



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 03:30 AM EDT

PDB ID : 8W8N / pdb_00008w8n
Title : Thermus thermophilus initiation transcription complex in the pre-translocated state
Authors : Li, L.; Zhang, Y.
Deposited on : 2023-09-04
Resolution : 2.69 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

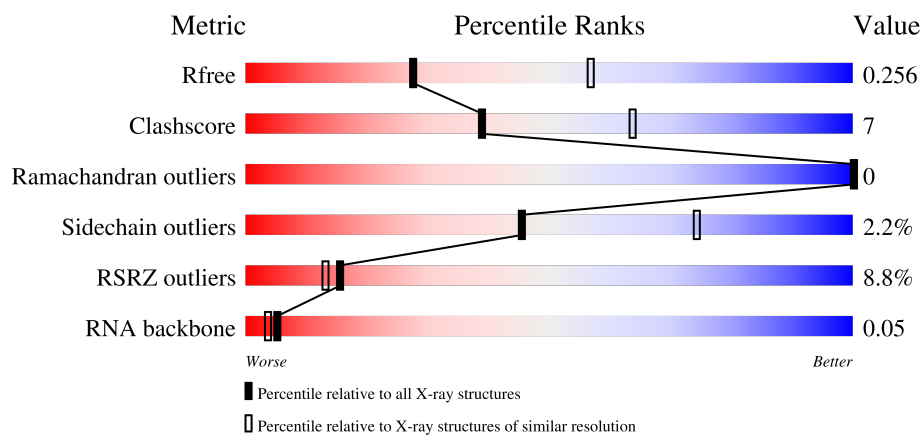
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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 $\leq 5\%$. 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	57% 14% • 28%
1	B	315	3% 55% 17% 28%
2	C	1119	8% 80% 19% ••
3	D	1524	10% 79% 18% •

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Mol	Chain	Length	Quality of chain
4	E	99	3% 79% 15% 5%
5	F	443	10% 66% 12% 22%
6	G	21	10% 38% 38% 24%
7	H	27	7% 44% 41% 15%
8	I	3	33% 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28636 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	227	Total	C	N	O	S	0	0	0
			1787	1141	311	333	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8761	5541	1562	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	1	0
			11706	7425	2060	2186	35			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	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 (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			326	154	62	94	16			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	23	Total	C	N	O	P	0	0	0
			476	227	91	136	22			

- Molecule 8 is a RNA chain called RNA (5'-D(*PP*PP*P)-R(*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			75	29	12	29	5			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

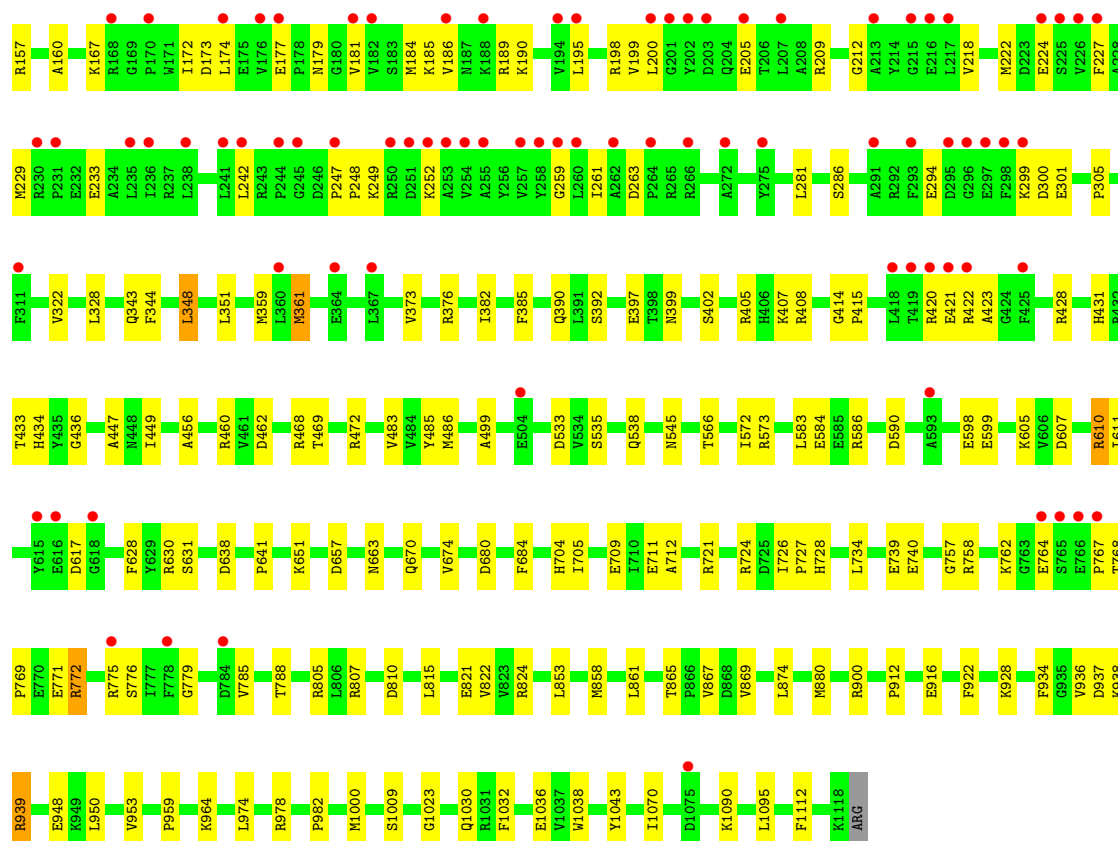
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Mg 1	0	0
9	D	3	Total 3	Mg 3	0	0
9	F	2	Total 2	Mg 2	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

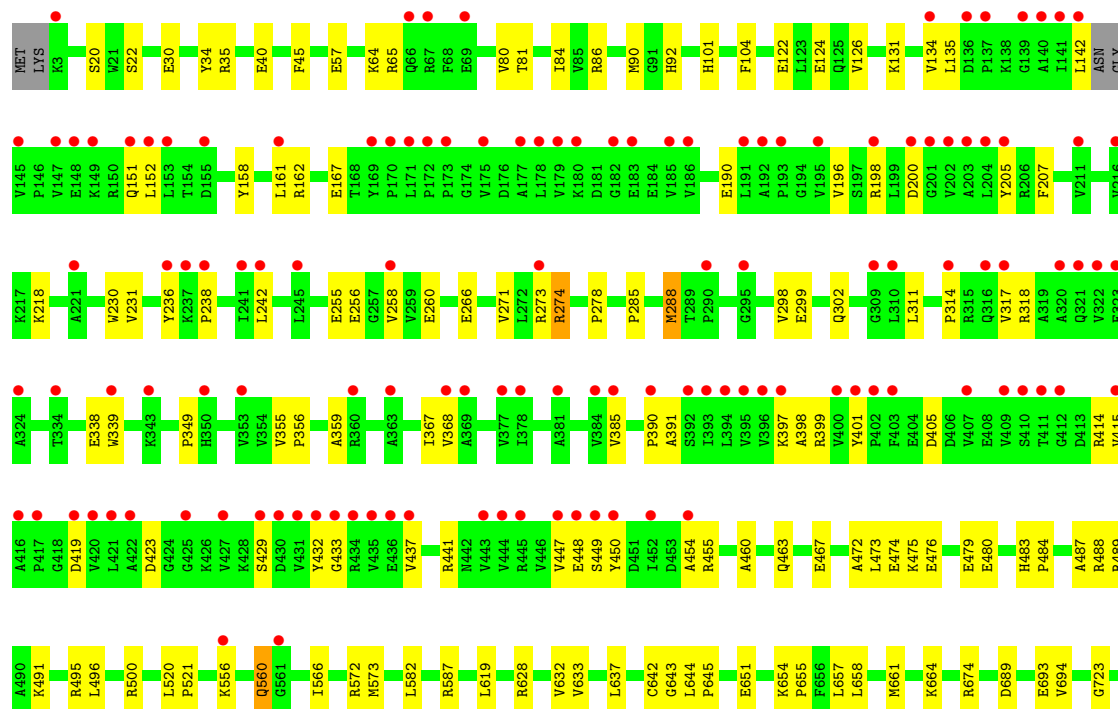
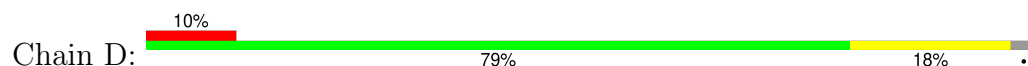
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total 2	Zn 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	3	Total 3	O 3	0	0
11	B	4	Total 4	O 4	0	0
11	C	47	Total 47	O 47	0	0
11	D	72	Total 72	O 72	0	0
11	E	2	Total 2	O 2	0	0
11	F	6	Total 6	O 6	0	0
11	G	5	Total 5	O 5	0	0
11	I	1	Total 1	O 1	0	0

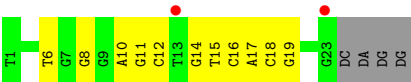


• Molecule 3: DNA-directed RNA polymerase subunit beta'





● Molecule 7: DNA (27-MER)



● Molecule 8: RNA (5'-D(*PP*PP*P)-R(*GP*GP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.42Å 103.70Å 295.44Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	48.86 – 2.69 48.86 – 2.69	Depositor EDS
% Data completeness (in resolution range)	74.9 (48.86-2.69) 74.9 (48.86-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.212 , 0.260 0.213 , 0.256	Depositor DCC
R_{free} test set	2002 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.5	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	0.91	EDS
Total number of atoms	28636	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: GTP, 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	0.15	0/1819	0.35	0/2473
1	B	0.13	0/1821	0.34	0/2476
2	C	0.14	0/8927	0.36	0/12074
3	D	0.16	0/11914	0.35	0/16111
4	E	0.13	0/775	0.31	0/1045
5	F	0.14	0/2852	0.31	0/3837
6	G	0.18	0/365	0.38	0/560
7	H	0.22	0/535	0.43	0/826
8	I	0.12	0/47	0.26	0/71
All	All	0.15	0/29055	0.35	0/39473

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	1787	0	1839	29	0
1	B	1789	0	1841	33	0
2	C	8761	0	8859	135	0
3	D	11706	0	11929	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	761	0	778	11	0
5	F	2807	0	2882	33	0
6	G	326	0	179	8	0
7	H	476	0	261	8	0
8	I	75	0	33	0	0
9	B	1	0	0	0	0
9	D	3	0	0	0	0
9	F	2	0	0	0	0
10	D	2	0	0	0	0
11	A	3	0	0	0	0
11	B	4	0	0	0	0
11	C	47	0	0	1	0
11	D	72	0	0	0	0
11	E	2	0	0	0	0
11	F	6	0	0	0	0
11	G	5	0	0	0	0
11	I	1	0	0	0	0
All	All	28636	0	28601	383	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 7.

The worst 5 of 383 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:11:DG:H2'	6:G:12:DA:C8	2.20	0.76
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.68	0.74
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.69	0.72
3:D:65:ARG:NH1	5:F:378:GLY:O	2.21	0.72
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.70	0.72

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	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	221 (98%)	4 (2%)	0	100	100
2	C	1108/1119 (99%)	1078 (97%)	30 (3%)	0	100	100
3	D	1479/1524 (97%)	1448 (98%)	31 (2%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	341 (99%)	3 (1%)	0	100	100
All	All	3473/3815 (91%)	3400 (98%)	73 (2%)	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	199/273 (73%)	194 (98%)	5 (2%)	42	71
1	B	200/273 (73%)	196 (98%)	4 (2%)	48	76
2	C	934/941 (99%)	914 (98%)	20 (2%)	47	75
3	D	1247/1279 (98%)	1222 (98%)	25 (2%)	48	76
4	E	83/88 (94%)	81 (98%)	2 (2%)	43	72
5	F	301/388 (78%)	293 (97%)	8 (3%)	39	69
All	All	2964/3242 (91%)	2900 (98%)	64 (2%)	45	74

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	141	VAL
5	F	156	VAL
2	C	764	GLU
2	C	762	LYS
5	F	279	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	737	ASN
3	D	1489	GLN
5	F	269	ASN
5	F	83	GLN
2	C	117	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/3 (33%)	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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	227/315 (72%)	0.21	1 (0%) 88 87	26, 41, 65, 77	0
1	B	227/315 (72%)	0.60	11 (4%) 35 32	25, 52, 80, 109	0
2	C	1112/1119 (99%)	0.18	87 (7%) 19 16	7, 36, 97, 122	0
3	D	1484/1524 (97%)	0.38	160 (10%) 11 9	8, 38, 96, 123	1 (0%)
4	E	94/99 (94%)	0.09	3 (3%) 50 46	17, 38, 73, 83	0
5	F	346/443 (78%)	0.76	45 (13%) 7 6	17, 55, 91, 111	0
6	G	16/21 (76%)	0.60	2 (12%) 8 7	29, 49, 123, 131	0
7	H	23/27 (85%)	0.99	2 (8%) 16 13	52, 72, 120, 136	0
8	I	2/3 (66%)	2.47	1 (50%) 0 0	23, 23, 23, 38	2 (100%)
All	All	3531/3866 (91%)	0.35	312 (8%) 15 13	7, 41, 95, 136	3 (0%)

The worst 5 of 312 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	203	ALA	6.0
3	D	420	VAL	5.6
3	D	142	LEU	5.5
2	C	275	TYR	5.1
3	D	1252	ILE	4.8

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
9	MG	B	401	1/1	0.81	0.11	60,60,60,60	0
9	MG	D	1605	1/1	0.86	0.09	41,41,41,41	0
9	MG	F	501	1/1	0.91	0.07	41,41,41,41	0
9	MG	F	502	1/1	0.91	0.22	43,43,43,43	0
9	MG	D	1604	1/1	0.92	0.20	33,33,33,33	0
9	MG	D	1603	1/1	0.99	0.05	18,18,18,18	0
10	ZN	D	1601	1/1	0.99	0.03	23,23,23,23	0
10	ZN	D	1602	1/1	1.00	0.01	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.