



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 02:25 PM BST

PDB ID : 4J3N
Title : Human Topoisomerase Iibeta in complex with DNA
Authors : Wu, C.C.; Li, T.K.; Li, Y.C.; Chan, N.L.
Deposited on : 2013-02-06
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

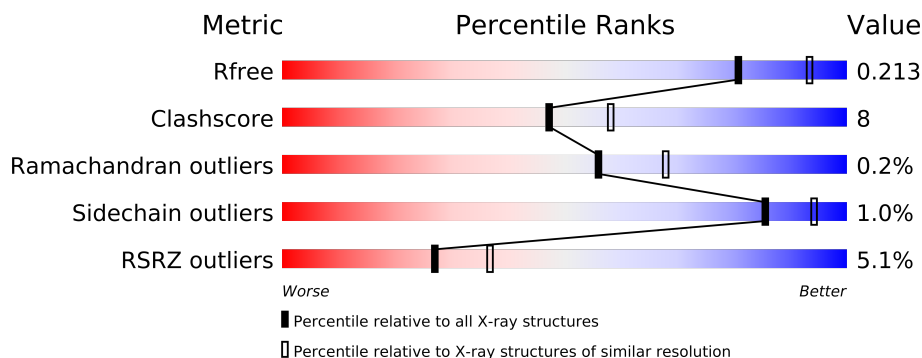
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable23004
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	803	
1	B	803	
2	C	8	
2	E	8	
3	D	12	
3	F	12	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	1302	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12463 atoms, of which 0 are hydrogen and 0 are deuterium.

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 topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	18	0
			5480	3501	941	1013	25			
1	B	670	Total	C	N	O	S	0	11	0
			5474	3491	950	1009	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	EXPRESSION TAG	UNP Q02880
A	420	ALA	-	EXPRESSION TAG	UNP Q02880
A	421	SER	-	EXPRESSION TAG	UNP Q02880
A	422	TRP	-	EXPRESSION TAG	UNP Q02880
A	423	SER	-	EXPRESSION TAG	UNP Q02880
A	424	HIS	-	EXPRESSION TAG	UNP Q02880
A	425	PRO	-	EXPRESSION TAG	UNP Q02880
A	426	GLN	-	EXPRESSION TAG	UNP Q02880
A	427	PHE	-	EXPRESSION TAG	UNP Q02880
A	428	GLU	-	EXPRESSION TAG	UNP Q02880
A	429	LYS	-	EXPRESSION TAG	UNP Q02880
A	430	GLY	-	EXPRESSION TAG	UNP Q02880
A	431	ALA	-	EXPRESSION TAG	UNP Q02880
A	432	ASP	-	EXPRESSION TAG	UNP Q02880
A	433	ASP	-	EXPRESSION TAG	UNP Q02880
A	434	ASP	-	EXPRESSION TAG	UNP Q02880
A	435	ASP	-	EXPRESSION TAG	UNP Q02880
A	436	LYS	-	EXPRESSION TAG	UNP Q02880
A	437	VAL	-	EXPRESSION TAG	UNP Q02880
A	438	PRO	-	EXPRESSION TAG	UNP Q02880
A	439	ASP	-	EXPRESSION TAG	UNP Q02880
A	440	PRO	-	EXPRESSION TAG	UNP Q02880
A	441	THR	-	EXPRESSION TAG	UNP Q02880
A	442	SER	-	EXPRESSION TAG	UNP Q02880
A	443	VAL	-	EXPRESSION TAG	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASP	-	EXPRESSION TAG	UNP Q02880
A	1202	GLY	-	EXPRESSION TAG	UNP Q02880
A	1203	ALA	-	EXPRESSION TAG	UNP Q02880
A	1204	PRO	-	EXPRESSION TAG	UNP Q02880
A	1205	GLY	-	EXPRESSION TAG	UNP Q02880
A	1206	PHE	-	EXPRESSION TAG	UNP Q02880
A	1207	SER	-	EXPRESSION TAG	UNP Q02880
A	1208	SER	-	EXPRESSION TAG	UNP Q02880
A	1209	ILE	-	EXPRESSION TAG	UNP Q02880
A	1210	SER	-	EXPRESSION TAG	UNP Q02880
A	1211	ALA	-	EXPRESSION TAG	UNP Q02880
A	1212	HIS	-	EXPRESSION TAG	UNP Q02880
A	1213	HIS	-	EXPRESSION TAG	UNP Q02880
A	1214	HIS	-	EXPRESSION TAG	UNP Q02880
A	1215	HIS	-	EXPRESSION TAG	UNP Q02880
A	1216	HIS	-	EXPRESSION TAG	UNP Q02880
A	1217	HIS	-	EXPRESSION TAG	UNP Q02880
A	1218	HIS	-	EXPRESSION TAG	UNP Q02880
A	1219	HIS	-	EXPRESSION TAG	UNP Q02880
A	1220	HIS	-	EXPRESSION TAG	UNP Q02880
A	1221	HIS	-	EXPRESSION TAG	UNP Q02880
B	419	MET	-	EXPRESSION TAG	UNP Q02880
B	420	ALA	-	EXPRESSION TAG	UNP Q02880
B	421	SER	-	EXPRESSION TAG	UNP Q02880
B	422	TRP	-	EXPRESSION TAG	UNP Q02880
B	423	SER	-	EXPRESSION TAG	UNP Q02880
B	424	HIS	-	EXPRESSION TAG	UNP Q02880
B	425	PRO	-	EXPRESSION TAG	UNP Q02880
B	426	GLN	-	EXPRESSION TAG	UNP Q02880
B	427	PHE	-	EXPRESSION TAG	UNP Q02880
B	428	GLU	-	EXPRESSION TAG	UNP Q02880
B	429	LYS	-	EXPRESSION TAG	UNP Q02880
B	430	GLY	-	EXPRESSION TAG	UNP Q02880
B	431	ALA	-	EXPRESSION TAG	UNP Q02880
B	432	ASP	-	EXPRESSION TAG	UNP Q02880
B	433	ASP	-	EXPRESSION TAG	UNP Q02880
B	434	ASP	-	EXPRESSION TAG	UNP Q02880
B	435	ASP	-	EXPRESSION TAG	UNP Q02880
B	436	LYS	-	EXPRESSION TAG	UNP Q02880
B	437	VAL	-	EXPRESSION TAG	UNP Q02880
B	438	PRO	-	EXPRESSION TAG	UNP Q02880
B	439	ASP	-	EXPRESSION TAG	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	EXPRESSION TAG	UNP Q02880
B	441	THR	-	EXPRESSION TAG	UNP Q02880
B	442	SER	-	EXPRESSION TAG	UNP Q02880
B	443	VAL	-	EXPRESSION TAG	UNP Q02880
B	444	ASP	-	EXPRESSION TAG	UNP Q02880
B	1202	GLY	-	EXPRESSION TAG	UNP Q02880
B	1203	ALA	-	EXPRESSION TAG	UNP Q02880
B	1204	PRO	-	EXPRESSION TAG	UNP Q02880
B	1205	GLY	-	EXPRESSION TAG	UNP Q02880
B	1206	PHE	-	EXPRESSION TAG	UNP Q02880
B	1207	SER	-	EXPRESSION TAG	UNP Q02880
B	1208	SER	-	EXPRESSION TAG	UNP Q02880
B	1209	ILE	-	EXPRESSION TAG	UNP Q02880
B	1210	SER	-	EXPRESSION TAG	UNP Q02880
B	1211	ALA	-	EXPRESSION TAG	UNP Q02880
B	1212	HIS	-	EXPRESSION TAG	UNP Q02880
B	1213	HIS	-	EXPRESSION TAG	UNP Q02880
B	1214	HIS	-	EXPRESSION TAG	UNP Q02880
B	1215	HIS	-	EXPRESSION TAG	UNP Q02880
B	1216	HIS	-	EXPRESSION TAG	UNP Q02880
B	1217	HIS	-	EXPRESSION TAG	UNP Q02880
B	1218	HIS	-	EXPRESSION TAG	UNP Q02880
B	1219	HIS	-	EXPRESSION TAG	UNP Q02880
B	1220	HIS	-	EXPRESSION TAG	UNP Q02880
B	1221	HIS	-	EXPRESSION TAG	UNP Q02880

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total 165	C 77	N 34	O 46	P 8	0	0	0
2	E	8	Total 165	C 77	N 34	O 46	P 8	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total 245	C 116	N 43	O 74	P 12	0	0	0
3	F	11	Total 224	C 106	N 38	O 69	P 11	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

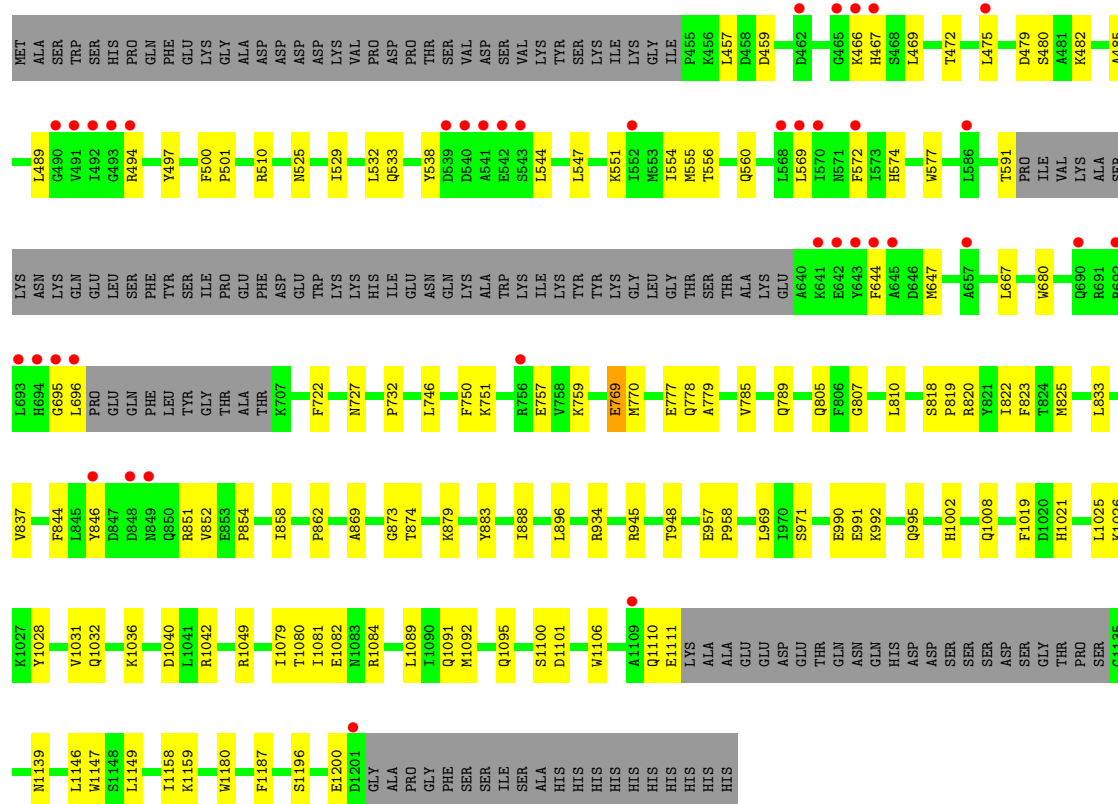
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	266	Total 266	O 266	0	0
5	B	340	Total 340	O 340	0	0
5	C	23	Total 23	O 23	0	0
5	D	30	Total 30	O 30	0	0
5	E	26	Total 26	O 26	0	0
5	F	18	Total 18	O 18	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

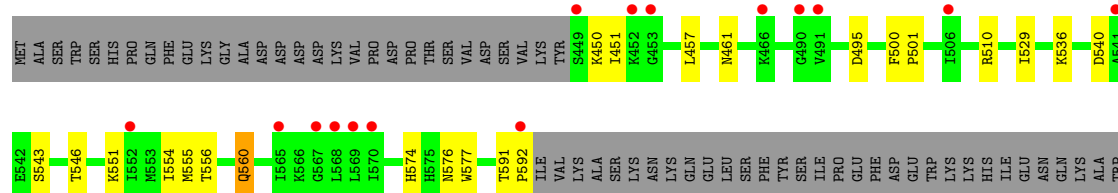
- Molecule 1: DNA topoisomerase 2-beta

Chain A: 



- Molecule 1: DNA topoisomerase 2-beta

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.95Å 176.37Å 94.22Å 90.00° 112.06° 90.00°	Depositor
Resolution (Å)	27.31 – 2.30 27.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.31-2.30) 92.7 (27.31-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4.486)	Depositor
R, R_{free}	0.176 , 0.218 0.173 , 0.213	Depositor DCC
R_{free} test set	4948 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 103794 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12463	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/5637	0.51	0/7590
1	B	0.40	0/5609	0.52	1/7551 (0.0%)
2	C	0.71	0/185	1.35	1/283 (0.4%)
2	E	0.91	0/185	1.56	3/283 (1.1%)
3	D	0.74	0/273	1.55	7/419 (1.7%)
3	F	0.78	0/248	1.65	6/378 (1.6%)
All	All	0.43	0/12137	0.66	18/16504 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	13	DG	O4'-C1'-N9	9.30	114.51	108.00
2	E	2	DG	O4'-C1'-N9	9.14	114.40	108.00
3	D	19	DC	C1'-O4'-C4'	-8.73	101.37	110.10
3	D	17	DG	O4'-C1'-N9	-7.97	102.42	108.00
3	F	19	DC	C1'-O4'-C4'	-7.90	102.20	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5480	0	5564	92	0
1	B	5474	0	5554	92	0
2	C	165	0	89	4	0
2	E	165	0	89	1	0
3	D	245	0	136	11	0
3	F	224	0	126	3	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	266	0	0	4	0
5	B	340	0	0	15	0
5	C	23	0	0	2	0
5	D	30	0	0	1	0
5	E	26	0	0	1	0
5	F	18	0	0	1	0
All	All	12463	0	11558	186	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 186 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1032[A]:GLN:HG2	5:A:1582:HOH:O	1.58	1.03
1:B:510:ARG:HH22	1:B:574:HIS:HD2	1.14	0.93
1:A:805:GLN:HE21	1:A:807:GLY:H	1.15	0.89
1:B:560:GLN:H	1:B:560:GLN:HE21	1.22	0.87
1:B:797:ILE:H	1:B:867:ASN:HD21	1.20	0.86

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	676/803 (84%)	654 (97%)	21 (3%)	1 (0%)	59 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	671/803 (84%)	650 (97%)	19 (3%)	2 (0%)	50	60
All	All	1347/1606 (84%)	1304 (97%)	40 (3%)	3 (0%)	56	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	852	VAL
1	A	852	VAL
1	B	1101	ASP

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	603/704 (86%)	596 (99%)	7 (1%)	82	92
1	B	599/704 (85%)	594 (99%)	5 (1%)	89	96
All	All	1202/1408 (85%)	1190 (99%)	12 (1%)	85	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	945	ARG
1	A	971	SER
1	B	759	LYS
1	A	825	MET
1	B	560	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1197	GLN
1	B	574	HIS
1	B	1095	GLN
1	B	560	GLN
1	B	583	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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.

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	666/803 (82%)	-0.02	39 (5%) 22 30	24, 44, 81, 112	0
1	B	670/803 (83%)	-0.08	29 (4%) 34 44	25, 40, 72, 96	0
2	C	8/8 (100%)	-0.35	1 (12%) 5 7	37, 40, 62, 82	0
2	E	8/8 (100%)	-0.46	0 100 100	30, 33, 55, 78	0
3	D	12/12 (100%)	-0.23	0 100 100	29, 38, 80, 88	0
3	F	11/12 (91%)	-0.15	0 100 100	37, 49, 72, 86	0
All	All	1375/1646 (83%)	-0.06	69 (5%) 27 38	24, 42, 77, 112	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	5.7
1	A	849	ASN	5.5
1	B	693	LEU	4.8
1	A	490	GLY	4.4
1	A	492	ILE	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 carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	1302	1/1	0.48	8.63	67,67,67,67	0
4	MG	D	101	1/1	0.11	0.53	55,55,55,55	0
4	MG	A	1303	1/1	0.12	-0.36	56,56,56,56	0
4	MG	F	101	1/1	0.07	-1.38	62,62,62,62	0
4	MG	B	1302	1/1	0.09	-1.61	61,61,61,61	0
4	MG	A	1301	1/1	0.05	-1.97	46,46,46,46	0
4	MG	B	1301	1/1	0.04	-2.78	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.