



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 06:48 PM EST

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 : unknown
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

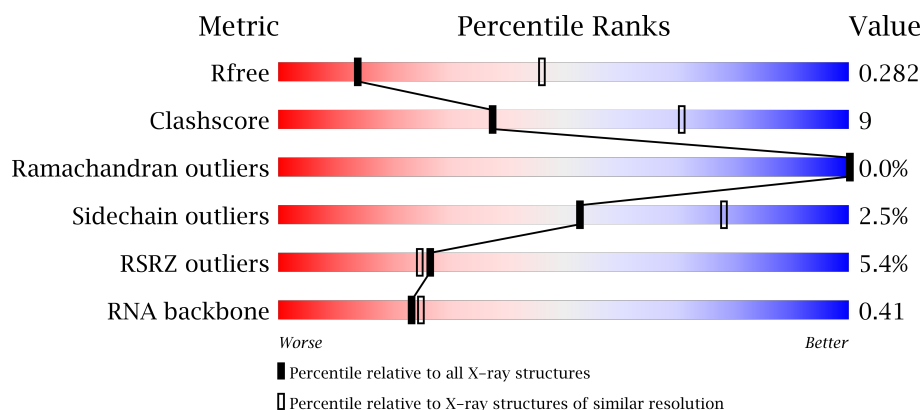
1 Overall quality at a glance

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.





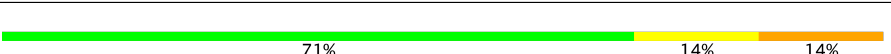
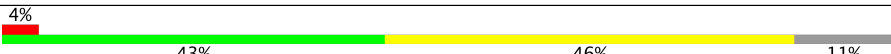
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>61% 12% 27%</div> </div>
1	B	315	<div> <div>0%</div> <div>53% 17% 29%</div> </div>
2	C	1119	<div> <div>4%</div> <div>76% 23% ..</div> </div>
3	D	1524	<div> <div>6%</div> <div>74% 23% .</div> </div>

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MG	D	2004	-	-	-	X

2 Entry composition

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
1	A	231	Total	C	N	O	S	0	1	0
			1814	1158	316	338	2			
1	B	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	3	0
			8792	5562	1570	1636	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	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
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
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
6	G	18	Total	C	N	O	P	0	0	0
			372	176	73	106	17			

- 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
7	I	7	Total	C	N	O	P	0	0	0
			142	65	24	47	6			

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

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

- 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).

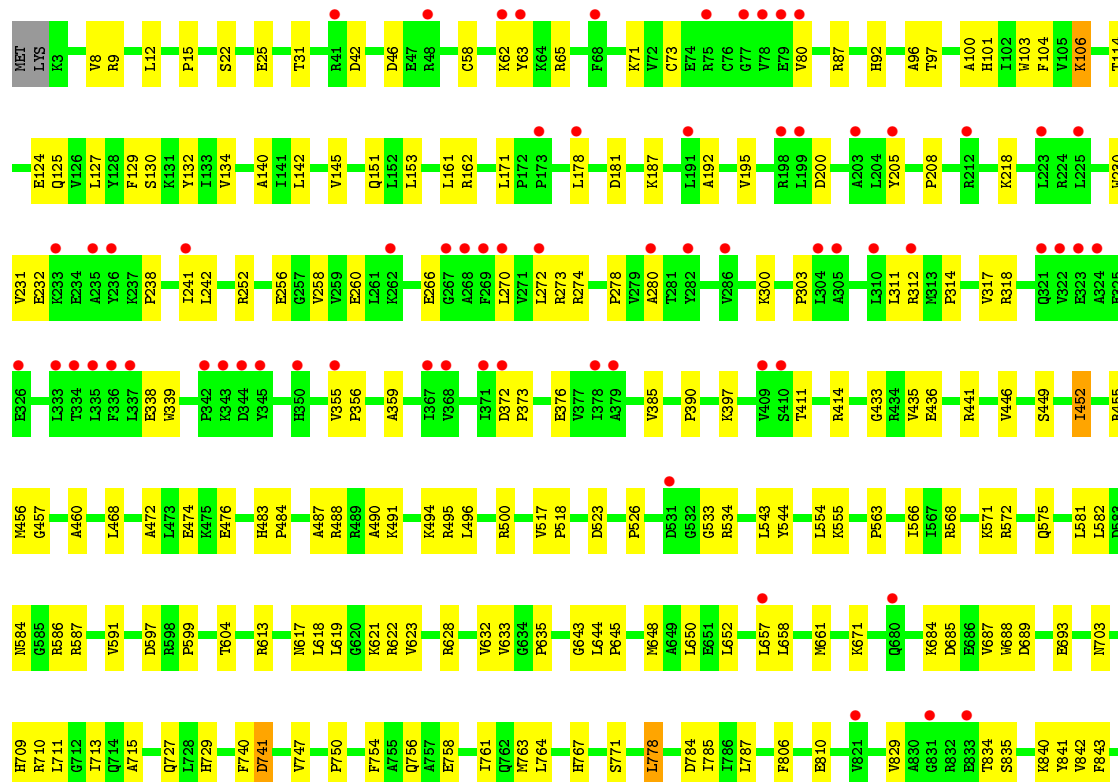
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

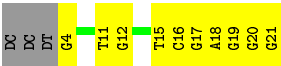
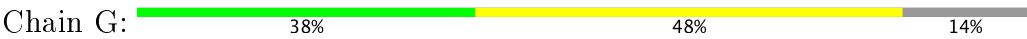
- Molecule 11 is water.

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 1: DNA-directed RNA polymerase subunit alpha



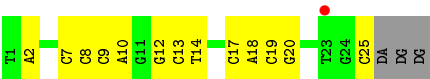




- Molecule 7: RNA (5'-R(*CP*CP*CP*UP*CP*GP*A)-3')



- Molecule 8: DNA (28-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.9	Depositor
R, R_{free}	0.238 , 0.284 0.238 , 0.282	Depositor DCC
R_{free} test set	3826 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	101.6	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28645	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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:1096:ARG:NH1	3:D:1440:PHE:O	2.35	0.60
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.66	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:HD3	3:D:894:LYS:H	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
8:H:13:DC:C3'	8:H:14:DT:H72	2.35	0.57
6:G:4:DG:H1	8:H:25:DC:H42	1.53	0.57
1:B:191:ASP:N	1:B:191:ASP:OD1	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
2:C:223:ASP:OD2	2:C:225:SER:OG	2.21	0.56
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.87	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:1036:GLU:OE2	2:C:1036:GLU:N	2.40	0.54
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.38	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:208:PRO:HA	3:D:390:PRO:HA	1.91	0.52
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.92	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: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
3:D:761:ILE:HD12	4:E:20:THR:HA	1.92	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:187:LYS:N	3:D:200:ASP:OD2	2.34	0.51
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.46	0.51
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.93	0.51
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.93	0.51
3:D:314:PRO:HB2	3:D:317:VAL:HG12	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:N	4:E:37:ASN:OD1	2.42	0.49
5:F:208:SER:OG	8:H:9:DC:N4	2.44	0.49
2:C:551:GLU:N	2:C:551:GLU:OE2	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: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
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.48	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
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
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.28	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
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
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.46	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:396:ASP:HA	2:C:633:GLN:HE22	1.80	0.47
2:C:42:VAL:O	2:C:45:GLN:HB3	2.13	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:N	2:C:881:ASN:OD1	2.48	0.47
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.97	0.47
3:D:42:ASP:N	3:D:46:ASP:OD2	2.38	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
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
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.96	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:1112:CYS:HB3	3:D:1196:THR:OG1	2.15	0.46
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.97	0.46
2:C:1019:GLN:CG	2:C:1058:ASP:HB3	2.45	0.46
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.98	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:1402:ALA:O	3:D:1405:GLU:HG2	2.16	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

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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:102:LYS:HB2	1:A:102:LYS:HE3	1.74	0.46
1:A:70:GLY:H	2:C:607:ASP:CG	2.19	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:1225:ALA:O	3:D:1229:ILE:HG13	2.16	0.46
3:D:103:TRP:HZ2	3:D:604:THR:HG1	1.64	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
3:D:411:THR:HG23	3:D:436:GLU:HA	1.98	0.45
2:C:1043:TYR:OH	3:D:713:ILE:O	2.28	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:1019:GLN:HE21	3:D:621:LYS:HE3	1.80	0.45
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.97	0.45
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.75	0.45
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.52	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:1258:ARG:NH1	3:D:1261:GLU:OE2	2.47	0.45
3:D:923:GLY:O	3:D:927:THR:OG1	2.25	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:615:TYR:OH	2:C:623:TYR:OH	2.15	0.44
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.17	0.44
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	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
2:C:134:ARG:NH2	6:G:21:DG:O3'	2.35	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: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
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
2:C:578:VAL:HA	2:C:900:ARG:HG2	2.00	0.44
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.52	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
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:1101:THR:OG1	2:C:1109:VAL:O	2.33	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
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:1274:ILE:HD11	3:D:1334:GLN:HB3	2.00	0.44
3:D:966:GLU:O	3:D:969:ARG:HG2	2.18	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:1010:ASN:OD1	3:D:1014:ASN:ND2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:487:ALA:O	3:D:491:LYS:HG2	2.18	0.43
3:D:913:ASP:O	3:D:917:GLN:HG2	2.18	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:1048:PRO:HD3	3:D:1075:HIS:CD2	2.54	0.43
3:D:96:ALA:HB3	3:D:554:LEU:HD23	2.00	0.43
3:D:31:THR:HG21	5:F:257:THR:HG22	2.00	0.43
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.00	0.43
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.99	0.43
3:D:230:TRP:CZ3	3:D:232:GLU:HG2	2.53	0.43
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.51	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:217:LEU:HA	2:C:217:LEU:HD13	1.82	0.43
2:C:458:TYR:HB3	2:C:470:PRO:HG3	2.01	0.43
2:C:91:GLN:HB3	2:C:119:PRO:HA	2.00	0.43
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.53	0.43
3:D:543:LEU:HD13	3:D:581:LEU:HA	2.01	0.43
3:D:63:TYR:HE2	3:D:73:CYS:HA	1.82	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:1056:LYS:HB3	3:D:623:VAL:HB	2.00	0.43
2:C:859:PRO:O	2:C:867:VAL:HG22	2.19	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:1140:ILE:O	3:D:1144:LEU:HB2	2.18	0.43
3:D:125:GLN:HA	3:D:130:SER:HB3	2.01	0.43
4:E:83:ASP:N	4:E:83:ASP:OD1	2.52	0.43
2:C:1005:MET:HE2	2:C:1005:MET:HB3	1.92	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
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:1463:LYS:HE2	3:D:1463:LYS:HB3	1.78	0.42
3:D:787:LEU:HD21	3:D:947:ILE:HG21	2.02	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:1144:LEU:HD23	3:D:1144:LEU:HA	1.76	0.42
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.85	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:N	5:F:318:GLU:OE1	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:85:LEU:HA	1:B:124:ASN:HD21	1.85	0.42
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.89	0.42
2:C:389:SER:OG	2:C:390:GLN:N	2.53	0.42
2:C:390:GLN:HB2	2:C:390:GLN:HE21	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:678:PRO:HA	2:C:683:ASN:HD21	1.84	0.42
2:C:571:LEU:HD22	2:C:700:TYR:HA	2.02	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:1100:ASP:O	3:D:1103:HIS:HD2	2.03	0.41
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.55	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: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
3:D:22:SER:HB2	3:D:92:HIS:HB3	2.02	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:H2'	8:H:19:DC:H6	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: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
2:C:713:ARG:CZ	3:D:533:GLY:HA3	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:HD23	3:D:12:LEU:HA	1.89	0.41
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.46	0.41
3:D:597:ASP:O	3:D:599:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:68:LEU:HA	4:E:68:LEU:HD12	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:1095:LEU:HD13	3:D:103:TRP:CH2	2.56	0.40
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.76	0.40
2:C:206:THR:O	2:C:210:GLU:HB2	2.20	0.40
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.21	0.40
3:D:373:PRO:HA	3:D:376:GLU:HG3	2.03	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:1053:PHE:CE2	3:D:1072:ILE:HG23	2.56	0.40
3:D:134:VAL:HG23	3:D:151:GLN:O	2.21	0.40
3:D:1407:LEU:O	3:D:1412:LYS:N	2.53	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
5:F:295:MET:HB3	5:F:299:TRP:CG	2.55	0.40
5:F:93:LEU:HD23	5:F:93:LEU:HA	1.89	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/315 (73%)	227 (99%)	3 (1%)	0	100	100
1	B	221/315 (70%)	216 (98%)	4 (2%)	1 (0%)	32	66
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 ⓘ

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%)	80	88
1	B	196/273 (72%)	193 (98%)	3 (2%)	70	85
2	C	939/941 (100%)	913 (97%)	26 (3%)	49	76
3	D	1255/1279 (98%)	1224 (98%)	31 (2%)	53	78
4	E	82/88 (93%)	80 (98%)	2 (2%)	54	79
5	F	291/388 (75%)	281 (97%)	10 (3%)	42	73
All	All	2964/3242 (91%)	2890 (98%)	74 (2%)	53	78

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

Mol	Chain	Res	Type
1	A	6	LEU

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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
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 carbohydrates 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	0.11	13 (5%) 25 23	74, 114, 142, 189	0
1	B	223/315 (70%)	-0.10	2 (0%) 84 83	66, 99, 137, 157	0
2	C	1112/1119 (99%)	0.21	47 (4%) 37 34	55, 114, 176, 217	0
3	D	1486/1524 (97%)	0.24	87 (5%) 23 22	50, 97, 174, 205	1 (0%)
4	E	94/99 (94%)	0.21	4 (4%) 36 34	76, 124, 176, 182	0
5	F	335/443 (75%)	0.54	37 (11%) 6 5	88, 138, 224, 236	0
6	G	18/21 (85%)	-0.15	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%)	0.06	1 (4%) 39 36	102, 124, 181, 209	0
All	All	3531/3871 (91%)	0.22	191 (5%) 26 25	50, 110, 179, 236	1 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	766	GLU	7.0
5	F	381	HIS	6.8
3	D	409	VAL	6.7
2	C	63	GLY	6.5
5	F	390	PHE	6.3
5	F	149	GLU	5.9
3	D	282	TYR	5.7
1	A	233	VAL	5.6
3	D	324	ALA	5.6
2	C	769	PRO	5.3
3	D	368	VAL	5.2
3	D	1495	ILE	5.2
3	D	322	VAL	5.0
1	A	234	ALA	5.0
3	D	326	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
3	D	367	ILE	4.9
3	D	269	PHE	4.8
3	D	1313	VAL	4.8
1	A	232	ALA	4.8
3	D	241	ILE	4.7
2	C	66	LEU	4.7
2	C	372	LEU	4.7
3	D	305	ALA	4.6
3	D	344	ASP	4.6
2	C	365	ASP	4.6
3	D	350	HIS	4.5
5	F	375	LEU	4.4
2	C	98	LEU	4.4
5	F	373	LYS	4.4
3	D	1294	VAL	4.3
3	D	345	TYR	4.1
3	D	268	ALA	4.0
5	F	331	ASP	4.0
2	C	643	VAL	4.0
3	D	1297	GLU	3.9
2	C	823	VAL	3.9
3	D	310	LEU	3.8
2	C	650	ARG	3.8
3	D	78	VAL	3.8
2	C	811	PRO	3.7
3	D	355	VAL	3.7
3	D	1277	ILE	3.5
1	A	231	ALA	3.5
3	D	280	ALA	3.5
2	C	100	LEU	3.5
2	C	367	LEU	3.4
3	D	77	GLY	3.4
5	F	330	GLY	3.4
3	D	1299	PHE	3.4
2	C	814	GLU	3.4
5	F	332	PHE	3.4
2	C	104	ASP	3.4
2	C	729	LEU	3.3
3	D	75	ARG	3.3
3	D	1499	ARG	3.3
3	D	212	ARG	3.3
5	F	386	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
5	F	397	ILE	3.3
3	D	335	LEU	3.2
2	C	421	GLU	3.2
5	F	392	VAL	3.2
2	C	109	LYS	3.2
4	E	87	LYS	3.1
5	F	414	ARG	3.1
5	F	163	LEU	3.1
4	E	32	ARG	3.1
3	D	1280	VAL	3.1
3	D	821	VAL	3.1
3	D	178	LEU	3.0
3	D	236	TYR	3.0
8	H	23	DT	3.0
3	D	333	LEU	3.0
3	D	974	ILE	3.0
3	D	343	LYS	3.0
3	D	1318	TYR	2.9
3	D	223	LEU	2.9
3	D	312	ARG	2.9
3	D	1058	ARG	2.9
5	F	173	TYR	2.9
3	D	1292	VAL	2.8
2	C	603	VAL	2.8
3	D	41	ARG	2.8
3	D	379	ALA	2.8
2	C	822	VAL	2.8
4	E	85	LEU	2.8
5	F	422	LEU	2.8
5	F	376	ILE	2.8
5	F	382	THR	2.8
2	C	68	PHE	2.8
3	D	833	GLU	2.8
3	D	1487	VAL	2.8
5	F	421	PHE	2.8
3	D	531	ASP	2.8
5	F	389	PHE	2.7
1	A	95	GLN	2.7
3	D	198	ARG	2.7
5	F	147	LEU	2.7
1	A	85	LEU	2.7
3	D	68	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	79	GLU	2.7
3	D	1182	GLU	2.7
1	A	94	LEU	2.7
3	D	680	GLN	2.7
3	D	1296	SER	2.7
3	D	1278	ASP	2.7
2	C	649	VAL	2.7
3	D	286	VAL	2.6
3	D	62	LYS	2.6
5	F	196	VAL	2.6
3	D	371	ILE	2.6
2	C	375	SER	2.6
2	C	219	GLN	2.6
3	D	378	ILE	2.6
3	D	1279	GLY	2.6
1	A	230	ALA	2.6
3	D	267	GLY	2.6
2	C	52	PHE	2.6
3	D	233	LYS	2.6
2	C	606	VAL	2.5
2	C	726	ILE	2.5
2	C	777	ILE	2.5
3	D	235	ALA	2.5
3	D	63	TYR	2.5
5	F	146	GLY	2.5
5	F	410	TYR	2.5
4	E	89	MET	2.5
3	D	304	LEU	2.4
5	F	307	THR	2.4
2	C	767	PRO	2.4
2	C	503	LEU	2.4
3	D	270	LEU	2.4
2	C	739	GLU	2.4
5	F	377	ASP	2.4
3	D	272	LEU	2.4
2	C	299	LYS	2.4
2	C	741	GLY	2.4
3	D	80	VAL	2.4
3	D	334	THR	2.4
3	D	203	ALA	2.3
3	D	1183	ILE	2.3
2	C	116	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	96	THR	2.3
2	C	230	ARG	2.3
2	C	611	ILE	2.3
3	D	225	LEU	2.3
5	F	148	LYS	2.3
3	D	321	GLN	2.3
1	B	120	VAL	2.3
2	C	251	ASP	2.3
2	C	755	LEU	2.3
5	F	404	ALA	2.3
1	A	73	GLU	2.3
3	D	191	LEU	2.3
3	D	336	PHE	2.3
2	C	511	GLU	2.2
5	F	374	GLY	2.2
3	D	342	PRO	2.2
5	F	371	LEU	2.2
3	D	1311	LEU	2.2
3	D	262	LYS	2.2
3	D	372	ASP	2.2
1	A	132	LEU	2.2
2	C	373	VAL	2.2
3	D	831	GLY	2.2
1	A	72	LYS	2.2
3	D	48	ARG	2.2
3	D	657	LEU	2.1
3	D	323	GLU	2.1
2	C	439	CYS	2.1
5	F	232	ARG	2.1
5	F	155	THR	2.1
2	C	654	LEU	2.1
5	F	393	THR	2.1
2	C	543	ASN	2.1
5	F	127	ILE	2.1
5	F	217	ASN	2.1
3	D	205	TYR	2.1
5	F	391	GLY	2.1
5	F	191	ASN	2.1
5	F	192	LEU	2.1
2	C	808	ARG	2.1
3	D	173	PRO	2.0
2	C	781	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	106	PRO	2.0
1	A	19	GLU	2.0
3	D	410	SER	2.0
2	C	807[A]	ARG	2.0
3	D	199	LEU	2.0
2	C	250	ARG	2.0
3	D	337	LEU	2.0
3	D	1312	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 carbohydrates 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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	MG	D	2004	1/1	0.96	0.50	3.88	65,65,65,65	0
10	ZN	D	2001	1/1	0.99	0.14	-0.53	73,73,73,73	0
10	ZN	D	2002	1/1	0.94	0.09	-1.73	163,163,163,163	0
9	MG	F	2001	1/1	0.91	0.04	-3.63	135,135,135,135	0
9	MG	D	2003	1/1	0.90	0.21	-	53,53,53,53	0
9	MG	B	2001	1/1	0.58	0.35	-	118,118,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.