



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 04:43 PM BST

PDB ID : 6KQH
Title : Thermus thermophilus initial transcription complex comprising sigma A and 5'-OH RNA of 7 nt
Authors : Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on : 2019-08-17
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	2.13.1
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)	:	2.13.1

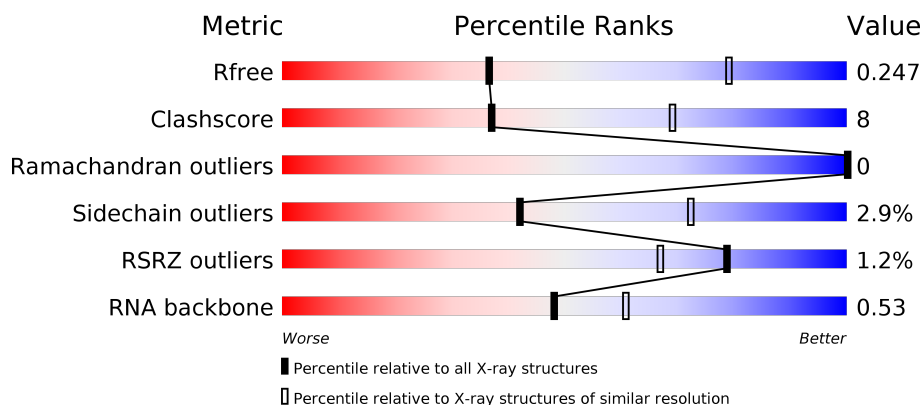
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)
RNA backbone	3102	1054 (3.50-2.86)

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 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	<div> <div></div> <div>59%14%27%</div> </div>
1	B	315	<div> <div>51%19%29%</div> </div>
2	C	1119	<div> <div>80%18%..</div> </div>
3	D	1524	<div> <div>78%18%..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>86%</div><div>8%</div><div>5%</div></div>
5	F	443	<div><div>3%</div><div></div><div>61%</div><div>14%</div><div>24%</div></div>
6	G	21	<div><div></div><div>52%</div><div>33%</div><div>14%</div></div>
7	H	27	<div><div></div><div>30%</div><div>59%</div><div>11%</div></div>
8	I	7	<div><div>14%</div><div></div><div>43%</div><div>43%</div><div>14%</div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 28728 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
			1757	1124	304	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
			8787	5560	1570	1633	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	3	0
			11718	7434	2060	2188	36			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	337	Total	C	N	O	S	0	0	0
			2737	1726	499	508	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 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*G)-3').

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

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

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

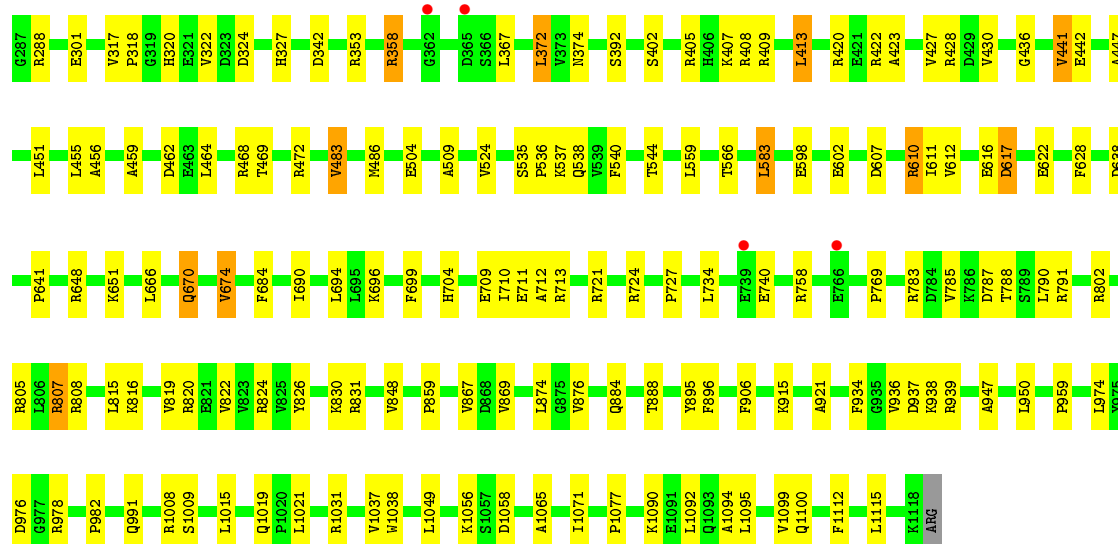
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Mg 2 2	0	0
9	D	1	Total Mg 1 1	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

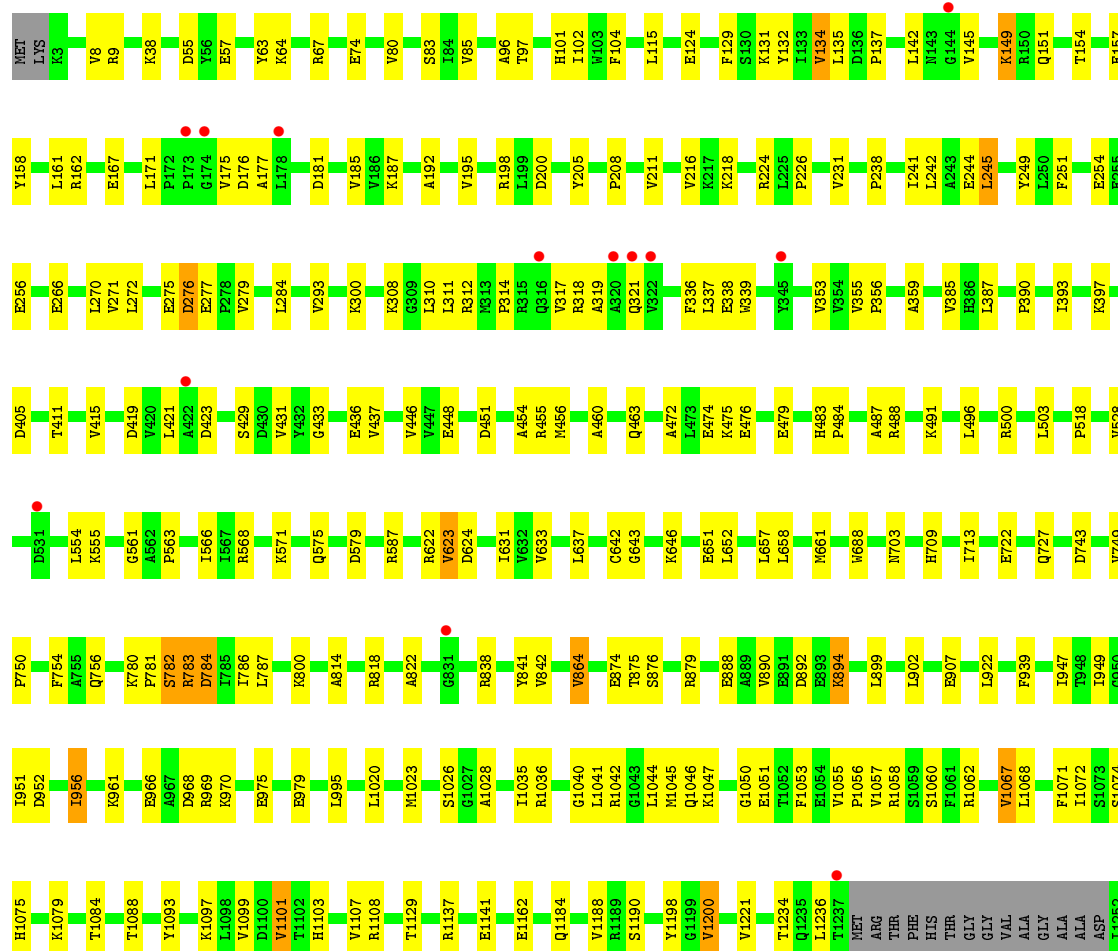
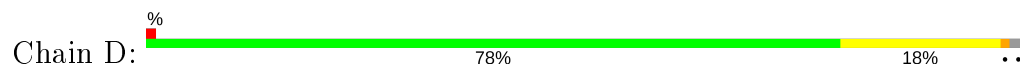
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	11	Total O 11 11	0	0
11	B	8	Total O 8 8	0	0
11	C	43	Total O 43 43	0	0
11	D	56	Total O 56 56	0	0
11	E	3	Total O 3 3	0	0
11	F	7	Total O 7 7	0	0
11	G	4	Total O 4 4	0	0
11	H	5	Total O 5 5	0	0
11	I	2	Total O 2 2	0	0



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



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

Chain I: 14% 43% 43% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.01Å 103.57Å 294.94Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	39.82 – 3.18 39.82 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.2 (39.82-3.18) 93.2 (39.82-3.18)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.203 , 0.247 0.203 , 0.247	Depositor DCC
R_{free} test set	4268 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.023 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28728	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/1849	0.48	0/2515
1	B	0.29	0/1789	0.48	0/2433
2	C	0.26	0/8964	0.45	0/12122
3	D	0.27	0/11933	0.45	0/16138
4	E	0.31	0/775	0.45	0/1045
5	F	0.25	0/2779	0.40	0/3737
6	G	0.52	0/418	0.84	0/645
7	H	0.55	0/556	0.94	0/858
8	I	0.34	0/157	0.90	0/242
All	All	0.28	0/29220	0.48	0/39735

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	32	0
1	B	1757	0	1806	48	0
2	C	8787	0	8897	144	0
3	D	11718	0	11939	191	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	761	0	778	7	0
5	F	2737	0	2819	49	0
6	G	372	0	203	10	0
7	H	495	0	272	15	0
8	I	142	0	78	9	0
9	B	2	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	A	11	0	0	0	0
11	B	8	0	0	3	0
11	C	43	0	0	1	0
11	D	56	0	0	2	0
11	E	3	0	0	0	0
11	F	7	0	0	0	0
11	G	4	0	0	0	0
11	H	5	0	0	2	0
11	I	2	0	0	0	0
All	All	28728	0	28661	441	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.

The worst 5 of 441 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)
3:D:783:ARG:HB3	3:D:1028:ALA:O	1.41	1.16
2:C:769:PRO:CB	5:F:375:LEU:CD2	2.30	1.09
2:C:769:PRO:HB2	5:F:375:LEU:HD22	1.33	1.05
2:C:769:PRO:HB2	5:F:375:LEU:CD2	1.88	1.03
2:C:769:PRO:HB3	5:F:375:LEU:HD23	1.45	0.95

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%)	229 (100%)	1 (0%)	0	100	100
1	B	221/315 (70%)	216 (98%)	5 (2%)	0	100	100
2	C	1111/1119 (99%)	1095 (99%)	16 (1%)	0	100	100
3	D	1485/1524 (97%)	1466 (99%)	19 (1%)	0	100	100
4	E	92/99 (93%)	92 (100%)	0	0	100	100
5	F	333/443 (75%)	332 (100%)	1 (0%)	0	100	100
All	All	3472/3815 (91%)	3430 (99%)	42 (1%)	0	100	100

There are no Ramachandran outliers to report.

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%)	194 (96%)	7 (4%)	36	68
1	B	196/273 (72%)	193 (98%)	3 (2%)	65	85
2	C	938/941 (100%)	911 (97%)	27 (3%)	42	72
3	D	1248/1279 (98%)	1209 (97%)	39 (3%)	40	71
4	E	83/88 (94%)	82 (99%)	1 (1%)	71	87
5	F	293/388 (76%)	282 (96%)	11 (4%)	33	66
All	All	2959/3242 (91%)	2871 (97%)	88 (3%)	42	72

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	149	LYS
3	D	623	VAL
5	F	136	LEU
3	D	175	VAL
3	D	245	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	538	GLN

5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	2	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 ⓘ

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%)	-0.39	3 (1%) 77 65	40, 57, 84, 136	0
1	B	223/315 (70%)	-0.31	0 100 100	38, 63, 100, 115	0
2	C	1112/1119 (99%)	-0.38	8 (0%) 87 81	23, 51, 114, 158	0
3	D	1486/1524 (97%)	-0.23	18 (1%) 79 67	19, 55, 119, 152	1 (0%)
4	E	94/99 (94%)	-0.43	0 100 100	27, 50, 89, 106	0
5	F	337/443 (76%)	-0.08	12 (3%) 42 27	42, 75, 128, 154	0
6	G	18/21 (85%)	-0.07	0 100 100	44, 74, 149, 158	0
7	H	24/27 (88%)	-0.10	0 100 100	64, 88, 146, 171	0
8	I	7/7 (100%)	-0.11	1 (14%) 2 1	41, 44, 95, 112	0
All	All	3532/3870 (91%)	-0.28	42 (1%) 79 67	19, 58, 117, 171	1 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	6.2
1	A	232	ALA	5.2
3	D	144	GLY	4.8
5	F	149	GLU	4.8
5	F	146	GLY	4.4

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

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

6.3 Carbohydrates ⓘ

There are no 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(\AA^2)	Q<0.9
9	MG	B	2001	1/1	0.91	0.25	73,73,73,73	0
9	MG	F	2001	1/1	0.96	0.14	70,70,70,70	0
9	MG	B	2002	1/1	0.98	0.22	45,45,45,45	0
9	MG	D	2003	1/1	0.99	0.19	23,23,23,23	0
10	ZN	D	2002	1/1	0.99	0.06	73,73,73,73	0
10	ZN	D	2001	1/1	1.00	0.16	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.