Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 03:25 AM JST

PDB ID	:	6KQE
Title	:	Thermus thermophilus initial transcription complex comprising sigma A and 5'-OH RNA of 4 nt
Authors	:	Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on	:	2019-08-17
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

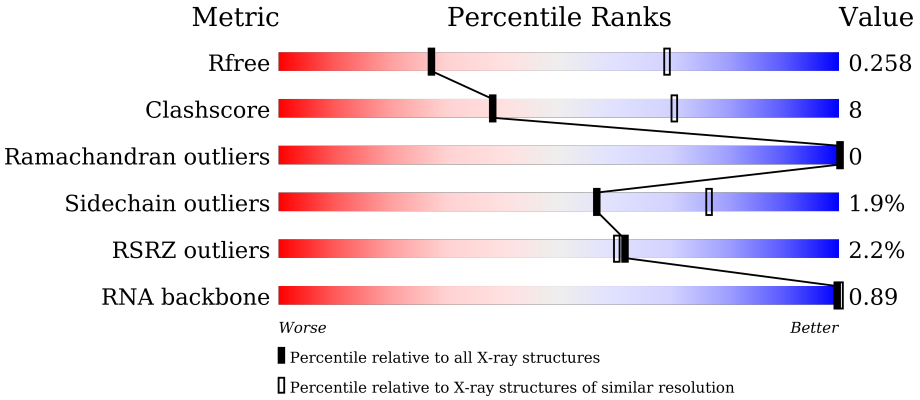
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	.% 60% 13% 27%
1	B	315	58% 13% • 28%
2	C	1119	2% 82% 16% ••
3	D	1524	3% 79% 18% •

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Mol	Chain	Length	Quality of chain
4	E	99	80% 15% 5%
5	F	443	% 65% 13% 22%
6	G	21	48% 33% 19%
7	H	27	33% 56% 11%
8	I	4	100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28688 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	1809	1155	315	337	2	0	0	0
1	B	227	1784	1140	309	333	2	0	0	0

- 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	8762	5544	1559	1635	24	0	0	0

- 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	11751	7450	2070	2195	36	0	2	0

- 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	759	484	132	139	4	0	0	0

- 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	346	2801	1767	506	524	4	0	0	0

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*TP*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	17	350	166	68	100	16	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	4	82	38	15	26	3	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

- 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.

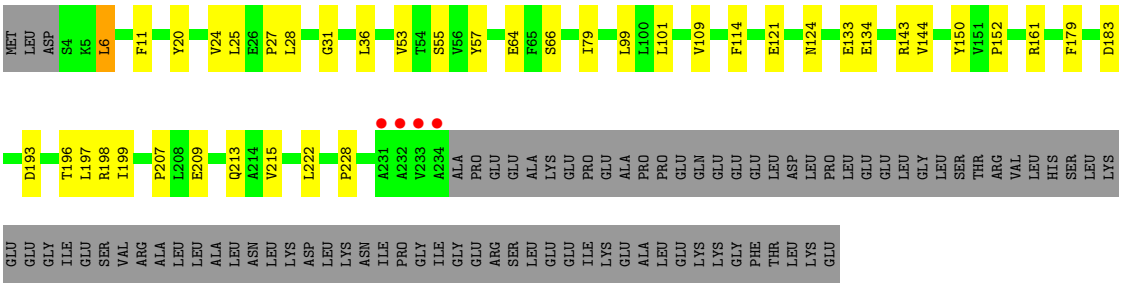
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	8	Total O 8 8	0	0
11	B	4	Total O 4 4	0	0
11	C	23	Total O 23 23	0	0
11	D	39	Total O 39 39	0	0
11	E	2	Total O 2 2	0	0
11	F	9	Total O 9 9	0	0
11	G	3	Total O 3 3	0	0
11	H	1	Total O 1 1	0	0
11	I	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

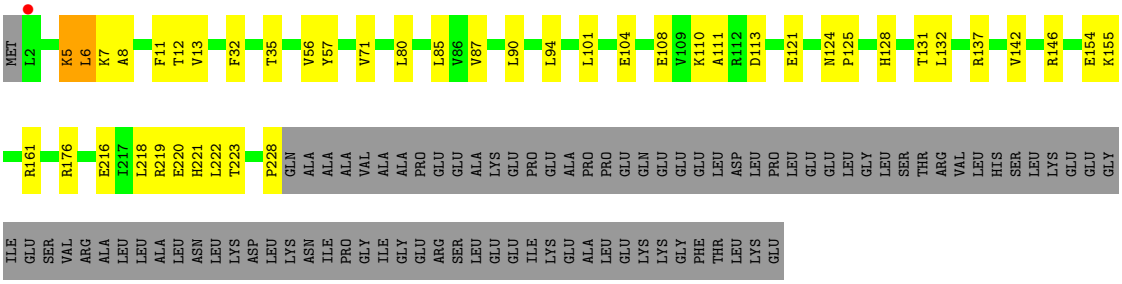
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



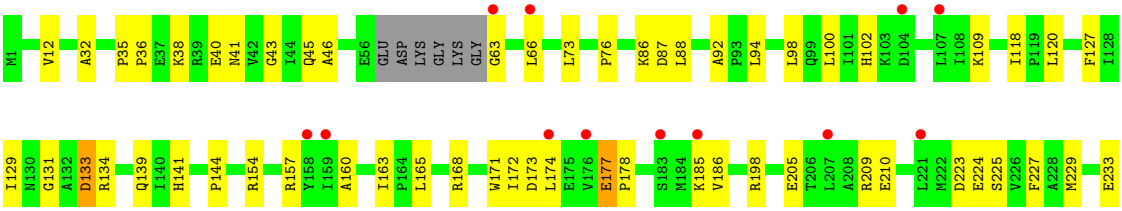
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



P247 P248 I261 R266 Y267 D268 R274 Y275 L281 L304 P305 F311 D326 R331 D342 Q343 L351 M361 D365 S366 L367 T368 L372 V373 F385 L391 E397 S402 L413 L418 T419 F425 D426 V427 R428 H434 I449

G450 L451 A456 A459 D462 R468 R472 T501 P502 L503 I508 V513 N545 R557 S562 T566 L571 M580 T581 G582 L583 E584 E598 K605 R610 I611 V612 E616 D617 G618 R619 E622 R627 F628 S631 N632 D638 Q639

R640 K651 D657 N663 Q670 V674 V689 E693 K696 R697 S702 E709 I710 E711 T715 R721 L729 E739 I745 G757 R758 T768 P769 E770 E771 R775 D784 V785 T788 S789 L790 V801 L806 R807 V822 V823 R824

K851 M858 V867 D868 V869 S878 P904 I905 F906 D907 P912 E916 F926 R929 F934 G935 V936 D937 K938 R939 L944 L950 G951 L952 P959 L963 D976 G977 R978 P982 S1009 S1014 L1015 I1016 Q1019 R1031 E1036 V1037 W1038

T1054 L1055 D1058 A1066 Y1067 I1070 E1083 K1090 E1091 L1092 Q1093 A1094 V1099 D1110 G1114 L1115 A1116 S1117 K1118 ARG

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

Chain D: 3% 79% 18%

MET LYS K3 L12 E25 K28 P29 E30 T31 R35 E40 R41 Y63 K64 R65 E74 V85 R86 R87 Y88 R89 M90 G91 H92 A96 T97 H101 F104 V105 K106 E124 Y128 F129 Y132 I133 V134 P137 L142 N143 G144 Q151 L152

Y158 L161 K165 Q166 E167 L171 P172 P173 G174 K180 D181 G182 E183 R198 V202 A203 L204 Y205 R206 F207 P208 V211 K218 G222 L223 R224 L225 A229 W230 V231 E232 A235 Y236 K237 P238 I241 L242 A243 E244 L245 F251 E254 E260 L261 K262

E266 G267 A268 F269 L272 R273 P278 V279 A280 P290 V298 Q302 A305 L310 L311 R312 M313 P314 V317 R318 A319 V322 E323 A324 L333 T334 L335 F336 L337 E338 W339 Y345 H350 M351 M352 V355 P356 E357 G358 A359 R360 W368 I371 D372

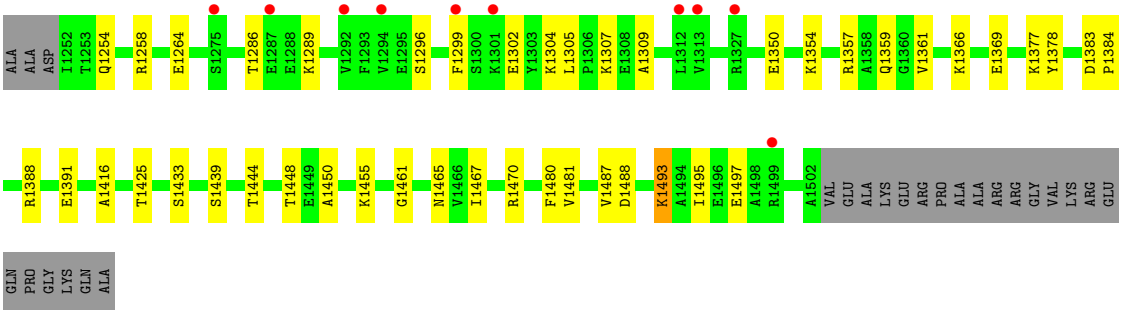
P373 V377 V385 P390 T393 L394 D405 V409 S410 T411 V415 D419 A422 D423 V427 G433 E436 S449 I452 D453 A454 R455 M456 A460 A472 L473 E474 K475 E476 E479 K482 H483 A487 R488 R489 A490 K491 L496 R500

P518 P521 V530 K555 G561 A562 P563 I566 I567 R568 K571 D579 R586 R587 R613 F614 L618 L619 R622 R628 I631 G634 L637 G643 K646 E651 L657 L658 M661 R674 D685 E686 V687 W688 L701 L702

N703 R704 T707 L708 H709 R710 L711 G712 I713 Q714 A715 Q727 L728 H729 P730 A738 D743 F754 R760 I761 Q762 M763 L764 L778 D784 R818 G819 E820 V821 A822 A825 V829 K840 Y841 V842 F843 V864 T865 L881 R884 I885 E888 A889 V890

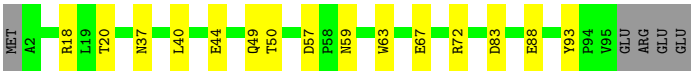
E891 D892 E893 K894 V895 L899 L911 V915 Y916 Q917 L922 F939 A954 K961 L964 K970 I974 E975 E979 L995 E1001 K1002 V1003 N1010 N1014 N1018 P1019 L1020 Q1034 I1035 L1038 C1039 G1040 L1041 M1045 Q1046 K1047 E1051 V1055

P1056 V1057 R1058 S1059 S1060 F1061 R1062 L1065 T1066 V1067 L1068 E1069 I1072 T1084 A1085 L1086 R1087 T1088 V1099 D1100 R1108 T1129 R1130 S1131 L1132 L1144 R1147 V1188 R1189 S1190 Y1198 C1204 Y1205 P1232 L1236 T1237 MET ARG THR PHE HIS THR GLY GLY VAL ALA GLY



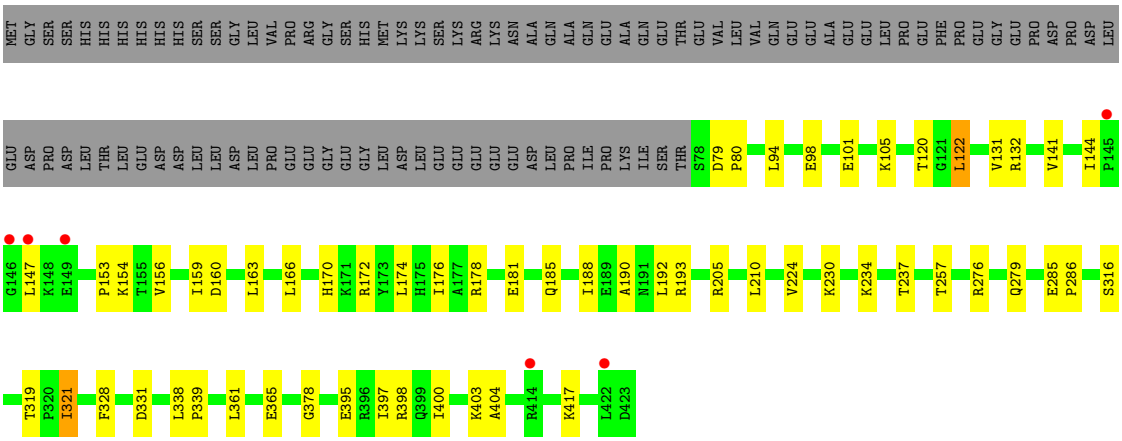
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



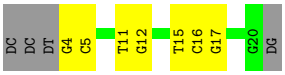
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



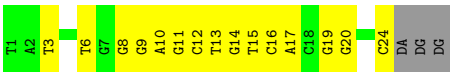
• Molecule 6: DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3')

Chain G:



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

Chain H:



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

Chain I: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.57Å 103.76Å 295.98Å 90.00° 98.70° 90.00°	Depositor
Resolution (Å)	48.95 – 3.30 48.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.95-3.30) 99.9 (48.95-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.217 , 0.258 0.217 , 0.258	Depositor DCC
R_{free} test set	4156 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28688	wwPDB-VP
Average B, all atoms (Å^2)	95.0	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.25	0/1841	0.46	0/2504
1	B	0.26	0/1816	0.48	1/2469 (0.0%)
2	C	0.27	0/8929	0.46	0/12078
3	D	0.24	0/11963	0.45	0/16173
4	E	0.24	0/773	0.42	0/1042
5	F	0.24	0/2846	0.41	0/3830
6	G	0.42	0/393	0.91	0/606
7	H	0.39	0/556	0.94	0/858
8	I	0.23	0/91	0.63	0/140
All	All	0.26	0/29208	0.48	1/39700 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	ALA	C-N-CD	5.15	139.21	128.40

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	1809	0	1863	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1784	0	1830	38	0
2	C	8762	0	8855	135	0
3	D	11751	0	11993	187	0
4	E	759	0	771	10	0
5	F	2801	0	2871	35	0
6	G	350	0	192	16	0
7	H	495	0	272	41	0
8	I	82	0	44	0	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
11	A	8	0	0	1	0
11	B	4	0	0	0	0
11	C	23	0	0	1	0
11	D	39	0	0	1	0
11	E	2	0	0	1	0
11	F	9	0	0	0	0
11	G	3	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
All	All	28688	0	28691	433	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 8.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:425:PHE:CE1	3:D:1086:LEU:HD12	1.74	1.23
7:H:16:DC:H2"	7:H:17:DA:C8	1.78	1.18
7:H:19:DG:H2"	7:H:20:DG:C8	1.80	1.16
6:G:4:DG:H2"	6:G:5:DC:C6	1.82	1.13
6:G:4:DG:H2"	6:G:5:DC:C5	1.82	1.13
7:H:11:DG:H3'	7:H:12:DC:H5"	1.26	1.10
2:C:425:PHE:HE1	3:D:1086:LEU:CD1	1.65	1.08
2:C:425:PHE:HE1	3:D:1086:LEU:HD12	0.98	1.07
2:C:906:PHE:CD2	3:D:1067:VAL:HG12	1.95	1.01
7:H:19:DG:C5	7:H:20:DG:C6	2.52	0.97
6:G:11:DT:H2"	6:G:12:DG:C8	2.00	0.97
6:G:4:DG:C2'	6:G:5:DC:C5	2.47	0.97
7:H:19:DG:H2"	7:H:20:DG:H8	1.29	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HE2	1:B:7:LYS:N	1.88	0.88
7:H:19:DG:C2'	7:H:20:DG:C8	2.56	0.88
7:H:11:DG:H3'	7:H:12:DC:C5'	2.04	0.87
2:C:418:LEU:HD21	7:H:14:DG:C8	2.10	0.87
7:H:16:DC:C2'	7:H:17:DA:C8	2.59	0.86
7:H:15:DT:C4	7:H:16:DC:N4	2.44	0.86
2:C:628:PHE:H	2:C:638:ASP:HB3	1.42	0.84
7:H:16:DC:H2"	7:H:17:DA:N7	1.95	0.79
2:C:418:LEU:HD21	7:H:14:DG:N7	1.97	0.78
1:B:5:LYS:HD2	1:B:5:LYS:O	1.85	0.77
2:C:906:PHE:CE2	3:D:1067:VAL:HA	2.19	0.77
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.67	0.76
2:C:906:PHE:HE2	3:D:1067:VAL:N	1.83	0.76
1:A:228:PRO:HA	1:B:11:PHE:CD2	2.20	0.76
2:C:428:ARG:HD3	2:C:449:ILE:O	1.86	0.75
7:H:8:DG:H2"	7:H:9:DG:O5'	1.87	0.75
6:G:4:DG:H1	7:H:24:DC:H42	1.35	0.74
2:C:139:GLN:HB2	2:C:391:LEU:HD21	1.70	0.73
2:C:906:PHE:CE2	3:D:1067:VAL:CA	2.73	0.72
2:C:425:PHE:CE1	3:D:1086:LEU:CD1	2.53	0.71
7:H:19:DG:C6	7:H:20:DG:C6	2.79	0.71
2:C:906:PHE:CE2	3:D:1067:VAL:N	2.59	0.70
2:C:904:PRO:HB2	2:C:907:ASP:O	1.92	0.70
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.74	0.70
3:D:134:VAL:HG22	3:D:151:GLN:H	1.56	0.70
1:B:6:LEU:HD13	1:B:6:LEU:O	1.93	0.69
2:C:266:ARG:NH1	7:H:11:DG:O6	2.26	0.69
6:G:4:DG:C2'	6:G:5:DC:H5	2.06	0.69
1:B:6:LEU:O	1:B:6:LEU:HD22	1.93	0.68
5:F:316:SER:HB3	5:F:319:THR:HG23	1.75	0.68
7:H:15:DT:C4	7:H:16:DC:C4	2.82	0.67
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.77	0.67
1:B:6:LEU:C	1:B:7:LYS:HE2	2.15	0.66
3:D:208:PRO:HA	3:D:390:PRO:HA	1.78	0.66
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.78	0.66
1:B:5:LYS:HB2	1:B:7:LYS:HZ1	1.62	0.65
3:D:224:ARG:H	3:D:251:PHE:HE1	1.44	0.65
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.79	0.65
7:H:19:DG:C4	7:H:20:DG:C5	2.85	0.65
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.30	0.65
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:ARG:NH1	5:F:378:GLY:O	2.31	0.64
2:C:906:PHE:HD2	3:D:1067:VAL:HG12	1.59	0.64
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.80	0.64
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.31	0.64
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.80	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.63
3:D:657:LEU:HG	3:D:661:MET:HE2	1.80	0.63
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.79	0.63
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.79	0.63
2:C:904:PRO:HD2	2:C:907:ASP:O	1.99	0.63
7:H:15:DT:N3	7:H:16:DC:C4	2.67	0.63
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.99	0.63
3:D:619:LEU:HD11	3:D:1439:SER:HB3	1.79	0.63
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.80	0.62
6:G:4:DG:H2'	6:G:5:DC:C5	2.33	0.62
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.80	0.62
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.81	0.62
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.80	0.62
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.33	0.62
2:C:1067:TYR:OH	3:D:674[A]:ARG:NH1	2.32	0.62
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.64	0.62
3:D:1439:SER:OG	3:D:1467:ILE:HD11	2.00	0.62
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.81	0.62
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.82	0.62
7:H:19:DG:C6	7:H:20:DG:N1	2.69	0.61
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.82	0.61
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.81	0.61
3:D:41:ARG:NH2	11:D:2104:HOH:O	2.32	0.61
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.82	0.61
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.34	0.60
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.83	0.60
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.82	0.60
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.83	0.59
6:G:11:DT:C2'	6:G:12:DG:C8	2.82	0.59
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.35	0.59
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.35	0.59
3:D:622:ARG:NH1	6:G:17:DG:OP1	2.36	0.59
2:C:906:PHE:HE2	3:D:1066:THR:C	2.07	0.58
6:G:4:DG:H2'	6:G:5:DC:H5	1.66	0.58
3:D:1045[B]:MET:HE1	3:D:1057:VAL:HG23	1.84	0.58
2:C:689:VAL:HG13	2:C:851:LYS:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.85	0.58
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.84	0.58
1:B:220:GLU:O	1:B:223:THR:OG1	2.20	0.58
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.35	0.57
3:D:433:GLY:HA2	3:D:449:SER:H	1.70	0.57
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.85	0.57
7:H:19:DG:C5	7:H:20:DG:C5	2.93	0.57
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.87	0.57
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.38	0.57
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.28	0.56
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.87	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.17	0.56
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.87	0.56
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.36	0.56
2:C:425:PHE:HD1	2:C:425:PHE:N	2.03	0.56
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.87	0.56
2:C:425:PHE:N	2:C:425:PHE:CD1	2.73	0.56
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.88	0.56
2:C:402:SER:HA	2:C:566:THR:HG23	1.87	0.56
2:C:905:ILE:HG13	2:C:905:ILE:O	2.04	0.56
7:H:12:DC:H2"	7:H:13:DT:C6	2.41	0.56
7:H:17:DA:OP2	7:H:17:DA:H2'	2.06	0.56
7:H:19:DG:N7	7:H:20:DG:O6	2.39	0.56
2:C:223:ASP:OD1	2:C:225:SER:OG	2.23	0.55
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.88	0.55
3:D:864:VAL:HG12	3:D:865:THR:H	1.71	0.55
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.88	0.55
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.89	0.55
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.89	0.55
2:C:41:ASN:O	2:C:46:ALA:HB2	2.07	0.55
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.87	0.55
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.25	0.54
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.88	0.54
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.90	0.54
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.89	0.54
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.41	0.54
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.89	0.53
1:B:6:LEU:H	1:B:6:LEU:CD1	2.21	0.53
2:C:1067:TYR:OH	3:D:674[B]:ARG:NH1	2.42	0.53
3:D:890:VAL:HG23	3:D:892:ASP:H	1.73	0.53
2:C:758:ARG:HH21	2:C:788:THR:HB	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.91	0.53
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.91	0.53
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.90	0.53
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.91	0.53
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.42	0.53
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.90	0.53
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.89	0.53
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.73	0.52
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.91	0.52
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.90	0.52
2:C:598:GLU:O	2:C:651:LYS:NZ	2.36	0.52
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.91	0.52
2:C:674:VAL:HG23	2:C:869:VAL:HB	1.91	0.52
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.92	0.52
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.90	0.52
3:D:411:THR:HG23	3:D:436:GLU:HA	1.92	0.52
3:D:658:LEU:HA	3:D:661:MET:HE3	1.92	0.52
6:G:12:DG:H5"	6:G:12:DG:H8	1.75	0.52
2:C:168:ARG:O	2:C:267:TYR:HA	2.10	0.52
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.91	0.52
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.45	0.51
1:B:94:LEU:O	1:B:146:ARG:NH2	2.43	0.51
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.91	0.51
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.91	0.51
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.91	0.51
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.92	0.51
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.45	0.51
7:H:16:DC:H2"	7:H:17:DA:H8	1.59	0.51
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.93	0.51
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.44	0.51
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.11	0.51
2:C:571:LEU:HD23	2:C:702:SER:HB3	1.93	0.51
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.11	0.51
5:F:237:THR:HG21	7:H:3:DT:H5"	1.91	0.51
5:F:276:ARG:O	5:F:279:GLN:HG3	2.11	0.51
1:B:6:LEU:HD22	1:B:6:LEU:C	2.31	0.51
7:H:16:DC:C2'	7:H:17:DA:N7	2.69	0.51
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.92	0.51
1:A:209:GLU:O	1:A:213:GLN:HG2	2.10	0.50
2:C:557:ARG:NH2	11:C:1202:HOH:O	2.38	0.50
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:701:LEU:HD22	3:D:763:MET:HE2	1.94	0.50
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.94	0.50
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.93	0.50
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.46	0.50
7:H:16:DC:H1'	7:H:17:DA:C8	2.47	0.50
7:H:19:DG:C5	7:H:20:DG:O6	2.64	0.50
1:B:5:LYS:HB2	1:B:7:LYS:NZ	2.27	0.50
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.44	0.50
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.94	0.50
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.12	0.50
7:H:19:DG:N7	7:H:20:DG:C6	2.79	0.50
2:C:1031:ARG:HG2	6:G:16:DC:H5"	1.93	0.49
3:D:241:ILE:HA	3:D:312:ARG:HB3	1.93	0.49
3:D:894:LYS:H	3:D:894:LYS:HD3	1.77	0.49
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.94	0.49
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.94	0.49
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.93	0.49
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.12	0.49
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.34	0.49
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.94	0.49
1:A:228:PRO:HG3	1:B:11:PHE:HE2	1.78	0.49
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.95	0.49
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.94	0.49
1:A:121:GLU:OE1	11:A:401:HOH:O	2.20	0.49
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.93	0.49
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.44	0.49
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.95	0.48
2:C:1031:ARG:NE	6:G:16:DC:OP1	2.43	0.48
2:C:1036:GLU:OE2	2:C:1036:GLU:N	2.47	0.48
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.25	0.48
1:A:31:GLY:N	1:A:193:ASP:OD2	2.46	0.48
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.95	0.48
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.95	0.48
7:H:16:DC:C1'	7:H:17:DA:C8	2.96	0.48
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.45	0.48
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.77	0.48
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.96	0.48
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.49	0.48
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.96	0.48
2:C:326:ASP:HA	2:C:331:ARG:HD2	1.95	0.48
3:D:864:VAL:HG12	3:D:865:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1232:PRO:HG3	3:D:1361:VAL:HG11	1.96	0.48
3:D:487:ALA:O	3:D:491:LYS:HG2	2.13	0.48
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.48	0.48
2:C:198:ARG:HE	2:C:227:PHE:HA	1.78	0.48
2:C:397:GLU:HG2	2:C:632:ASN:HB2	1.95	0.47
2:C:580:MET:SD	2:C:584:GLU:HG3	2.54	0.47
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.95	0.47
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.96	0.47
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.96	0.47
7:H:19:DG:C8	7:H:20:DG:N7	2.82	0.47
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.49	0.47
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.48	0.47
1:A:228:PRO:CA	1:B:11:PHE:CD2	2.95	0.47
2:C:426:ASP:OD1	2:C:426:ASP:N	2.48	0.47
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.97	0.47
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.50	0.47
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.96	0.47
5:F:79:ASP:OD2	7:H:8:DG:N1	2.35	0.47
5:F:122:LEU:HD21	5:F:159:ILE:HD12	1.97	0.46
5:F:328:PHE:HB2	5:F:331:ASP:OD2	2.14	0.46
3:D:975:GLU:O	3:D:979:GLU:HG2	2.15	0.46
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.97	0.46
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.46
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.97	0.46
2:C:154:ARG:HE	2:C:157:ARG:HG3	1.80	0.46
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.98	0.46
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.98	0.46
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.97	0.46
1:B:155:LYS:HD3	1:B:155:LYS:HA	1.70	0.46
2:C:906:PHE:HE2	3:D:1067:VAL:CA	2.19	0.46
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.97	0.46
2:C:109:LYS:HE2	2:C:368:THR:HG22	1.97	0.46
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.77	0.46
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.98	0.46
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.33	0.46
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.69	0.46
1:B:5:LYS:HD3	1:B:7:LYS:HZ2	1.81	0.45
2:C:905:ILE:O	2:C:906:PHE:HB2	2.15	0.45
2:C:361:MET:SD	2:C:361:MET:N	2.90	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.97	0.45
3:D:784:ASP:HB2	3:D:939:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.16	0.45
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.81	0.45
1:A:11:PHE:O	1:B:228:PRO:HA	2.16	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
3:D:613:ARG:HG3	3:D:618:LEU:HD23	1.98	0.45
3:D:1057:VAL:HG12	3:D:1059:SER:H	1.82	0.45
3:D:1205:TYR:O	3:D:1366:LYS:HD3	2.16	0.45
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.98	0.45
1:A:99:LEU:HD23	1:A:114:PHE:CG	2.52	0.45
2:C:100:LEU:HD13	2:C:367:LEU:O	2.17	0.45
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.99	0.45
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.99	0.45
1:B:6:LEU:HD13	1:B:6:LEU:H	1.82	0.44
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.52	0.44
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.98	0.44
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.98	0.44
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.52	0.44
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.99	0.44
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.99	0.44
2:C:94:LEU:HD22	2:C:118:ILE:HD11	1.98	0.44
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.42	0.44
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.18	0.44
2:C:63:GLY:HA2	2:C:102:HIS:HD2	1.82	0.44
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.00	0.44
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.51	0.44
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.52	0.44
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	2.00	0.44
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.90	0.44
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.99	0.44
2:C:693:GLU:HG3	2:C:697:ARG:HH12	1.81	0.44
2:C:784:ASP:OD1	2:C:784:ASP:N	2.50	0.44
3:D:1047:LYS:N	3:D:1051:GLU:O	2.34	0.44
6:G:15:DT:H2'	6:G:16:DC:C6	2.53	0.44
2:C:163:ILE:HG23	2:C:171:TRP:NE1	2.32	0.44
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.18	0.44
3:D:472:ALA:O	3:D:476:GLU:HG2	2.18	0.44
3:D:881:LEU:O	3:D:885:ILE:HG13	2.18	0.44
3:D:1286:THR:HB	3:D:1289:LYS:H	1.82	0.44
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.99	0.44
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.40	0.44
2:C:205:GLU:O	2:C:209:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:230:TRP:CZ3	3:D:232:GLU:HG2	2.52	0.44
5:F:181:GLU:O	5:F:185:GLN:HG2	2.18	0.44
3:D:895:VAL:HG11	3:D:922:LEU:HD21	2.00	0.44
5:F:172:ARG:O	5:F:176:ILE:HG12	2.18	0.44
7:H:15:DT:C2	7:H:16:DC:C4	3.06	0.44
1:B:12:THR:HG22	1:B:13:VAL:N	2.32	0.43
2:C:769:PRO:HG3	3:D:65:ARG:HH12	1.83	0.43
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.99	0.43
1:A:215:VAL:HG13	1:B:222:LEU:HB3	2.00	0.43
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	2.00	0.43
3:D:96:ALA:HB2	3:D:555:LYS:HG2	2.00	0.43
3:D:715:ALA:HB3	3:D:764:LEU:HA	2.00	0.43
3:D:1481:VAL:HA	4:E:18:ARG:HH21	1.82	0.43
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.31	0.43
3:D:631:ILE:HD11	3:D:743:ASP:HB2	2.00	0.43
7:H:15:DT:C2	7:H:16:DC:C5	3.05	0.43
7:H:15:DT:O4	7:H:16:DC:N4	2.51	0.43
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.99	0.43
3:D:634:GLY:HA3	3:D:637:LEU:HD12	2.01	0.43
3:D:784:ASP:HB2	3:D:939:PHE:HE1	1.83	0.43
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.88	0.43
4:E:83:ASP:OD1	4:E:83:ASP:N	2.51	0.43
6:G:4:DG:N2	6:G:5:DC:C2	2.86	0.43
2:C:745:ILE:HD12	2:C:801:VAL:O	2.18	0.43
2:C:926:PHE:HE1	2:C:929:ARG:HH21	1.66	0.43
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.73	0.43
3:D:106:LYS:HA	3:D:106:LYS:HD2	1.86	0.43
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.00	0.43
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.81	0.43
1:B:176:ARG:HD3	3:D:884:ARG:NH2	2.34	0.43
2:C:418:LEU:CD2	7:H:14:DG:C8	2.91	0.43
3:D:760:ARG:O	3:D:764:LEU:HB2	2.19	0.43
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.00	0.43
2:C:86:LYS:HB2	2:C:88:LEU:HG	2.00	0.43
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.19	0.43
4:E:37:ASN:OD1	4:E:37:ASN:N	2.41	0.43
2:C:462:ASP:HB3	2:C:468:ARG:HD2	2.01	0.43
2:C:858:MET:HE2	2:C:867:VAL:O	2.19	0.43
3:D:614:PHE:HA	3:D:618:LEU:HB2	2.01	0.43
3:D:761:ILE:HD12	4:E:20:THR:HA	2.01	0.43
3:D:1010:ASN:OD1	3:D:1014:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:59:ASN:O	4:E:63:TRP:HD1	2.01	0.43
1:A:101:LEU:HD21	1:A:109:VAL:HG11	2.01	0.42
3:D:229:ALA:HB1	3:D:245:LEU:HD12	2.00	0.42
7:H:10:DA:H2"	7:H:11:DG:O5'	2.18	0.42
2:C:274:ARG:HG3	2:C:275:TYR:N	2.34	0.42
3:D:167:GLU:O	3:D:394:LEU:HD12	2.19	0.42
1:A:25:LEU:HB3	1:A:28:LEU:HD11	2.01	0.42
2:C:1009:SER:HB3	3:D:651:GLU:O	2.18	0.42
1:A:53:VAL:HG22	1:A:144:VAL:HG22	2.01	0.42
3:D:1038:LEU:O	3:D:1060:SER:HB2	2.19	0.42
6:G:4:DG:H1	7:H:24:DC:N4	2.11	0.42
2:C:807:ARG:H	2:C:807:ARG:HG2	1.70	0.42
3:D:90:MET:SD	3:D:521:PRO:HD3	2.58	0.42
3:D:762:GLN:HA	11:E:101:HOH:O	2.19	0.42
5:F:321:ILE:HA	5:F:321:ILE:HD13	1.78	0.42
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.20	0.42
3:D:31:THR:HG21	5:F:257:THR:HG22	2.01	0.42
3:D:333:LEU:HB3	3:D:335:LEU:HD13	2.01	0.42
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.54	0.42
3:D:899:LEU:HD22	3:D:917:GLN:HB3	2.02	0.42
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.02	0.42
2:C:43:GLY:O	2:C:46:ALA:HB3	2.20	0.42
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.19	0.42
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	2.02	0.42
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.51	0.42
2:C:127:PHE:O	2:C:133:ASP:HA	2.20	0.42
2:C:281:LEU:HD13	2:C:305:PRO:HB2	2.02	0.42
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.26	0.42
3:D:134:VAL:CG2	3:D:151:GLN:H	2.29	0.42
3:D:142:LEU:HB2	3:D:161:LEU:HD11	2.02	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.96	0.42
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.55	0.42
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.85	0.41
2:C:1094:ALA:HA	3:D:518:PRO:HB2	2.02	0.41
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.91	0.41
1:A:199:ILE:HB	1:A:207:PRO:HB3	2.02	0.41
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.84	0.41
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.53	0.41
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.02	0.41
3:D:206:ARG:HA	3:D:206:ARG:HD2	1.91	0.41
5:F:94:LEU:HG	5:F:190:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:GLU:O	2:C:45:GLN:HG2	2.20	0.41
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.02	0.41
2:C:456:ALA:HB3	2:C:459:ALA:HB2	2.02	0.41
3:D:371:ILE:HG23	5:F:230:LYS:HD2	2.02	0.41
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.30	0.41
3:D:1444:THR:O	3:D:1448:THR:HG23	2.19	0.41
1:A:133:GLU:HG2	1:A:134:GLU:H	1.85	0.41
2:C:224:GLU:CD	2:C:224:GLU:H	2.24	0.41
3:D:106:LYS:O	3:D:586:ARG:NH1	2.53	0.41
3:D:818:ARG:HE	3:D:820:GLU:CD	2.24	0.41
3:D:964:LEU:HD23	3:D:964:LEU:HA	1.94	0.41
7:H:16:DC:C2	7:H:17:DA:C6	3.09	0.41
2:C:912:PRO:O	2:C:916:GLU:HG3	2.21	0.41
3:D:319:ALA:HA	3:D:337:LEU:HD23	2.02	0.41
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.84	0.41
3:D:1302:GLU:OE1	3:D:1304:LYS:HE3	2.20	0.41
4:E:57:ASP:O	4:E:63:TRP:NE1	2.49	0.41
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.56	0.41
2:C:657:ASP:OD2	2:C:663:ASN:N	2.50	0.41
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	2.03	0.41
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.90	0.41
3:D:1045[B]:MET:HE3	3:D:1045[B]:MET:HB2	1.89	0.41
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	2.02	0.41
5:F:120:THR:HG22	5:F:122:LEU:HD13	2.03	0.41
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.95	0.41
1:B:90:LEU:HD21	1:B:121:GLU:HB2	2.02	0.41
2:C:141:HIS:HE1	2:C:144:PRO:HD3	1.85	0.41
3:D:28:LYS:HA	3:D:29:PRO:HD3	1.88	0.41
3:D:222:GLY:HA2	3:D:333:LEU:O	2.21	0.41
3:D:1296:SER:N	3:D:1299:PHE:O	2.52	0.41
2:C:605:LYS:HB3	2:C:610:ARG:HH11	1.86	0.40
2:C:771:GLU:O	2:C:775:ARG:HB2	2.21	0.40
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.86	0.40
3:D:841:TYR:HB2	3:D:864:VAL:HG13	2.02	0.40
5:F:234:LYS:HE2	5:F:234:LYS:HB3	1.96	0.40
5:F:156:VAL:O	5:F:160:ASP:HB2	2.21	0.40
1:B:124:ASN:OD1	1:B:124:ASN:N	2.53	0.40
2:C:428:ARG:CD	2:C:449:ILE:O	2.63	0.40
2:C:627:ARG:CZ	2:C:640:ARG:HG3	2.51	0.40
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.37	0.40
3:D:479:GLU:HA	3:D:482:LYS:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:911:LEU:O	3:D:915:VAL:HG23	2.21	0.40
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.55	0.40
1:A:124:ASN:OD1	1:A:124:ASN:N	2.53	0.40
2:C:582:GLY:N	2:C:584:GLU:OE2	2.55	0.40
3:D:1439:SER:OG	3:D:1467:ILE:CD1	2.69	0.40
1:B:101:LEU:HD11	1:B:113:ASP:HB2	2.03	0.40
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.56	0.40
3:D:231:VAL:O	3:D:236:TYR:OH	2.39	0.40
3:D:1084:THR:O	3:D:1088:THR:HG23	2.22	0.40
3:D:1493:LYS:H	3:D:1493:LYS:HG2	1.63	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	229/315 (73%)	226 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	218 (97%)	7 (3%)	0	100	100
2	C	1108/1119 (99%)	1077 (97%)	31 (3%)	0	100	100
3	D	1484/1524 (97%)	1447 (98%)	37 (2%)	0	100	100
4	E	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3482/3815 (91%)	3395 (98%)	87 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	200/273 (73%)	198 (99%)	2 (1%)	76	86
1	B	198/273 (72%)	195 (98%)	3 (2%)	65	81
2	C	934/941 (99%)	910 (97%)	24 (3%)	46	71
3	D	1255/1279 (98%)	1236 (98%)	19 (2%)	65	81
4	E	82/88 (93%)	79 (96%)	3 (4%)	34	63
5	F	300/388 (77%)	294 (98%)	6 (2%)	55	76
All	All	2969/3242 (92%)	2912 (98%)	57 (2%)	57	77

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	66	SER
1	B	5	LYS
1	B	6	LEU
1	B	154	GLU
2	C	133	ASP
2	C	177	GLU
2	C	261	ILE
2	C	274	ARG
2	C	342	ASP
2	C	361	MET
2	C	402	SER
2	C	419	THR
2	C	425	PHE
2	C	426	ASP
2	C	434	HIS
2	C	513	VAL
2	C	562	SER
2	C	583	LEU
2	C	584	GLU
2	C	610	ARG
2	C	640	ARG

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Mol	Chain	Res	Type
2	C	657	ASP
2	C	670	GLN
2	C	715	THR
2	C	784	ASP
2	C	807	ARG
2	C	907	ASP
2	C	1014	SER
3	D	35	ARG
3	D	183	GLU
3	D	530	VAL
3	D	628	ARG
3	D	687	VAL
3	D	709	HIS
3	D	754	PHE
3	D	784	ASP
3	D	894	LYS
3	D	1001	GLU
3	D	1055	VAL
3	D	1062	ARG
3	D	1100	ASP
3	D	1129	THR
3	D	1188	VAL
3	D	1307	LYS
3	D	1433	SER
3	D	1487	VAL
3	D	1493	LYS
4	E	49	GLN
4	E	50	THR
4	E	93	TYR
5	F	122	LEU
5	F	141	VAL
5	F	154	LYS
5	F	205	ARG
5	F	321	ILE
5	F	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	219	GLN
2	C	498	GLN
3	D	714	GLN

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Mol	Chain	Res	Type
3	D	855	HIS
3	D	976	GLN
3	D	1334	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	3/4 (75%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.04	4 (1%)	70	68	63, 91, 117, 162	0
1	B	227/315 (72%)	-0.11	1 (0%)	92	93	63, 95, 124, 155	0
2	C	1112/1119 (99%)	0.02	23 (2%)	63	62	45, 88, 139, 167	0
3	D	1486/1524 (97%)	0.09	45 (3%)	50	49	46, 86, 145, 169	1 (0%)
4	E	94/99 (94%)	-0.22	0	100	100	65, 97, 135, 142	0
5	F	346/443 (78%)	-0.02	6 (1%)	70	68	65, 103, 147, 164	0
6	G	17/21 (80%)	-0.33	0	100	100	70, 105, 177, 184	0
7	H	24/27 (88%)	-0.46	0	100	100	96, 126, 176, 188	0
8	I	4/4 (100%)	-0.13	0	100	100	69, 72, 79, 89	0
All	All	3541/3867 (91%)	0.02	79 (2%)	62	60	45, 91, 142, 188	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	9.0
1	A	232	ALA	4.6
3	D	322	VAL	4.4
3	D	203	ALA	4.3
3	D	173	PRO	4.2
3	D	1292	VAL	4.0
5	F	146	GLY	3.9
3	D	1313	VAL	3.7
5	F	145	PRO	3.7
3	D	974	ILE	3.4
3	D	409	VAL	3.4
1	A	231	ALA	3.3
1	A	233	VAL	3.3
2	C	365	ASP	3.2
2	C	311	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	393	ILE	3.1
3	D	324	ALA	3.1
3	D	144	GLY	3.1
3	D	202	VAL	3.0
2	C	372	LEU	3.0
2	C	66	LEU	2.9
3	D	368	VAL	2.9
3	D	235	ALA	2.9
1	B	2	LEU	2.9
3	D	262	LYS	2.8
2	C	367	LEU	2.8
2	C	104	ASP	2.8
2	C	729	LEU	2.8
2	C	176	VAL	2.8
5	F	149	GLU	2.7
2	C	174	LEU	2.7
2	C	159	ILE	2.7
2	C	739	GLU	2.6
2	C	107	LEU	2.6
3	D	345	TYR	2.6
2	C	221	LEU	2.6
2	C	158	TYR	2.5
3	D	360	ARG	2.5
3	D	269	PHE	2.5
3	D	241	ILE	2.5
3	D	1301	LYS	2.5
3	D	352	ASN	2.5
1	A	234	ALA	2.4
3	D	377	VAL	2.4
3	D	1312	LEU	2.4
3	D	422	ALA	2.4
3	D	211	VAL	2.4
3	D	821	VAL	2.4
3	D	142	LEU	2.3
2	C	207	LEU	2.3
3	D	152	LEU	2.3
3	D	174	GLY	2.3
3	D	1327	ARG	2.3
3	D	1275	SER	2.3
3	D	335	LEU	2.2
5	F	422	LEU	2.2
5	F	147	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	806	LEU	2.2
3	D	305	ALA	2.2
3	D	350	HIS	2.2
3	D	1130	ARG	2.2
3	D	1294	VAL	2.2
2	C	185	LYS	2.2
3	D	290	PRO	2.2
3	D	1299	PHE	2.1
2	C	757	GLY	2.1
3	D	225	LEU	2.1
3	D	1132	LEU	2.1
3	D	1287	GLU	2.1
2	C	368	THR	2.1
2	C	183	SER	2.1
3	D	165	LYS	2.1
3	D	829	VAL	2.1
2	C	616	GLU	2.1
3	D	1499	ARG	2.1
5	F	414	ARG	2.0
2	C	611	ILE	2.0
3	D	268	ALA	2.0
3	D	427	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	B	2001	1/1	0.88	0.25	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	D	2003	1/1	0.90	0.18	52,52,52,52	0
9	MG	D	2004	1/1	0.95	0.47	63,63,63,63	0
10	ZN	D	2002	1/1	0.97	0.07	111,111,111,111	0
10	ZN	D	2001	1/1	0.99	0.21	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.