



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 11:43 AM EDT

PDB ID : 5E18  
Title : T. thermophilus transcription initiation complex having a YYY discriminator sequence and a nontemplate-strand length corresponding to TSS selection at position 8 (RPO-CCC-8)  
Authors : Zhang, Y.; Ebright, R.H.  
Deposited on : 2015-09-29  
Resolution : 3.30 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](mailto: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>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

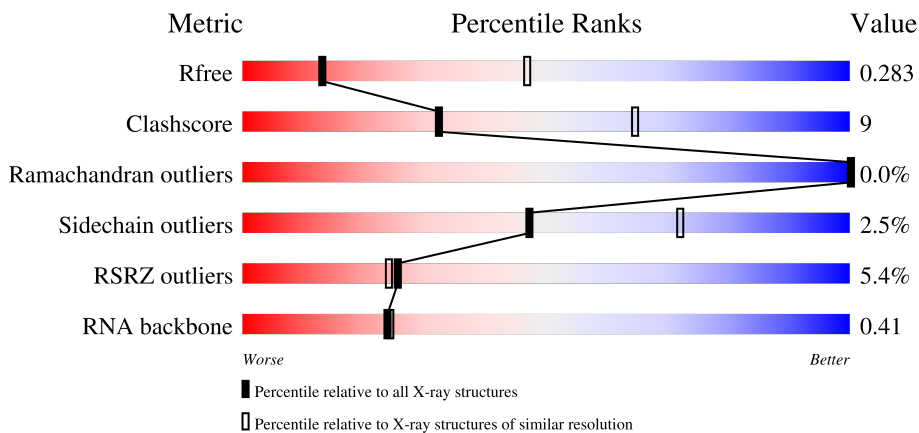
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.



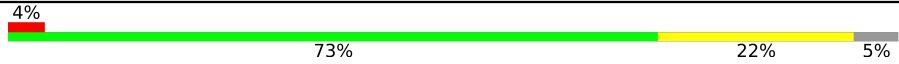

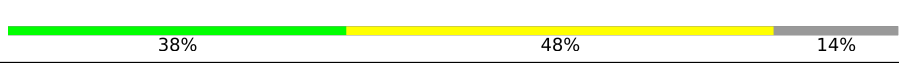

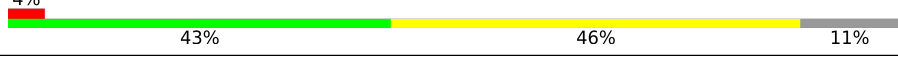
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 4% 61% 12% 23%
1	B	315	 53% 17% 29%
2	C	1119	 4% 76% 23% 2%
3	D	1524	 6% 74% 23% 2%

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Mol	Chain	Length	Quality of chain
4	E	99	
5	F	443	
6	G	21	
7	I	7	
8	H	28	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 28645 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
2	C	1112	Total	C	N	O	S	0	3	0
			8792	5562	1570	1636	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1486	Total	C	N	O	S	0	2	0
			11751	7450	2070	2195	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	Total	C	N	O	S	0	0	0
			758	483	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	335	Total	C	N	O	S	0	0	0
			2718	1713	497	504	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
			Total	C	N	O	P			
6	G	18	372	176	73	106	17	0	0	0

- Molecule 7 is a RNA chain called RNA (5'-R(\*CP\*CP\*CP\*UP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	I	7	142	65	24	47	6	0	0	0

- Molecule 8 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	H	25	508	243	93	148	24	0	0	0

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

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

- Molecule 11 is water.

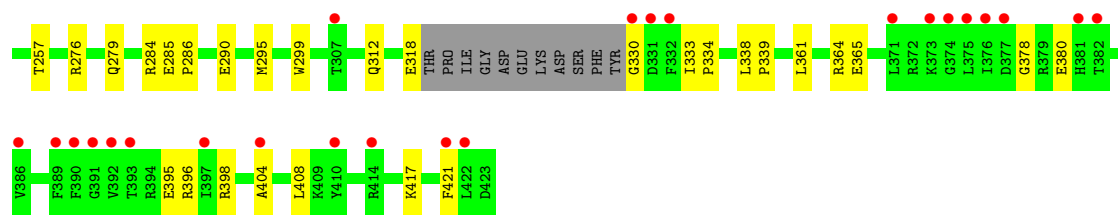
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O 1 1	0	0
11	B	3	Total O 3 3	0	0
11	C	8	Total O 8 8	0	0
11	D	10	Total O 10 10	0	0
11	E	1	Total O 1 1	0	0
11	F	2	Total O 2 2	0	0
11	H	1	Total O 1 1	0	0





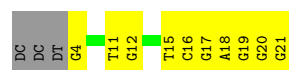






- Molecule 6: DNA (5'-D(\*CP\*CP\*T\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*GP\*AP\*GP\*GP\*G)-3')

Chain G: 38% 48% 14%



- Molecule 7: RNA (5'-R(\*CP\*CP\*CP\*UP\*CP\*GP\*A)-3')

Chain I: 71% 14% 14%



- Molecule 8: DNA (28-MER)

Chain H: 4% 43% 46% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.92Å 103.24Å 298.40Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	38.34 – 3.30 39.66 – 3.28	Depositor EDS
% Data completeness (in resolution range)	90.3 (38.34-3.30) 90.4 (39.66-3.28)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.9	Depositor
R, $R_{free}$	0.238 , 0.284 0.241 , 0.283	Depositor DCC
$R_{free}$ test set	3869 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.6	Xtrriage
Anisotropy	0.584	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: ZN, MG

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	0/1849	0.43	0/2515
1	B	0.24	0/1790	0.47	0/2435
2	C	0.25	0/8969	0.44	0/12129
3	D	0.26	0/11963	0.44	0/16173
4	E	0.24	0/772	0.41	0/1040
5	F	0.29	0/2759	0.44	0/3709
6	G	0.53	0/418	0.80	0/645
7	I	0.26	0/157	0.72	0/242
8	H	0.64	0/569	0.91	0/876
All	All	0.27	0/29246	0.47	0/39764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1814	0	1869	23	0
1	B	1758	0	1808	40	0
2	C	8792	0	8902	164	0
3	D	11751	0	11994	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	758	0	770	16	0
5	F	2718	0	2803	53	0
6	G	372	0	203	12	0
7	I	142	0	78	3	0
8	H	508	0	283	35	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	1	0	0	0	0
11	B	3	0	0	0	0
11	C	8	0	0	0	0
11	D	10	0	0	3	0
11	E	1	0	0	0	0
11	F	2	0	0	0	0
11	H	1	0	0	0	0
All	All	28645	0	28710	498	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 9.

All (498) 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)
6:G:20:DG:H1	7:I:2:C:H42	1.18	0.88
8:H:13:DC:O3'	8:H:14:DT:H72	1.74	0.86
5:F:209:PHE:HB2	8:H:9:DC:C4	2.12	0.84
2:C:628:PHE:H	2:C:638:ASP:HB3	1.43	0.83
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.66	0.77
2:C:167:LYS:HA	8:H:13:DC:C6	2.21	0.75
5:F:209:PHE:H	8:H:9:DC:N4	1.83	0.75
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.20	0.75
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.69	0.74
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.71	0.72
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.23	0.71
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.73	0.70
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.25	0.69
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.74	0.69
2:C:637:LEU:HG	2:C:659:PRO:HG3	1.73	0.69
3:D:65:ARG:NH1	5:F:378:GLY:O	2.27	0.67
8:H:13:DC:C2'	8:H:14:DT:H72	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.77	0.67
3:D:622:ARG:NH1	6:G:17:DG:OP1	2.27	0.67
3:D:1484:THR:O	4:E:25:LYS:NZ	2.21	0.66
5:F:209:PHE:H	8:H:9:DC:H42	1.41	0.66
2:C:1019:GLN:HG3	2:C:1058:ASP:HB3	1.75	0.66
1:B:14:ARG:HB3	1:B:22:GLU:HB2	1.79	0.65
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.77	0.65
2:C:244:PRO:O	5:F:82:ARG:NH1	2.29	0.65
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.78	0.65
3:D:63:TYR:HB2	3:D:80:VAL:HG21	1.79	0.65
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.78	0.65
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.78	0.65
2:C:26:TYR:OH	2:C:119:PRO:O	2.13	0.64
2:C:711:GLU:O	2:C:758:ARG:NH1	2.29	0.64
5:F:194:LEU:O	5:F:197:SER:OG	2.14	0.64
8:H:9:DC:H2''	8:H:10:DA:C8	2.32	0.64
8:H:13:DC:O3'	8:H:14:DT:C7	2.44	0.64
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.15	0.64
1:A:31:GLY:N	1:A:193:ASP:OD2	2.31	0.63
6:G:17:DG:H2'	6:G:18:DA:C8	2.34	0.62
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.81	0.62
1:B:77:GLU:OE1	3:D:867:ARG:NH2	2.32	0.62
3:D:140:ALA:HB2	3:D:452:ILE:HG12	1.81	0.61
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.82	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.61
3:D:1219:GLU:OE1	4:E:17:TYR:OH	2.17	0.61
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.83	0.61
2:C:428:ARG:NH2	2:C:447:ALA:O	2.32	0.61
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.81	0.61
6:G:21:DG:O6	7:I:1:C:N4	2.34	0.61
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.82	0.61
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.81	0.60
2:C:237:ARG:O	2:C:240:THR:OG1	2.18	0.60
2:C:343:GLN:NE2	2:C:384:GLU:OE2	2.33	0.60
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.83	0.60
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.66	0.60
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.66	0.60
3:D:1096:ARG:NH1	3:D:1440:PHE:O	2.35	0.60
1:A:133:GLU:OE1	2:C:610:ARG:NH1	2.35	0.60
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.83	0.60
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.84	0.59
2:C:805:ARG:HG2	2:C:807[A]:ARG:HE	1.66	0.59
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.84	0.59
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.84	0.59
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.83	0.59
3:D:1479:ASP:OD1	3:D:1482:ARG:NE	2.36	0.59
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	1.84	0.58
2:C:167:LYS:HA	8:H:13:DC:H6	1.67	0.58
2:C:326:ASP:HA	2:C:331:ARG:HD2	1.86	0.58
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.84	0.58
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.37	0.58
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.85	0.58
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.84	0.58
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.86	0.58
3:D:894:LYS:H	3:D:894:LYS:HD3	1.68	0.58
1:B:38:ASN:ND2	2:C:978:ARG:O	2.35	0.57
3:D:1149:LEU:HD12	3:D:1164:ARG:HB3	1.87	0.57
2:C:946:ARG:NH1	11:D:2101:HOH:O	2.36	0.57
3:D:252:ARG:HA	3:D:303:PRO:HA	1.87	0.57
6:G:4:DG:H1	8:H:25:DC:H42	1.53	0.57
8:H:13:DC:C3'	8:H:14:DT:H72	2.35	0.57
1:B:191:ASP:OD1	1:B:191:ASP:N	2.33	0.57
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.87	0.56
5:F:116:LEU:HD11	5:F:174:LEU:HA	1.86	0.56
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.87	0.56
2:C:223:ASP:OD2	2:C:225:SER:OG	2.21	0.56
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.87	0.56
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.88	0.56
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.36	0.56
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.41	0.56
2:C:399:ASN:O	2:C:402:SER:OG	2.20	0.56
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.88	0.56
3:D:162:ARG:O	3:D:414:ARG:NH1	2.37	0.56
8:H:13:DC:H2''	8:H:14:DT:H72	1.87	0.56
2:C:884:GLN:O	2:C:888:THR:OG1	2.23	0.56
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.88	0.56
5:F:209:PHE:CB	8:H:9:DC:C4	2.87	0.56
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.87	0.55
2:C:168:ARG:O	2:C:267:TYR:HA	2.06	0.55
5:F:209:PHE:N	8:H:9:DC:N4	2.55	0.55
2:C:971:LYS:HG2	2:C:988:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:LYS:HD3	8:H:13:DC:H2'	1.88	0.55
2:C:1019:GLN:OE1	3:D:617:ASN:ND2	2.29	0.55
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.88	0.55
3:D:256:GLU:OE2	3:D:300:LYS:NZ	2.27	0.55
3:D:433:GLY:HA2	3:D:449:SER:H	1.72	0.55
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.39	0.55
2:C:627:ARG:HD3	2:C:638:ASP:HB2	1.89	0.55
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.89	0.54
1:B:84:GLU:OE2	3:D:867:ARG:NH1	2.37	0.54
3:D:1468:LEU:HD23	3:D:1470:ARG:HD2	1.88	0.54
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.38	0.54
2:C:1036:GLU:OE2	2:C:1036:GLU:N	2.40	0.54
1:A:223:THR:O	1:A:226:SER:OG	2.21	0.54
1:B:30:ARG:HH21	2:C:854:PRO:HB3	1.73	0.54
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.41	0.54
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.89	0.54
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.90	0.54
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.90	0.54
3:D:741:ASP:OD1	3:D:741:ASP:N	2.40	0.54
3:D:1045[B]:MET:HE1	3:D:1057:VAL:HG23	1.88	0.54
5:F:171:LYS:O	5:F:175:HIS:ND1	2.30	0.54
2:C:167:LYS:CA	8:H:13:DC:C6	2.90	0.54
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.40	0.54
5:F:209:PHE:N	8:H:9:DC:H42	2.05	0.54
2:C:614:ARG:NH2	2:C:618:GLY:O	2.41	0.53
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.89	0.53
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.43	0.53
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.08	0.53
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.89	0.53
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.89	0.53
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.40	0.53
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.26	0.53
1:A:133:GLU:HG2	1:A:134:GLU:H	1.73	0.53
1:A:209:GLU:O	1:A:213:GLN:HG2	2.08	0.53
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.23	0.53
2:C:550:LEU:HD23	2:C:906:PHE:HE1	1.74	0.53
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.42	0.53
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.90	0.52
3:D:435:VAL:HG22	3:D:446:VAL:HG22	1.91	0.52
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.89	0.52
6:G:15:DT:H2'	6:G:16:DC:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.91	0.52
3:D:657:LEU:HG	3:D:661:MET:HE2	1.91	0.52
8:H:12:DG:C8	8:H:12:DG:H5''	2.45	0.52
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.91	0.52
2:C:657:ASP:OD2	2:C:663:ASN:N	2.37	0.52
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.92	0.52
3:D:208:PRO:HA	3:D:390:PRO:HA	1.91	0.52
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.45	0.52
2:C:203:ASP:OD1	2:C:204:GLN:N	2.43	0.52
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.44	0.52
3:D:834:THR:OG1	3:D:835:SER:N	2.42	0.52
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.92	0.52
3:D:761:ILE:HD12	4:E:20:THR:HA	1.92	0.52
3:D:1047:LYS:HD3	3:D:1051:GLU:HB3	1.91	0.52
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.10	0.52
1:A:59:GLU:OE1	1:A:139[B]:ASN:ND2	2.30	0.51
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.91	0.51
5:F:193:ARG:HG2	8:H:7:DC:H5''	1.93	0.51
2:C:617:ASP:OD1	2:C:617:ASP:N	2.43	0.51
2:C:705:ILE:HA	2:C:828:ALA:HA	1.91	0.51
2:C:495:THR:N	2:C:530:GLU:OE1	2.42	0.51
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.93	0.51
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.92	0.51
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.45	0.51
2:C:669:GLY:HA3	2:C:995:MET:HA	1.93	0.51
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.46	0.51
3:D:187:LYS:N	3:D:200:ASP:OD2	2.34	0.51
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.93	0.51
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.93	0.51
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.93	0.51
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.92	0.50
6:G:18:DA:H2'	6:G:19:DG:C8	2.45	0.50
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.47	0.50
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	1.94	0.50
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.12	0.50
8:H:13:DC:H1'	8:H:14:DT:C7	2.41	0.50
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.93	0.50
1:B:8:ALA:HB1	1:B:9:PRO:HA	1.93	0.50
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.12	0.50
3:D:58:CYS:SG	3:D:62:LYS:N	2.85	0.50
3:D:890:VAL:HB	3:D:922:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:O	1:B:228:PRO:HA	2.11	0.49
3:D:132:TYR:HB2	3:D:153:LEU:HB2	1.94	0.49
4:E:37:ASN:OD1	4:E:37:ASN:N	2.42	0.49
5:F:208:SER:OG	8:H:9:DC:N4	2.44	0.49
2:C:551:GLU:OE2	2:C:551:GLU:N	2.35	0.49
3:D:534:ARG:HH12	5:F:312:GLN:HB3	1.77	0.49
5:F:189:GLU:O	5:F:192:LEU:HB2	2.11	0.49
5:F:228:GLU:OE1	5:F:231:ARG:NH2	2.31	0.49
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.37	0.49
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.12	0.49
3:D:1232:PRO:HG2	3:D:1356:TYR:HE1	1.77	0.49
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.47	0.49
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.93	0.49
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.93	0.49
3:D:256:GLU:OE1	3:D:274:ARG:NH1	2.45	0.49
3:D:472:ALA:O	3:D:476:GLU:HG2	2.12	0.49
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.93	0.49
3:D:100:ALA:HB3	3:D:575:GLN:HE22	1.78	0.49
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.48	0.49
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.94	0.49
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.12	0.49
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.94	0.49
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.95	0.49
5:F:203:THR:HB	8:H:9:DC:O2	2.13	0.49
2:C:471:TYR:OH	2:C:516:ARG:NH2	2.45	0.49
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.95	0.48
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.28	0.48
2:C:496:ILE:HG12	2:C:531:PHE:HB2	1.95	0.48
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.95	0.48
3:D:898:GLU:OE2	3:D:921:ARG:NH2	2.46	0.48
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.94	0.48
5:F:276:ARG:O	5:F:279:GLN:HG3	2.12	0.48
1:B:150:TYR:CE2	1:B:170:VAL:HG22	2.49	0.48
5:F:170:HIS:HA	5:F:173:TYR:HD2	1.78	0.48
4:E:67:GLU:O	4:E:70:THR:OG1	2.25	0.48
5:F:181:GLU:O	5:F:184:ARG:HB3	2.13	0.48
8:H:8:DC:H2"	8:H:9:DC:OP2	2.14	0.48
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.46	0.48
2:C:170:PRO:HA	8:H:14:DT:O4	2.14	0.48
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.95	0.48
5:F:172:ARG:O	5:F:176:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:778:LEU:HD12	3:D:778:LEU:HA	1.60	0.48
3:D:613:ARG:HG3	3:D:618:LEU:HD23	1.96	0.48
5:F:223:ALA:HB2	5:F:242:TRP:HB2	1.97	0.47
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.95	0.47
4:E:57:ASP:O	4:E:63:TRP:NE1	2.41	0.47
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.75	0.47
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.96	0.47
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.96	0.47
2:C:42:VAL:O	2:C:45:GLN:HB3	2.13	0.47
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.80	0.47
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.96	0.47
4:E:39:VAL:O	4:E:72:ARG:NH1	2.42	0.47
8:H:19:DC:H2''	8:H:20:DG:C8	2.49	0.47
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.48	0.47
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.96	0.47
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.96	0.47
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.78	0.47
2:C:881:ASN:OD1	2:C:881:ASN:N	2.48	0.47
3:D:42:ASP:N	3:D:46:ASP:OD2	2.38	0.47
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.97	0.47
1:B:208:LEU:O	1:B:212:ASN:ND2	2.48	0.47
2:C:704:HIS:O	2:C:829:GLN:HG2	2.15	0.47
2:C:18:LEU:HD13	2:C:404:LEU:HD21	1.97	0.47
2:C:184:MET:HE3	2:C:303:PHE:HE1	1.79	0.47
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.97	0.47
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.96	0.46
2:C:41:ASN:O	2:C:46:ALA:HB2	2.16	0.46
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.97	0.46
5:F:169:GLU:O	5:F:172:ARG:HB3	2.16	0.46
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.50	0.46
2:C:437:ARG:NH2	2:C:491:GLU:OE2	2.47	0.46
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.97	0.46
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.15	0.46
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.98	0.46
2:C:1019:GLN:CG	2:C:1058:ASP:HB3	2.45	0.46
1:A:99:LEU:HD21	1:A:122:ILE:HD11	1.98	0.46
1:B:124:ASN:OD1	1:B:124:ASN:N	2.48	0.46
3:D:178:LEU:HG	3:D:192:ALA:HA	1.98	0.46
3:D:452:ILE:H	3:D:452:ILE:HG13	1.36	0.46
3:D:761:ILE:HD13	4:E:19:LEU:HG	1.97	0.46
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HB3	1:A:27:PRO:O	2.15	0.46
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.81	0.46
3:D:1258:ARG:NH2	3:D:1262:LEU:HD21	2.30	0.46
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.97	0.46
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.98	0.46
3:D:1486:VAL:HG22	4:E:22:VAL:HG13	1.98	0.46
1:A:70:GLY:H	2:C:607:ASP:CG	2.19	0.46
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.74	0.46
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.47	0.46
3:D:758:GLU:OE1	3:D:1476:THR:OG1	2.26	0.46
2:C:874:LEU:HB3	3:D:1029:ARG:HG3	1.98	0.46
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.98	0.46
3:D:103:TRP:HZ2	3:D:604:THR:HG1	1.64	0.46
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.16	0.46
3:D:106:LYS:O	3:D:586:ARG:NH1	2.50	0.45
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.51	0.45
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.51	0.45
2:C:1043:TYR:OH	3:D:713:ILE:O	2.28	0.45
3:D:411:THR:HG23	3:D:436:GLU:HA	1.98	0.45
6:G:20:DG:N2	7:I:2:C:N3	2.46	0.45
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.83	0.45
3:D:633:VAL:O	3:D:635:PRO:HD3	2.16	0.45
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.17	0.45
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.82	0.45
1:B:14:ARG:O	1:B:22:GLU:N	2.45	0.45
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.97	0.45
2:C:1019:GLN:HE21	3:D:621:LYS:HE3	1.80	0.45
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.52	0.45
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.75	0.45
8:H:13:DC:O3'	8:H:14:DT:C5	2.69	0.45
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.52	0.45
3:D:923:GLY:O	3:D:927:THR:OG1	2.25	0.45
3:D:1258:ARG:NH1	3:D:1261:GLU:OE2	2.47	0.45
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.99	0.45
3:D:1296:SER:OG	3:D:1297:GLU:N	2.50	0.45
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.17	0.45
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.82	0.45
2:C:139:GLN:HB2	2:C:391:LEU:HD11	1.99	0.45
2:C:553:ASP:OD2	2:C:843:HIS:ND1	2.37	0.45
2:C:286:SER:OG	2:C:301:GLU:OE2	2.26	0.45
2:C:317:VAL:O	2:C:320:HIS:ND1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:224:GLU:CD	2:C:224:GLU:H	2.20	0.44
2:C:261:ILE:HG22	2:C:262:ALA:N	2.32	0.44
3:D:939:PHE:O	3:D:942:SER:OG	2.29	0.44
2:C:134:ARG:NH2	6:G:21:DG:O3'	2.35	0.44
2:C:615:TYR:OH	2:C:623:TYR:OH	2.15	0.44
3:D:584:ASN:HD21	3:D:591:VAL:H	1.65	0.44
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.53	0.44
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	0.44
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.17	0.44
2:C:712:ALA:O	2:C:820:ARG:N	2.49	0.44
3:D:881:LEU:O	3:D:885:ILE:HG13	2.17	0.44
3:D:924:MET:HE2	3:D:924:MET:HB2	1.88	0.44
3:D:658:LEU:HD23	3:D:661:MET:HE1	2.00	0.44
3:D:684:LYS:HB3	3:D:684:LYS:HE2	1.78	0.44
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.50	0.44
3:D:1351:GLU:O	3:D:1354:LYS:HB2	2.16	0.44
3:D:1444:THR:O	3:D:1448:THR:HG23	2.17	0.44
2:C:578:VAL:HA	2:C:900:ARG:HG2	2.00	0.44
3:D:101:HIS:CE1	3:D:582:LEU:HD13	2.52	0.44
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.00	0.44
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.52	0.44
5:F:364:ARG:HH12	5:F:396:ARG:NH2	2.15	0.44
1:B:110:LYS:HD3	1:B:128:HIS:HA	2.00	0.44
2:C:343:GLN:HG3	2:C:385:PHE:CD1	2.53	0.44
2:C:390:GLN:HB3	2:C:415:PRO:HD3	2.00	0.44
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.33	0.44
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.30	0.44
5:F:361:LEU:HD11	5:F:408:LEU:HG	1.99	0.44
8:H:12:DG:H4'	8:H:13:DC:OP2	2.17	0.44
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.99	0.44
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.52	0.44
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.99	0.44
3:D:65:ARG:HA	3:D:65:ARG:HD3	1.69	0.44
3:D:806:PHE:HB2	3:D:829:VAL:HG22	2.00	0.44
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.00	0.44
3:D:966:GLU:O	3:D:969:ARG:HG2	2.18	0.44
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	2.00	0.44
1:B:156:HIS:CG	1:B:157:GLY:H	2.35	0.43
2:C:193:LEU:HD23	2:C:307:LEU:HD22	2.00	0.43
2:C:551:GLU:HB2	3:D:1065:LEU:H	1.83	0.43
3:D:487:ALA:O	3:D:491:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:913:ASP:O	3:D:917:GLN:HG2	2.18	0.43
3:D:1010:ASN:OD1	3:D:1014:ASN:ND2	2.46	0.43
1:B:156:HIS:CG	1:B:157:GLY:N	2.86	0.43
2:C:1048:THR:O	2:C:1052:MET:HG2	2.18	0.43
3:D:31:THR:HG21	5:F:257:THR:HG22	2.00	0.43
3:D:96:ALA:HB3	3:D:554:LEU:HD23	2.00	0.43
3:D:1048:PRO:HD3	3:D:1075:HIS:CD2	2.54	0.43
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.00	0.43
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.51	0.43
3:D:230:TRP:CZ3	3:D:232:GLU:HG2	2.53	0.43
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.99	0.43
5:F:107:GLU:HG3	5:F:229:TYR:HD2	1.83	0.43
6:G:11:DT:H2''	6:G:12:DG:H5''	2.00	0.43
3:D:648:MET:O	3:D:652:LEU:HG	2.18	0.43
3:D:911:LEU:O	3:D:915:VAL:HG23	2.19	0.43
6:G:4:DG:H1	8:H:25:DC:N4	2.13	0.43
2:C:91:GLN:HB3	2:C:119:PRO:HA	2.00	0.43
2:C:217:LEU:HD13	2:C:217:LEU:HA	1.82	0.43
2:C:458:TYR:HB3	2:C:470:PRO:HG3	2.01	0.43
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.53	0.43
3:D:63:TYR:HE2	3:D:73:CYS:HA	1.82	0.43
3:D:543:LEU:HD13	3:D:581:LEU:HA	2.01	0.43
3:D:879:ARG:HD3	3:D:902:LEU:O	2.18	0.43
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.18	0.43
1:B:90:LEU:HD21	1:B:121:GLU:HB2	2.01	0.43
2:C:859:PRO:O	2:C:867:VAL:HG22	2.19	0.43
2:C:1056:LYS:HB3	3:D:623:VAL:HB	2.00	0.43
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.83	0.43
3:D:356:PRO:HB3	3:D:441:ARG:HA	2.00	0.43
1:B:8:ALA:HB1	1:B:27:PRO:HD2	2.00	0.43
2:C:40:GLU:O	2:C:45:GLN:HG2	2.18	0.43
3:D:125:GLN:HA	3:D:130:SER:HB3	2.01	0.43
3:D:1140:ILE:O	3:D:1144:LEU:HB2	2.18	0.43
4:E:83:ASP:OD1	4:E:83:ASP:N	2.52	0.43
2:C:139:GLN:NE2	2:C:413:LEU:O	2.52	0.43
2:C:891:GLY:O	2:C:991:GLN:HB2	2.18	0.43
2:C:1005:MET:HE2	2:C:1005:MET:HB3	1.92	0.43
3:D:523:ASP:O	3:D:526:PRO:HG3	2.19	0.43
3:D:671:LYS:NZ	5:F:421:PHE:HA	2.34	0.43
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.51	0.43
3:D:618:LEU:HD12	3:D:1467:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:196:VAL:HG11	8:H:7:DC:H4'	2.01	0.43
3:D:771:SER:HB2	3:D:778:LEU:HD22	2.00	0.43
3:D:843:PHE:HE2	3:D:864:VAL:HG21	1.84	0.43
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.83	0.42
2:C:32:ALA:HB2	2:C:73:LEU:HD12	2.01	0.42
1:A:221:HIS:O	1:A:224:TYR:HB2	2.20	0.42
2:C:419:THR:HG23	2:C:422:ARG:HG3	2.01	0.42
3:D:161:LEU:HB3	3:D:452:ILE:HD11	2.01	0.42
6:G:17:DG:H2'	6:G:18:DA:H8	1.80	0.42
8:H:12:DG:H3'	8:H:13:DC:O4'	2.19	0.42
2:C:543:ASN:HD21	2:C:566:THR:HG22	1.84	0.42
2:C:627:ARG:HH22	2:C:640:ARG:HG3	1.84	0.42
3:D:787:LEU:HD21	3:D:947:ILE:HG21	2.02	0.42
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.78	0.42
2:C:236:ILE:O	2:C:240:THR:HG23	2.20	0.42
2:C:595:LEU:HB3	2:C:655:LEU:HB2	2.02	0.42
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	2.35	0.42
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.85	0.42
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.76	0.42
5:F:107:GLU:HG3	5:F:229:TYR:CD2	2.54	0.42
2:C:144:PRO:HG2	2:C:165:LEU:HD23	2.01	0.42
2:C:299:LYS:HB2	2:C:299:LYS:HE3	1.84	0.42
3:D:1072:ILE:O	3:D:1075:HIS:HB2	2.20	0.42
3:D:1087:ARG:HD2	3:D:1236:LEU:O	2.19	0.42
5:F:163:LEU:HB3	5:F:174:LEU:HD22	2.02	0.42
5:F:318:GLU:OE1	5:F:318:GLU:N	2.50	0.42
2:C:888:THR:O	2:C:990:GLY:HA3	2.20	0.42
2:C:910:LYS:O	2:C:914:ILE:HG13	2.19	0.42
3:D:200:ASP:O	3:D:397:LYS:HG2	2.20	0.42
3:D:572:ARG:NH2	5:F:87:GLU:OE2	2.53	0.42
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.89	0.42
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.85	0.42
2:C:389:SER:OG	2:C:390:GLN:N	2.53	0.42
2:C:390:GLN:HE21	2:C:390:GLN:HB2	1.57	0.42
3:D:15:PRO:HG3	11:D:2105:HOH:O	2.20	0.42
3:D:258:VAL:HG12	3:D:273:ARG:O	2.20	0.42
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.20	0.42
5:F:184:ARG:O	5:F:188:ILE:HG13	2.20	0.42
2:C:944:LEU:HD21	2:C:963:LEU:HD23	2.02	0.42
2:C:992:MET:HG2	2:C:994:ILE:HG13	2.02	0.42
3:D:689:ASP:O	3:D:693:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:571:LEU:HD22	2:C:700:TYR:HA	2.02	0.42
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.84	0.42
5:F:181:GLU:O	5:F:185:GLN:HG2	2.20	0.42
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.84	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.84	0.41
5:F:231:ARG:HG3	8:H:2:DA:C2	2.54	0.41
8:H:13:DC:H1'	8:H:14:DT:H72	2.02	0.41
1:A:10:VAL:HG12	1:A:26:GLU:O	2.19	0.41
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.01	0.41
3:D:1000:THR:HG23	3:D:1041:LEU:HD11	2.02	0.41
2:C:1107:ASN:HA	2:C:1108:PRO:HD3	1.94	0.41
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.55	0.41
3:D:1100:ASP:O	3:D:1103:HIS:HD2	2.03	0.41
2:C:207:LEU:HD13	2:C:221:LEU:HD21	2.03	0.41
2:C:755:LEU:HB3	2:C:825:VAL:HG21	2.02	0.41
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.56	0.41
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.36	0.41
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.91	0.41
2:C:63:GLY:HA3	2:C:100:LEU:HD21	2.03	0.41
2:C:167:LYS:O	2:C:169:GLY:N	2.52	0.41
2:C:627:ARG:NH2	2:C:640:ARG:HG3	2.35	0.41
3:D:22:SER:HB2	3:D:92:HIS:HB3	2.02	0.41
3:D:106:LYS:HA	3:D:106:LYS:HD2	1.81	0.41
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	2.01	0.41
2:C:610:ARG:HG2	2:C:611:ILE:N	2.35	0.41
3:D:238:PRO:HD3	3:D:318:ARG:HG3	2.03	0.41
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.95	0.41
8:H:17:DC:H2''	8:H:18:DA:C8	2.56	0.41
8:H:19:DC:H6	8:H:19:DC:H2'	1.77	0.41
3:D:490:ALA:O	3:D:494:LYS:HG3	2.21	0.41
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.94	0.41
5:F:330:GLY:HA2	5:F:333:ILE:HD12	2.02	0.41
2:C:713:ARG:CZ	3:D:533:GLY:HA3	2.51	0.41
2:C:892:LEU:HB2	2:C:990:GLY:HA2	2.02	0.41
3:D:161:LEU:HB3	3:D:452:ILE:CD1	2.51	0.41
3:D:729:HIS:N	11:D:2102:HOH:O	2.53	0.41
1:B:94:LEU:HD11	1:B:96:THR:O	2.21	0.41
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.21	0.41
3:D:12:LEU:HA	3:D:12:LEU:HD23	1.89	0.41
3:D:597:ASP:O	3:D:599:PRO:HD3	2.21	0.41
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.88	0.41
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.90	0.41
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.88	0.40
1:B:94:LEU:O	1:B:146:ARG:NH2	2.46	0.40
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.76	0.40
2:C:1095:LEU:HD13	3:D:103:TRP:CH2	2.56	0.40
2:C:206:THR:O	2:C:210:GLU:HB2	2.20	0.40
3:D:373:PRO:HA	3:D:376:GLU:HG3	2.03	0.40
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.21	0.40
1:B:101:LEU:HD11	1:B:113:ASP:HB2	2.03	0.40
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.57	0.40
2:C:838:LYS:HE2	2:C:997:LEU:HD12	2.04	0.40
2:C:853:LEU:HB2	2:C:858:MET:SD	2.61	0.40
3:D:134:VAL:HG23	3:D:151:GLN:O	2.21	0.40
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.92	0.40
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.55	0.40
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.56	0.40
3:D:1407:LEU:O	3:D:1412:LYS:N	2.53	0.40
5:F:93:LEU:HA	5:F:93:LEU:HD23	1.89	0.40
5:F:295:MET:HB3	5:F:299:TRP:CG	2.55	0.40
8:H:13:DC:C1'	8:H:14:DT:H72	2.52	0.40
1:B:110:LYS:HD2	1:B:126:ASP:O	2.21	0.40
3:D:864:VAL:HG22	3:D:865:THR:H	1.86	0.40
3:D:895:VAL:O	3:D:899:LEU:HG	2.22	0.40
4:E:59:ASN:O	4:E:63:TRP:HD1	2.04	0.40
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.86	0.40
2:C:570:PRO:HB3	2:C:660:ALA:HB2	2.04	0.40
2:C:886:LEU:HD21	3:D:951:ILE:HG12	2.04	0.40
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.02	0.40
5:F:361:LEU:HB3	5:F:365:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/315 (73%)	227 (99%)	3 (1%)	0	100	100
1	B	221/315 (70%)	216 (98%)	4 (2%)	1 (0%)	29	61
2	C	1111/1119 (99%)	1076 (97%)	35 (3%)	0	100	100
3	D	1484/1524 (97%)	1433 (97%)	51 (3%)	0	100	100
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	331/443 (75%)	327 (99%)	4 (1%)	0	100	100
All	All	3469/3815 (91%)	3368 (97%)	100 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/273 (74%)	199 (99%)	2 (1%)	76	86
1	B	196/273 (72%)	193 (98%)	3 (2%)	65	81
2	C	939/941 (100%)	913 (97%)	26 (3%)	43	70
3	D	1255/1279 (98%)	1224 (98%)	31 (2%)	47	72
4	E	82/88 (93%)	80 (98%)	2 (2%)	49	73
5	F	291/388 (75%)	281 (97%)	10 (3%)	37	65
All	All	2964/3242 (91%)	2890 (98%)	74 (2%)	47	72

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	112	ARG
1	B	126	ASP
1	B	154	GLU
1	B	188	GLN
2	C	11	GLU
2	C	27	ARG
2	C	133	ASP
2	C	177	GLU
2	C	182	VAL
2	C	217	LEU
2	C	230	ARG
2	C	274	ARG
2	C	276	LYS
2	C	284	ARG
2	C	345	ARG
2	C	353	ARG
2	C	384	GLU
2	C	388	ARG
2	C	390	GLN
2	C	419	THR
2	C	443	THR
2	C	513	VAL
2	C	595	LEU
2	C	617	ASP
2	C	723	THR
2	C	775	ARG
2	C	807[A]	ARG
2	C	807[B]	ARG
2	C	888	THR
2	C	929	ARG
3	D	71	LYS
3	D	106	LYS
3	D	145	VAL
3	D	231	VAL
3	D	270	LEU
3	D	452	ILE
3	D	544	TYR
3	D	628	ARG
3	D	632	VAL
3	D	650	LEU
3	D	687	VAL
3	D	741	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	747	VAL
3	D	754	PHE
3	D	778	LEU
3	D	784	ASP
3	D	810	GLU
3	D	894	LYS
3	D	907	GLU
3	D	921	ARG
3	D	922	LEU
3	D	986	ARG
3	D	1129	THR
3	D	1207	TYR
3	D	1231	GLU
3	D	1234	THR
3	D	1252	ILE
3	D	1286	THR
3	D	1295	GLU
3	D	1307	LYS
3	D	1501	GLU
4	E	49	GLN
4	E	50	THR
5	F	88	ILE
5	F	122	LEU
5	F	186	HIS
5	F	193	ARG
5	F	205	ARG
5	F	209	PHE
5	F	218	GLN
5	F	233	PHE
5	F	380	GLU
5	F	417	LYS

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	156	HIS
1	B	212	ASN
2	C	99	GLN
2	C	343	GLN
2	C	390	GLN
2	C	543	ASN
2	C	1026	GLN

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Mol	Chain	Res	Type
3	D	66	GLN
3	D	669	ASN
3	D	717	GLN
3	D	762	GLN
3	D	1046	GLN
3	D	1075	HIS
3	D	1124	GLN
3	D	1172	HIS
3	D	1359	GLN
5	F	83	GLN
5	F	218	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	I	6/7 (85%)	1 (16%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	I	2	C

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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, 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%)	0.10	13 (5%) 24 23	74, 114, 142, 189	0
1	B	223/315 (70%)	-0.10	1 (0%) 92 93	66, 99, 137, 157	0
2	C	1112/1119 (99%)	0.20	48 (4%) 35 34	55, 114, 176, 217	0
3	D	1486/1524 (97%)	0.23	88 (5%) 22 22	50, 97, 174, 205	1 (0%)
4	E	94/99 (94%)	0.20	4 (4%) 35 34	76, 124, 176, 182	0
5	F	335/443 (75%)	0.53	37 (11%) 5 5	88, 138, 224, 236	0
6	G	18/21 (85%)	-0.18	0 100 100	73, 104, 196, 202	0
7	I	7/7 (100%)	-0.39	0 100 100	69, 76, 122, 132	0
8	H	25/28 (89%)	0.02	1 (4%) 38 36	102, 124, 181, 209	0
All	All	3531/3871 (91%)	0.21	192 (5%) 25 24	50, 110, 179, 236	1 (0%)

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	766	GLU	6.9
3	D	409	VAL	6.6
2	C	63	GLY	6.6
5	F	381	HIS	6.6
5	F	390	PHE	6.4
5	F	149	GLU	6.1
3	D	282	TYR	5.8
3	D	324	ALA	5.5
1	A	233	VAL	5.4
2	C	769	PRO	5.3
3	D	368	VAL	5.1
3	D	1495	ILE	5.1
3	D	326	GLU	4.9
3	D	1313	VAL	4.9
3	D	367	ILE	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	66	LEU	4.8
3	D	305	ALA	4.8
1	A	234	ALA	4.8
2	C	372	LEU	4.7
3	D	269	PHE	4.7
3	D	322	VAL	4.7
2	C	365	ASP	4.6
3	D	241	ILE	4.6
1	A	232	ALA	4.6
3	D	344	ASP	4.5
5	F	375	LEU	4.4
3	D	350	HIS	4.4
2	C	98	LEU	4.3
5	F	373	LYS	4.3
5	F	331	ASP	4.2
3	D	1294	VAL	4.2
3	D	268	ALA	4.0
3	D	345	TYR	4.0
2	C	643	VAL	3.9
2	C	811	PRO	3.8
2	C	823	VAL	3.8
2	C	650	ARG	3.8
3	D	78	VAL	3.8
3	D	1297	GLU	3.7
3	D	310	LEU	3.7
3	D	355	VAL	3.6
2	C	100	LEU	3.6
3	D	1277	ILE	3.5
2	C	367	LEU	3.5
5	F	330	GLY	3.5
3	D	280	ALA	3.5
5	F	332	PHE	3.4
3	D	77	GLY	3.4
2	C	814	GLU	3.4
1	A	231	ALA	3.4
2	C	104	ASP	3.4
5	F	397	ILE	3.3
3	D	1299	PHE	3.3
2	C	421	GLU	3.2
3	D	212	ARG	3.2
5	F	386	VAL	3.2
5	F	392	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	729	LEU	3.2
3	D	1499	ARG	3.2
3	D	335	LEU	3.2
3	D	75	ARG	3.1
2	C	109	LYS	3.1
4	E	32	ARG	3.1
5	F	163	LEU	3.1
3	D	821	VAL	3.1
3	D	1280	VAL	3.1
3	D	178	LEU	3.0
3	D	531	ASP	3.0
5	F	414	ARG	3.0
3	D	974	ILE	3.0
4	E	87	LYS	3.0
3	D	343	LYS	2.9
5	F	173	TYR	2.9
3	D	236	TYR	2.9
3	D	1318	TYR	2.9
3	D	223	LEU	2.9
8	H	23	DT	2.9
3	D	1058	ARG	2.9
3	D	333	LEU	2.9
5	F	389	PHE	2.9
3	D	379	ALA	2.9
3	D	198	ARG	2.8
3	D	1292	VAL	2.8
3	D	41	ARG	2.8
3	D	1182	GLU	2.8
2	C	822	VAL	2.8
2	C	68	PHE	2.8
5	F	376	ILE	2.8
5	F	147	LEU	2.8
5	F	382	THR	2.8
3	D	312	ARG	2.7
3	D	680	GLN	2.7
2	C	603	VAL	2.7
3	D	79	GLU	2.7
1	A	85	LEU	2.7
1	A	94	LEU	2.7
1	A	95	GLN	2.7
3	D	68	PHE	2.7
4	E	85	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	1487	VAL	2.7
5	F	422	LEU	2.6
3	D	833	GLU	2.6
2	C	649	VAL	2.6
3	D	1278	ASP	2.6
2	C	219	GLN	2.6
5	F	421	PHE	2.6
3	D	1296	SER	2.6
5	F	196	VAL	2.6
3	D	378	ILE	2.6
3	D	286	VAL	2.6
1	A	230	ALA	2.6
3	D	371	ILE	2.6
2	C	52	PHE	2.5
3	D	62	LYS	2.5
5	F	146	GLY	2.5
2	C	375	SER	2.5
2	C	606	VAL	2.5
3	D	267	GLY	2.5
3	D	1279	GLY	2.5
3	D	304	LEU	2.5
2	C	299	LYS	2.5
2	C	777	ILE	2.5
3	D	235	ALA	2.4
2	C	726	ILE	2.4
3	D	63	TYR	2.4
3	D	233	LYS	2.4
3	D	1183	ILE	2.4
2	C	767	PRO	2.4
3	D	272	LEU	2.4
2	C	251	ASP	2.4
3	D	80	VAL	2.4
5	F	307	THR	2.4
5	F	410	TYR	2.4
1	B	120	VAL	2.4
4	E	89	MET	2.4
3	D	203	ALA	2.4
2	C	741	GLY	2.3
5	F	148	LYS	2.3
3	D	191	LEU	2.3
3	D	270	LEU	2.3
1	A	96	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	755	LEU	2.3
3	D	1311	LEU	2.3
2	C	511	GLU	2.3
2	C	503	LEU	2.3
3	D	321	GLN	2.3
3	D	334	THR	2.3
5	F	377	ASP	2.3
2	C	739	GLU	2.3
3	D	225	LEU	2.3
2	C	230	ARG	2.2
5	F	404	ALA	2.2
2	C	611	ILE	2.2
5	F	374	GLY	2.2
1	A	132	LEU	2.2
1	A	73	GLU	2.2
2	C	116	GLY	2.2
3	D	336	PHE	2.2
3	D	342	PRO	2.2
5	F	393	THR	2.2
5	F	371	LEU	2.2
3	D	657	LEU	2.2
3	D	372	ASP	2.2
3	D	831	GLY	2.2
5	F	391	GLY	2.2
1	A	72	LYS	2.1
3	D	262	LYS	2.1
3	D	48	ARG	2.1
5	F	155	THR	2.1
5	F	127	ILE	2.1
2	C	373	VAL	2.1
3	D	70	GLY	2.1
3	D	173	PRO	2.1
2	C	250	ARG	2.1
3	D	410	SER	2.1
3	D	1312	LEU	2.1
2	C	439	CYS	2.1
2	C	781	LYS	2.1
3	D	205	TYR	2.1
2	C	254	VAL	2.0
2	C	362	GLY	2.0
5	F	232	ARG	2.0
3	D	323	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	217	ASN	2.0
2	C	654	LEU	2.0
2	C	368	THR	2.0
2	C	543	ASN	2.0
1	A	19	GLU	2.0
5	F	191	ASN	2.0
5	F	192	LEU	2.0
3	D	1287	GLU	2.0
3	D	199	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MG	B	2001	1/1	0.56	0.34	118,118,118,118	0
9	MG	D	2003	1/1	0.91	0.21	53,53,53,53	0
9	MG	F	2001	1/1	0.91	0.03	135,135,135,135	0
10	ZN	D	2002	1/1	0.94	0.09	163,163,163,163	0
9	MG	D	2004	1/1	0.96	0.50	65,65,65,65	0
10	ZN	D	2001	1/1	0.99	0.14	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.