	2.46	0.49
5:F:238:TYR:HH	7:H:1:DT:H6	1.59	0.48
1:B:54:THR:HG22	1:B:169:ALA:HB2	1.95	0.48
2:C:65:VAL:HG21	2:C:103:LYS:HE3	1.95	0.48
2:C:774:LEU:O	2:C:777:ILE:HD12	2.12	0.48
3:D:1114:THR:OG1	3:D:1195:GLN:NE2	2.45	0.48
3:D:530:VAL:HG12	3:D:531:ASP:H	1.77	0.48
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.94	0.48
7:H:24:DC:N3	7:H:25:DA:C6	2.81	0.48
2:C:1031:ARG:NE	6:G:16:DG:OP1	2.36	0.48
2:C:1035:MET:SD	6:G:15:DT:H4'	2.53	0.48
2:C:777:ILE:HA	5:F:405:LEU:CD1	2.33	0.48
3:D:846:PRO:N	12:D:2115:HOH:O	2.47	0.48
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.95	0.48
3:D:1128:VAL:HG23	3:D:1130:ARG:H	1.79	0.48
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.95	0.48
3:D:1229:ILE:HG23	3:D:1356:TYR:OH	2.14	0.48
2:C:960:GLU:HB2	12:C:1303:HOH:O	2.11	0.48
2:C:376:ARG:HD3	5:F:276:ARG:HD2	1.94	0.48
2:C:1102:LEU:HD11	3:D:9:ARG:HH11	1.78	0.48
5:F:361:LEU:HD11	5:F:408:LEU:CG	2.42	0.48
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.95	0.48
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.96	0.48
2:C:767:PRO:O	2:C:769:PRO:HD3	2.14	0.47
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.47	0.47
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.95	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.47
3:D:1042:ARG:HG3	3:D:1045:MET:HE3	1.96	0.47
3:D:264:LEU:HB3	12:D:2116:HOH:O	2.13	0.47
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.96	0.47
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.36	0.47
5:F:360:LYS:HD3	5:F:360:LYS:HA	1.63	0.47
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.97	0.47
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.96	0.47
1:A:109:VAL:HG22	12:A:404:HOH:O	2.13	0.47
2:C:405:ARG:NE	2:C:442:GLU:OE2	2.37	0.47
2:C:976:ASP:OD1	2:C:978:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.97	0.47
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.97	0.47
2:C:1058:ASP:OD1	3:D:621:LYS:HE2	2.14	0.47
2:C:1021:LEU:HD22	5:F:331:ASP:O	2.15	0.47
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.79	0.47
6:G:6:DA:N1	7:H:22:DT:C4	2.80	0.47
2:C:763:GLY:C	2:C:765:SER:N	2.68	0.47
3:D:272:LEU:O	3:D:279:VAL:N	2.47	0.47
3:D:658:LEU:HD11	3:D:674[A]:ARG:HH11	1.80	0.47
6:G:18:DA:H2''	6:G:19:DG:O5'	2.14	0.47
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.47	0.47
1:A:196:THR:HG21	2:C:934:PHE:CE2	2.47	0.47
3:D:683:ILE:HD11	3:D:688:TRP:CZ2	2.50	0.47
2:C:773:LEU:HD13	2:C:773:LEU:O	2.15	0.47
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.39	0.47
12:C:1315:HOH:O	3:D:1472:ILE:HG21	2.15	0.47
5:F:84:TYR:O	5:F:88:ILE:HG12	2.15	0.47
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.97	0.46
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.96	0.46
2:C:880:MET:HE1	3:D:1242:HIS:CG	2.49	0.46
3:D:65:ARG:NE	5:F:379:ARG:HB3	2.30	0.46
7:H:21:DA:C2'	7:H:22:DT:C5'	2.86	0.46
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.97	0.46
3:D:1088:THR:HG23	3:D:1238:MET:SD	2.56	0.46
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.96	0.46
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
3:D:1239:ARG:O	3:D:1241:PHE:CD1	2.68	0.46
3:D:737:ASN:ND2	3:D:1235:GLN:HE22	2.13	0.46
1:A:193:ASP:OD2	2:C:938:LYS:NZ	2.40	0.46
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.46
2:C:543:ASN:CB	12:C:1316:HOH:O	1.70	0.46
2:C:773:LEU:HD13	2:C:777:ILE:HG13	1.98	0.46
2:C:774:LEU:C	2:C:777:ILE:HD12	2.36	0.46
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.51	0.46
3:D:879:ARG:HD3	3:D:902:LEU:O	2.16	0.46
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.97	0.45
2:C:299:LYS:HE2	2:C:299:LYS:HA	1.96	0.45
1:A:90:LEU:HB2	1:A:119:ASP:HB3	1.98	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.65	0.45
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	0.45
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.75	0.45
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:LEU:HD22	1:A:141:GLU:HG2	1.98	0.45
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.98	0.45
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.17	0.45
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.30	0.45
5:F:357:ALA:HA	5:F:360:LYS:HB2	1.99	0.45
3:D:1091:SER:OG	3:D:1234:THR:CA	2.64	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
2:C:1118:LYS:HE2	3:D:20:SER:O	2.17	0.45
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.82	0.45
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.99	0.45
1:A:198:ARG:HD3	2:C:934:PHE:CE1	2.52	0.45
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.45
2:C:41:ASN:O	2:C:46:ALA:HB2	2.17	0.45
3:D:353:VAL:HG11	3:D:387:LEU:HD11	1.98	0.45
2:C:424:GLY:O	2:C:426:ASP:N	2.49	0.45
2:C:764:GLU:O	2:C:766:GLU:CG	2.61	0.45
3:D:238:PRO:HG3	3:D:318:ARG:HB2	1.99	0.45
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.87	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.16	0.44
3:D:264:LEU:CB	12:D:2116:HOH:O	2.65	0.44
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.50	0.44
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.00	0.44
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.82	0.44
4:E:95:VAL:O	4:E:95:VAL:HG12	2.16	0.44
2:C:367:LEU:HD13	2:C:372:LEU:HD21	2.00	0.44
2:C:763:GLY:O	2:C:765:SER:N	2.51	0.44
3:D:1232:PRO:HB3	3:D:1361:VAL:HG11	1.99	0.44
3:D:717:GLN:NE2	12:D:2118:HOH:O	2.50	0.44
5:F:109:GLY:O	5:F:113:ILE:HG13	2.17	0.44
5:F:362:SER:OG	5:F:365:GLU:HG2	2.18	0.44
2:C:422:ARG:HG2	7:H:15:DT:C6	2.52	0.44
2:C:1001:VAL:HG12	12:C:1317:HOH:O	2.17	0.44
3:D:260:GLU:HB3	3:D:271:VAL:HB	2.00	0.44
3:D:67:ARG:HG3	5:F:377:ASP:O	2.18	0.44
2:C:422:ARG:HG2	7:H:15:DT:OP2	2.18	0.44
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.99	0.44
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.99	0.44
3:D:1176:LYS:HE2	3:D:1176:LYS:HB3	1.79	0.44
3:D:1211:MET:HE3	3:D:1211:MET:HB2	1.89	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.17	0.44
3:D:265:GLU:N	12:D:2116:HOH:O	2.51	0.44
3:D:84:ILE:O	3:D:87:ARG:HG2	2.18	0.44
7:H:15:DT:H2"	7:H:16:DC:H5'	1.99	0.44
1:A:31:GLY:CA	12:A:403:HOH:O	2.64	0.44
2:C:1095:LEU:O	3:D:101:HIS:NE2	2.39	0.44
8:C:1201:ATP:H5'1	12:D:2123:HOH:O	2.16	0.44
3:D:135:LEU:O	3:D:453:ASP:HB3	2.18	0.44
2:C:324:ASP:HB3	2:C:327:HIS:HB2	2.00	0.44
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.50	0.44
2:C:194:VAL:HA	2:C:197:LEU:HD12	2.00	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.43
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.53	0.43
3:D:1487:VAL:HG11	3:D:1492:LEU:HD13	2.00	0.43
2:C:768:THR:HB	2:C:770:GLU:HB2	2.01	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.17	0.43
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.53	0.43
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.73	0.43
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.00	0.43
2:C:101:ILE:HG12	2:C:108:ILE:HG12	2.01	0.43
2:C:154:ARG:H	2:C:154:ARG:HG2	1.68	0.43
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.00	0.43
2:C:97:ARG:HG2	2:C:112:GLU:HB2	2.00	0.43
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.47	0.43
3:D:410:SER:H	5:F:164:LYS:NZ	2.16	0.43
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.43
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.43
2:C:996:LYS:CG	12:C:1321:HOH:O	2.29	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.01	0.43
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.87	0.43
3:D:1263:PHE:CD2	3:D:1375:MET:HE2	2.48	0.43
3:D:526:PRO:N	12:D:2119:HOH:O	2.51	0.43
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.53	0.43
5:F:355:GLU:HA	5:F:358:LEU:CG	2.49	0.43
2:C:773:LEU:HD23	5:F:373:LYS:HB3	1.91	0.43
7:H:23:DG:H2"	7:H:24:DC:C6	2.53	0.43
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.01	0.42
3:D:1086:LEU:HD12	3:D:1086:LEU:N	2.33	0.42
3:D:81:THR:OG1	3:D:82:LYS:N	2.52	0.42
4:E:37:ASN:N	4:E:37:ASN:OD1	2.44	0.42
2:C:562:SER:CA	12:C:1316:HOH:O	2.63	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.54	0.42
3:D:12:LEU:HA	3:D:12:LEU:HD23	1.85	0.42
3:D:1255:GLY:HA2	3:D:1355:VAL:HG13	2.01	0.42
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.19	0.42
4:E:68:LEU:HA	4:E:68:LEU:HD12	1.77	0.42
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.42
3:D:1254:GLN:O	3:D:1257:PRO:HB2	2.19	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.50	0.42
3:D:560:GLN:HE22	5:F:222:ARG:HH12	1.68	0.42
2:C:1091:GLU:OE2	3:D:606:ILE:HG21	2.19	0.42
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.84	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.00	0.42
2:C:218:VAL:O	2:C:222:MET:HG2	2.19	0.42
2:C:878:SER:N	12:C:1301:HOH:O	2.44	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
5:F:355:GLU:O	5:F:356:LYS:C	2.58	0.42
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.92	0.42
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.52	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.88	0.42
3:D:706:PRO:HG3	6:G:14:DG:H21	1.84	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.80	0.42
2:C:624:PRO:CA	12:C:1313:HOH:O	2.68	0.42
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.54	0.42
3:D:838:ARG:HD3	3:D:874:GLU:OE1	2.20	0.42
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.42
1:A:133:GLU:HG2	1:A:134:GLU:N	2.35	0.42
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.42
5:F:355:GLU:HA	5:F:358:LEU:HB2	2.02	0.42
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.02	0.41
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.20	0.41
3:D:801:GLY:HA3	3:D:821:VAL:HG13	2.01	0.41
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.41
2:C:768:THR:OG1	2:C:771:GLU:HG3	2.20	0.41
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.41
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.95	0.41
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.02	0.41
3:D:1253:THR:O	3:D:1257:PRO:CD	2.68	0.41
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.01	0.41
3:D:176:ASP:OD1	3:D:177:ALA:N	2.44	0.41
3:D:185:VAL:N	3:D:201:GLY:O	2.45	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.02	0.41
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.20	0.41
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.02	0.41
3:D:760:ARG:O	3:D:764:LEU:HB2	2.21	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.84	0.41
2:C:771:GLU:HB3	2:C:775:ARG:HH21	1.83	0.41
3:D:66:GLN:C	3:D:68:PHE:N	2.73	0.41
5:F:321:ILE:O	5:F:327:SER:HB3	2.20	0.41
5:F:358:LEU:HD11	5:F:370:LYS:NZ	1.97	0.41
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.02	0.41
2:C:765:SER:O	2:C:767:PRO:HD3	2.21	0.41
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.75	0.41
3:D:68:PHE:O	3:D:80:VAL:HG21	2.19	0.41
3:D:704:ARG:HB2	3:D:745:MET:HG2	2.03	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.96	0.41
5:F:88:ILE:CG2	5:F:193:ARG:HG2	2.50	0.41
6:G:5:DC:H1'	6:G:6:DA:H8	1.85	0.41
2:C:1102:LEU:HD11	3:D:9:ARG:HB2	2.03	0.41
2:C:408:ARG:NH1	2:C:456:ALA:O	2.53	0.41
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.03	0.41
3:D:538:SER:HB3	12:D:2119:HOH:O	2.03	0.41
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.01	0.41
1:B:124:ASN:N	1:B:124:ASN:OD1	2.53	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.03	0.41
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.02	0.41
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.03	0.41
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.56	0.41
3:D:675:ARG:HH22	5:F:420:ASP:HB3	1.85	0.41
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.03	0.41
2:C:773:LEU:C	2:C:773:LEU:CD1	2.89	0.41
2:C:946:ARG:HG3	12:C:1320:HOH:O	2.20	0.41
3:D:525:ARG:C	12:D:2119:HOH:O	2.59	0.41
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.86	0.41
1:A:109:VAL:CG2	12:A:404:HOH:O	2.69	0.41
2:C:773:LEU:HD13	2:C:777:ILE:CG1	2.51	0.41
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.85	0.41
3:D:613:ARG:HG3	3:D:618:LEU:HD22	2.03	0.41
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.35	0.40
3:D:226:PRO:HD3	3:D:249:TYR:CE2	2.56	0.40
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.93	0.40
7:H:21:DA:H1'	7:H:22:DT:C5'	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.95	0.40
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.55	0.40
2:C:848:VAL:HB	3:D:740:PHE:O	2.21	0.40
2:C:1104:GLU:HA	3:D:7:LYS:HE3	2.03	0.40
5:F:162:LYS:O	5:F:165:SER:OG	2.34	0.40
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.51	0.40
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.53	0.40
2:C:773:LEU:HD22	5:F:373:LYS:CD	2.42	0.40
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.40
3:D:403:PHE:CD2	3:D:444:VAL:HG23	2.57	0.40
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.56	0.40
6:G:15:DT:H2'	6:G:16:DG:H8	1.87	0.40
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.86	0.40
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.57	0.40
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.57	0.40
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.57	0.40
2:C:858:MET:HG2	2:C:867:VAL:O	2.22	0.40
3:D:907:GLU:HB2	3:D:1026:SER:HA	2.03	0.40

All (6) 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	Distance(Å)	Clash(Å)
3:D:306:GLU:OE1	7:H:1:DT:O5'[4.745]	1.70	0.50
2:C:318:PRO:CB	4:E:87:LYS:CG[1.545]	1.77	0.43
3:D:34:TYR:OH	3:D:327:GLU:OE1[4.755]	1.89	0.31
3:D:328:GLY:O	5:F:303:ARG:NH2[4.745]	2.11	0.09
2:C:37:GLU:OE1	3:D:1151:ARG:NH1[3.545]	2.12	0.08
2:C:49:ARG:NH2	5:F:390:PHE:O[1.545]	2.18	0.02

## 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	229/315 (73%)	226 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
2	C	1108/1119 (99%)	1076 (97%)	26 (2%)	6 (0%)	38	79
3	D	1491/1524 (98%)	1454 (98%)	33 (2%)	4 (0%)	50	85
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423 (81%)	336 (98%)	7 (2%)	1 (0%)	50	85
All	All	3489/3795 (92%)	3403 (98%)	75 (2%)	11 (0%)	50	85

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	425	PHE
2	C	765	SER
2	C	769	PRO
3	D	1240	THR
2	C	779	GLY
3	D	66	GLN
5	F	360	LYS
2	C	763	GLY
3	D	1253	THR
2	C	768	THR
3	D	1257	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	200/273 (73%)	196 (98%)	4 (2%)	68	92
1	B	200/273 (73%)	196 (98%)	4 (2%)	68	92
2	C	936/941 (100%)	907 (97%)	29 (3%)	52	88
3	D	1260/1279 (98%)	1229 (98%)	31 (2%)	60	91
4	E	83/88 (94%)	83 (100%)	0	100	100
5	F	301/371 (81%)	296 (98%)	5 (2%)	73	94
All	All	2980/3225 (92%)	2907 (98%)	73 (2%)	60	91

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	66	SER
1	A	96	THR
1	A	219	ARG
1	B	7	LYS
1	B	14	ARG
1	B	91	ASN
1	B	154	GLU
2	C	81	ASP
2	C	141	HIS
2	C	194	VAL
2	C	219	GLN
2	C	285	LEU
2	C	299	LYS
2	C	360	LEU
2	C	397	GLU
2	C	405	ARG
2	C	464	LEU
2	C	513	VAL
2	C	557	ARG
2	C	595	LEU
2	C	610	ARG
2	C	617	ASP
2	C	640	ARG
2	C	698	ASP
2	C	728	HIS
2	C	729	LEU
2	C	765	SER
2	C	767	PRO
2	C	768	THR
2	C	769	PRO
2	C	773	LEU
2	C	775	ARG
2	C	778	PHE
2	C	784	ASP
2	C	848	VAL
2	C	1078	GLU
3	D	66	GLN
3	D	67	ARG
3	D	87	ARG
3	D	134	VAL
3	D	276	ASP

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Mol	Chain	Res	Type
3	D	354	VAL
3	D	406	ASP
3	D	415	VAL
3	D	420	VAL
3	D	530	VAL
3	D	618	LEU
3	D	632	VAL
3	D	683	ILE
3	D	709	HIS
3	D	754	PHE
3	D	784	ASP
3	D	907	GLU
3	D	1083	ASP
3	D	1084	THR
3	D	1236	LEU
3	D	1237	THR
3	D	1238	MET
3	D	1243	THR
3	D	1252	ILE
3	D	1254	GLN
3	D	1256	LEU
3	D	1288	GLU
3	D	1307	LYS
3	D	1433	SER
3	D	1455	LYS
3	D	1488	ASP
5	F	95	THR
5	F	141	VAL
5	F	279	GLN
5	F	356	LYS
5	F	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
2	C	390	GLN
2	C	434	HIS
2	C	506	ASN
2	C	565	GLN
2	C	670	GLN
2	C	728	HIS

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Mol	Chain	Res	Type
2	C	860	HIS
3	D	316	GLN
3	D	560	GLN
3	D	669	ASN
3	D	717	GLN
3	D	768	ASN
3	D	855	HIS
3	D	976	GLN
3	D	1124	GLN
3	D	1195	GLN
3	D	1235	GLN
3	D	1242	HIS
3	D	1254	GLN
3	D	1441	GLN
5	F	83	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ATP	C	1201	10	33,33,33	1.30	5 (15%)	52,52,52	1.94	7 (13%)
11	2TM	D	2006	-	30,30,30	6.08	11 (36%)	44,47,47	2.24	15 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	C	1201	10	-	0/22/38/38	0/3/3/3
11	2TM	D	2006	-	-	0/18/38/38	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2006	2TM	PB-C1	-22.76	1.58	1.79
11	D	2006	2TM	PA-C1	-21.48	1.59	1.79
11	D	2006	2TM	PB-O3B	4.26	1.63	1.58
11	D	2006	2TM	C6-N1	-4.07	1.29	1.35
11	D	2006	2TM	C2'-C1'	-3.87	1.47	1.53
11	D	2006	2TM	PB-O1B	-3.74	1.46	1.56
11	D	2006	2TM	C5-C4	-3.55	1.32	1.40
11	D	2006	2TM	PA-O2A	-3.21	1.48	1.56
8	C	1201	ATP	C4-N9	-3.09	1.33	1.37
8	C	1201	ATP	PB-O3A	3.00	1.65	1.59
8	C	1201	ATP	C5-C4	2.84	1.46	1.40
11	D	2006	2TM	C4-N3	-2.73	1.30	1.35
8	C	1201	ATP	PA-O3A	2.36	1.64	1.59
11	D	2006	2TM	O4'-C4'	-2.32	1.39	1.45
11	D	2006	2TM	O4'-C1'	-2.14	1.38	1.41
8	C	1201	ATP	O4'-C1'	2.01	1.43	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1201	ATP	C5-C4-N3	-6.80	119.35	125.98
8	C	1201	ATP	N3-C4-N9	5.78	135.30	125.39
8	C	1201	ATP	C2'-C1'-N9	-5.71	97.79	113.35
8	C	1201	ATP	N3-C2-N1	-5.57	123.99	128.89
11	D	2006	2TM	O5'-PA-O1A	-5.13	100.97	114.15
11	D	2006	2TM	O3G-PG-O1G	4.65	125.58	110.36
11	D	2006	2TM	O4'-C1'-N1	4.22	117.33	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2006	2TM	C2'-C1'-N1	-3.99	102.43	113.34
11	D	2006	2TM	O1B-PB-O2B	3.78	122.18	110.40
11	D	2006	2TM	O3B-PB-O2B	-3.44	104.22	111.51
11	D	2006	2TM	C2-N3-C4	3.32	120.43	115.65
11	D	2006	2TM	C6-N1-C2	-3.19	116.11	121.28
11	D	2006	2TM	PB-C1-PA	3.12	124.86	119.02
11	D	2006	2TM	PA-O5'-C5'	-3.12	118.00	122.18
11	D	2006	2TM	C2-N1-C1'	3.04	123.16	119.03
11	D	2006	2TM	C6-C5-C4	2.76	118.83	117.51
11	D	2006	2TM	N4-C4-N3	2.65	121.55	116.61
11	D	2006	2TM	O5'-PA-C1	-2.47	97.21	104.26
8	C	1201	ATP	PB-O3B-PG	-2.36	125.38	131.93
11	D	2006	2TM	O2A-PA-O5'	2.25	113.02	105.82
8	C	1201	ATP	N6-C6-N1	2.17	123.73	119.11
8	C	1201	ATP	C2-N3-C4	2.11	119.35	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	231/315 (73%)	0.45	17 (7%) 14 17	36, 68, 92, 101	0
1	B	227/315 (72%)	0.50	17 (7%) 14 17	41, 69, 100, 122	0
2	C	1112/1119 (99%)	0.53	74 (6%) 17 21	25, 58, 115, 135	0
3	D	1494/1524 (98%)	0.64	149 (9%) 8 10	19, 58, 122, 214	0
4	E	94/99 (94%)	0.59	9 (9%) 8 11	34, 73, 111, 114	0
5	F	346/423 (81%)	1.02	64 (18%) 2 3	43, 79, 152, 176	0
6	G	18/22 (81%)	0.14	1 (5%) 24 28	55, 81, 139, 140	0
7	H	25/27 (92%)	0.27	3 (12%) 5 7	70, 100, 149, 169	0
All	All	3547/3844 (92%)	0.61	334 (9%) 9 11	19, 64, 124, 214	0

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	311	PHE	8.4
3	D	173	PRO	8.3
2	C	300	ASP	8.1
3	D	427	VAL	8.0
5	F	386	VAL	7.1
5	F	146	GLY	7.0
3	D	211	VAL	6.8
5	F	149	GLU	6.7
5	F	375	LEU	6.5
1	B	2	LEU	6.5
5	F	381	HIS	6.5
2	C	107	LEU	6.4
3	D	1499	ARG	6.2
3	D	1305	LEU	6.2
3	D	322	VAL	6.1
5	F	150	THR	6.1

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Mol	Chain	Res	Type	RSRZ
5	F	151	LEU	5.9
5	F	373	LYS	5.9
2	C	207	LEU	5.8
5	F	145	PRO	5.7
3	D	422	ALA	5.7
3	D	324	ALA	5.6
1	A	231	ALA	5.6
5	F	382	THR	5.6
3	D	1127	GLU	5.6
3	D	241	ILE	5.5
3	D	1297	GLU	5.4
5	F	147	LEU	5.4
2	C	365	ASP	5.2
3	D	1500	LYS	5.2
5	F	414	ARG	5.1
5	F	369	LEU	5.0
3	D	202	VAL	5.0
3	D	203	ALA	5.0
3	D	821	VAL	4.9
3	D	977	ALA	4.9
3	D	1495	ILE	4.8
3	D	1298	GLY	4.7
3	D	268	ALA	4.7
5	F	356	LYS	4.7
3	D	195	VAL	4.7
3	D	1497	GLU	4.6
5	F	143	HIS	4.5
3	D	1319	VAL	4.5
3	D	1299	PHE	4.5
5	F	376	ILE	4.4
3	D	267	GLY	4.4
3	D	976	GLN	4.4
4	E	85	LEU	4.4
2	C	104	ASP	4.4
5	F	388	ALA	4.4
2	C	64	LEU	4.4
1	A	97	VAL	4.3
3	D	830	ALA	4.3
3	D	1306	PRO	4.3
5	F	415	THR	4.2
5	F	349	LEU	4.2
3	D	339	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	217	LEU	4.1
3	D	983	LEU	4.1
5	F	361	LEU	4.1
1	A	230	ALA	4.1
3	D	982	PHE	4.1
1	A	94	LEU	4.1
2	C	811	PRO	4.1
5	F	153	PRO	4.1
3	D	393	ILE	4.0
5	F	127	ILE	4.0
2	C	629	TYR	4.0
3	D	1313	VAL	4.0
5	F	392	VAL	4.0
3	D	335	LEU	4.0
3	D	191	LEU	4.0
2	C	766	GLU	3.9
3	D	974	ILE	3.9
3	D	666	ILE	3.9
2	C	778	PHE	3.9
2	C	281	LEU	3.8
5	F	410	TYR	3.8
2	C	208	ALA	3.8
2	C	307	LEU	3.8
3	D	1058	ARG	3.7
3	D	368	VAL	3.7
5	F	397	ILE	3.7
2	C	296	GLY	3.7
5	F	421	PHE	3.7
2	C	189	ARG	3.7
4	E	89	MET	3.7
5	F	383	LEU	3.7
3	D	1242	HIS	3.7
5	F	377	ASP	3.7
2	C	52	PHE	3.7
2	C	769	PRO	3.7
5	F	173	TYR	3.7
5	F	385	GLU	3.6
2	C	219	GLN	3.6
5	F	359	SER	3.6
2	C	315	ALA	3.6
3	D	1128	VAL	3.6
3	D	174	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	D	1327	ARG	3.6
4	E	32	ARG	3.6
2	C	174	LEU	3.6
5	F	423	ASP	3.6
3	D	1287	GLU	3.6
3	D	1130	ARG	3.5
3	D	1490	LYS	3.5
3	D	1300	SER	3.5
2	C	242	LEU	3.5
3	D	310	LEU	3.5
2	C	298	PHE	3.5
5	F	390	PHE	3.5
3	D	144	GLY	3.5
3	D	320	ALA	3.5
5	F	345	ALA	3.5
2	C	617	ASP	3.4
3	D	488	ARG	3.4
3	D	212	ARG	3.4
2	C	729	LEU	3.4
2	C	226	VAL	3.4
3	D	667	ALA	3.4
2	C	511	GLU	3.4
3	D	409	VAL	3.4
3	D	428	LYS	3.4
2	C	763	GLY	3.4
2	C	299	LYS	3.4
3	D	674[A]	ARG	3.3
2	C	228	ALA	3.3
3	D	269	PHE	3.2
1	B	82	LEU	3.2
3	D	142	LEU	3.2
3	D	387	LEU	3.2
2	C	102	HIS	3.2
3	D	973	GLN	3.2
2	C	649	VAL	3.2
3	D	831	GLY	3.1
3	D	205	TYR	3.1
5	F	325	LYS	3.1
2	C	275	TYR	3.1
7	H	23	DG	3.1
3	D	1292	VAL	3.1
1	A	99	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	1405	GLU	3.0
3	D	373	PRO	3.0
1	B	118	ALA	3.0
2	C	196	LEU	3.0
2	C	200	LEU	3.0
3	D	213	VAL	3.0
1	B	3	ASP	3.0
3	D	807	ALA	3.0
3	D	1283	ILE	2.9
7	H	24	DC	2.9
2	C	304	LEU	2.9
5	F	142	ARG	2.9
1	A	100	LEU	2.9
3	D	216	VAL	2.9
5	F	379	ARG	2.9
3	D	336	PHE	2.9
1	B	120	VAL	2.9
2	C	185	LYS	2.9
2	C	297	GLU	2.9
5	F	346	THR	2.8
3	D	1408	ILE	2.8
3	D	317	VAL	2.8
1	B	189	ARG	2.8
3	D	340	THR	2.8
4	E	79	LEU	2.8
7	H	25	DA	2.8
3	D	345	TYR	2.8
3	D	217	LYS	2.8
3	D	1054	GLU	2.8
1	B	138	LEU	2.8
3	D	350	HIS	2.8
3	D	1491	THR	2.8
5	F	393	THR	2.8
5	F	419	ARG	2.7
1	A	233	VAL	2.7
2	C	367	LEU	2.7
2	C	739	GLU	2.7
3	D	1273	VAL	2.7
2	C	159	ILE	2.7
3	D	1239	ARG	2.7
3	D	1225	ALA	2.7
3	D	1325	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	378	ILE	2.7
3	D	1277	ILE	2.7
2	C	998	TYR	2.7
3	D	1129	THR	2.7
5	F	136	LEU	2.7
1	B	122	ILE	2.7
3	D	426	LYS	2.7
2	C	100	LEU	2.7
2	C	176	VAL	2.6
3	D	367	ILE	2.6
3	D	1238	MET	2.6
3	D	374	GLU	2.6
3	D	470	LEU	2.6
5	F	391	GLY	2.6
3	D	270	LEU	2.6
3	D	316	GLN	2.6
1	B	89	PHE	2.6
1	B	5	LYS	2.6
3	D	360	ARG	2.6
3	D	969	ARG	2.6
3	D	1304	LYS	2.6
2	C	762	LYS	2.6
3	D	805	GLU	2.5
2	C	105	THR	2.5
2	C	648	ARG	2.5
2	C	775	ARG	2.5
3	D	198	ARG	2.5
2	C	757	GLY	2.5
3	D	225	LEU	2.5
3	D	1314	LYS	2.5
3	D	410	SER	2.5
3	D	1414	PRO	2.5
5	F	342	VAL	2.5
2	C	188	LYS	2.5
3	D	804	LEU	2.5
4	E	75	PHE	2.5
3	D	484	PRO	2.5
5	F	400	ILE	2.5
2	C	157	ARG	2.5
5	F	394	ARG	2.5
5	F	352	GLU	2.5
5	F	159	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	2.4
2	C	227	PHE	2.4
3	D	321	GLN	2.4
2	C	1040	LEU	2.4
3	D	161	LEU	2.4
2	C	48	PHE	2.4
2	C	153	ALA	2.4
3	D	143	ASN	2.4
5	F	413	SER	2.4
3	D	687	VAL	2.4
2	C	764	GLU	2.4
3	D	314	PRO	2.4
2	C	41	ASN	2.4
2	C	51	THR	2.4
1	A	16	GLN	2.4
3	D	980	MET	2.4
1	B	6	LEU	2.4
4	E	73	LEU	2.4
3	D	1275	SER	2.4
2	C	1	MET	2.4
3	D	1328	GLY	2.4
2	C	650	ARG	2.4
1	A	234	ALA	2.4
2	C	254	VAL	2.3
3	D	377	VAL	2.3
3	D	1281	VAL	2.3
5	F	148	LYS	2.3
5	F	416	ARG	2.3
3	D	337	LEU	2.3
5	F	122	LEU	2.3
2	C	975	TYR	2.3
3	D	401	TYR	2.3
5	F	141	VAL	2.3
5	F	324	GLU	2.3
3	D	1044	LEU	2.3
4	E	54	LEU	2.3
2	C	422	ARG	2.3
3	D	445	ARG	2.3
1	B	186	LEU	2.3
4	E	51	LEU	2.3
3	D	1174	LEU	2.3
1	A	115	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	338	GLU	2.3
3	D	96	ALA	2.3
3	D	220	ARG	2.3
3	D	432	TYR	2.3
1	B	11	PHE	2.3
3	D	152	LEU	2.3
3	D	304	LEU	2.3
5	F	96	LEU	2.3
2	C	368	THR	2.3
3	D	135	LEU	2.2
1	B	111	ALA	2.2
1	B	190	THR	2.2
5	F	93	LEU	2.2
5	F	422	LEU	2.2
3	D	133	ILE	2.2
5	F	310	ILE	2.2
3	D	239	GLY	2.2
5	F	411	HIS	2.2
3	D	434	ARG	2.2
3	D	1310	ARG	2.2
3	D	833	GLU	2.2
1	A	208	LEU	2.2
2	C	512	ARG	2.2
3	D	1133	ARG	2.2
1	A	142	VAL	2.2
2	C	372	LEU	2.2
3	D	556	LYS	2.2
2	C	420	ARG	2.2
3	D	189	GLN	2.2
1	A	62	LEU	2.2
5	F	125	ASP	2.2
2	C	245	GLY	2.2
3	D	487	ALA	2.2
2	C	202	TYR	2.2
3	D	463	GLN	2.1
1	A	160	ASP	2.1
3	D	868	TYR	2.1
2	C	1070	ILE	2.1
6	G	3	DT	2.1
5	F	389	PHE	2.1
2	C	98	LEU	2.1
3	D	676	MET	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	80	VAL	2.1
1	A	217	ILE	2.1
3	D	452	ILE	2.1
1	A	85	LEU	2.1
3	D	54	LYS	2.1
3	D	194	GLY	2.1
3	D	1290	LEU	2.1
1	B	119	ASP	2.1
5	F	327	SER	2.1
5	F	420	ASP	2.0
1	B	58	ILE	2.0
2	C	616	GLU	2.0
3	D	201	GLY	2.0
4	E	40	LEU	2.0
2	C	366	SER	2.0
5	F	140	ARG	2.0
3	D	68	PHE	2.0
3	D	70	GLY	2.0
3	D	1156	LEU	2.0
3	D	1301	LYS	2.0
5	F	401	GLU	2.0
3	D	1413	THR	2.0
3	D	333	LEU	2.0
3	D	1307	LYS	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MG	D	2004	1/1	0.60	48.06	54,54,54,54	0
10	MG	D	2003	1/1	0.23	3.35	38,38,38,38	0
10	MG	D	2005	1/1	0.28	1.03	45,45,45,45	0
8	ATP	C	1201	31/31	0.18	-0.61	38,47,75,83	0
11	2TM	D	2006	29/29	0.18	-0.73	38,51,69,94	0
9	ZN	D	2001	1/1	0.16	-1.76	38,38,38,38	0
9	ZN	D	2002	1/1	0.04	-1.78	59,59,59,59	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.