



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:40 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

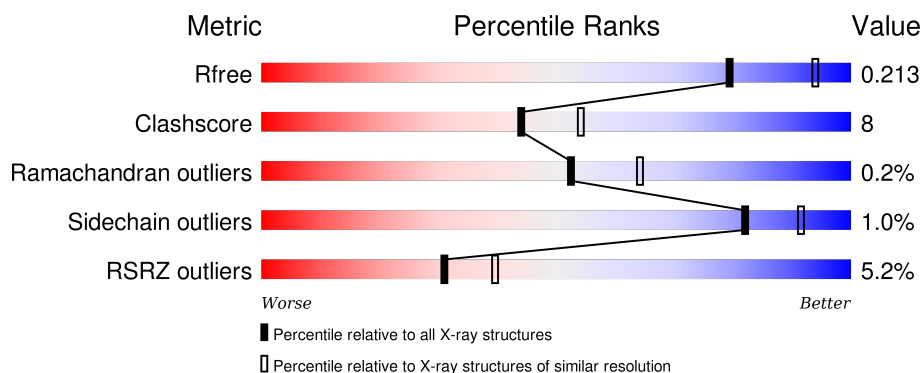
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	803	<div> <div>5%</div> <div>67% 16% 17%</div> </div>
1	B	803	<div> <div>4%</div> <div>70% 12% 17%</div> </div>
2	C	8	<div> <div>13%</div> <div>63% 38%</div> </div>
2	E	8	<div> <div>63% 25% 13%</div> </div>
3	D	12	<div> <div>33% 58% 8%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	12	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 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 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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) 92.8 (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 0.171 , 0.213	Depositor DCC
R_{free} test set	4957 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 , 53.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

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

All (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
2	E	8	DC	O4'-C1'-N1	7.59	113.32	108.00
3	D	20	DT	O4'-C4'-C3'	-7.58	101.45	106.00
2	C	8	DC	O4'-C1'-N1	7.19	113.03	108.00
3	D	13	DG	O4'-C1'-N9	7.15	113.00	108.00
2	E	1	DA	C1'-O4'-C4'	-7.07	103.03	110.10
3	F	11	DC	O4'-C1'-N1	7.03	112.92	108.00
3	D	9	DT	N3-C4-O4	6.29	123.67	119.90
3	D	20	DT	C1'-O4'-C4'	-6.20	103.90	110.10
1	B	743	ARG	NE-CZ-NH2	-6.18	117.21	120.30
3	F	14	DC	O4'-C4'-C3'	-5.99	102.10	104.50
3	F	17	DG	O4'-C1'-N9	-5.85	103.90	108.00
3	D	9	DT	C5-C4-O4	-5.53	121.03	124.90
3	F	19	DC	P-O5'-C5'	-5.01	112.88	120.90

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	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

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 (186) 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)
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
1:B:805:GLN:HE21	1:B:807:GLY:H	1.27	0.82
3:D:10:DG:H2''	3:D:11:DC:H5''	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:GLU:HB2	1:B:820[B]:ARG:HH11	1.47	0.78
3:D:10:DG:C2'	3:D:11:DC:H5''	2.16	0.75
1:A:510:ARG:HH22	1:A:574:HIS:HD2	1.33	0.74
1:A:1139:ASN:HD22	1:B:1147:TRP:HE1	1.34	0.73
1:B:536:LYS:HZ2	1:B:546:THR:HG21	1.53	0.73
2:C:1:DA:H5'	2:C:1:DA:C8	2.25	0.72
1:B:944:VAL:HG12	1:B:945:ARG:HG2	1.71	0.72
1:A:805:GLN:NE2	1:A:807:GLY:H	1.85	0.71
1:A:846:TYR:CZ	1:A:851:ARG:HG3	2.25	0.71
1:B:536:LYS:NZ	1:B:546:THR:HG21	2.07	0.70
1:B:805:GLN:NE2	1:B:807:GLY:H	1.89	0.70
1:B:868:GLY:HA2	5:B:1681:HOH:O	1.91	0.69
1:A:466:LYS:HG3	1:A:467:HIS:CD2	2.28	0.68
1:B:868:GLY:CA	5:B:1681:HOH:O	2.42	0.68
1:A:820[A]:ARG:HD3	3:F:9:DT:OP2	1.95	0.66
1:B:1087:LYS:HE2	5:B:1732:HOH:O	1.97	0.65
1:A:777:GLU:HB2	1:B:820[B]:ARG:NH1	2.12	0.64
1:B:879:LYS:HE2	5:D:218:HOH:O	1.97	0.64
1:A:466:LYS:HG3	1:A:467:HIS:HD2	1.62	0.63
1:A:820[B]:ARG:NH1	1:B:777:GLU:HB2	2.13	0.63
1:A:485:ALA:O	1:A:489:LEU:HB2	2.00	0.61
1:B:592:PRO:HG2	1:B:643:TYR:OH	1.99	0.61
1:A:732:PRO:HG3	1:A:869:ALA:HB1	1.81	0.61
3:D:11:DC:H2''	3:D:12:DA:H5'	1.84	0.60
1:A:510:ARG:HH22	1:A:574:HIS:CD2	2.19	0.59
1:A:759:LYS:HE3	5:B:1480:HOH:O	2.02	0.59
1:B:540:ASP:HB2	1:B:543:SER:H	1.69	0.58
1:B:574:HIS:HE1	1:B:662:ASP:OD2	1.87	0.58
1:B:938:GLU:OE2	1:B:983:LYS:HE3	2.02	0.58
1:B:457:LEU:HD22	1:B:529:ILE:HG12	1.85	0.58
1:B:732:PRO:HG2	1:B:869:ALA:HB1	1.86	0.57
1:A:1079:ILE:HD11	1:A:1092:MET:HE3	1.86	0.57
3:F:10:DG:H2''	3:F:11:DC:OP2	2.04	0.57
1:B:868:GLY:N	5:B:1681:HOH:O	2.38	0.56
1:B:1086:LYS:O	1:B:1090:ILE:HG12	2.05	0.56
1:B:510:ARG:HH22	1:B:574:HIS:CD2	2.06	0.56
3:D:10:DG:H2''	3:D:11:DC:C5'	2.33	0.56
1:A:1147:TRP:HE1	1:B:1139:ASN:HD22	1.52	0.56
1:A:778[B]:GLN:HG2	5:C:110:HOH:O	2.06	0.55
3:D:10:DG:H1'	3:D:11:DC:H5''	1.89	0.55
1:A:457:LEU:HD13	1:A:529:ILE:HD13	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778[A]:GLN:HB2	3:D:9:DT:H73	1.88	0.55
1:A:820[B]:ARG:HH11	1:B:777:GLU:HB2	1.70	0.54
1:B:560:GLN:N	1:B:560:GLN:HE21	1.98	0.54
1:B:536:LYS:NZ	1:B:546:THR:CG2	2.71	0.54
1:A:479:ASP:O	1:A:482:LYS:HB3	2.08	0.54
1:A:1026:LYS:HD3	1:A:1028:TYR:CZ	2.44	0.53
1:B:881:PRO:HB3	1:B:1011:LEU:HD21	1.89	0.53
1:A:746[B]:LEU:HG	1:A:750:PHE:CE2	2.42	0.53
1:B:810[A]:LEU:HD12	1:B:948:THR:HB	1.91	0.53
1:B:858:ILE:HG13	1:B:1042:ARG:HD2	1.91	0.53
1:A:883:TYR:CZ	1:A:1031[A]:VAL:HG21	2.44	0.53
1:B:543:SER:HA	5:B:1690:HOH:O	2.08	0.53
1:B:820[A]:ARG:HH21	3:D:9:DT:H2'	1.74	0.52
1:B:510:ARG:NH2	1:B:574:HIS:HD2	1.97	0.52
1:B:751:LYS:HE3	5:B:1556:HOH:O	2.08	0.52
1:A:459:ASP:O	1:A:494:ARG:NH1	2.40	0.52
3:D:10:DG:C1'	3:D:11:DC:H5''	2.40	0.52
1:B:727:ASN:ND2	1:B:874:THR:H	2.08	0.52
1:A:1089:LEU:HD12	1:A:1092:MET:HE2	1.92	0.51
1:B:993:LEU:HD12	1:B:993:LEU:O	2.11	0.51
1:B:560:GLN:NE2	1:B:560:GLN:H	2.01	0.51
1:A:533:GLN:HA	5:A:1630:HOH:O	2.10	0.51
1:B:858:ILE:O	1:B:858:ILE:HG23	2.11	0.51
1:A:769:GLU:HG2	1:A:770:MET:HG3	1.93	0.51
1:A:879:LYS:HE2	5:F:206:HOH:O	2.09	0.51
1:B:727:ASN:HD21	1:B:874:THR:H	1.57	0.51
1:A:1021:HIS:HD2	5:A:1659:HOH:O	1.93	0.51
1:A:934:ARG:HB3	1:A:990:GLU:HG2	1.92	0.51
1:A:751:LYS:HD3	1:A:770:MET:HE3	1.92	0.50
1:B:758[A]:VAL:HG12	1:B:824:THR:O	2.12	0.50
1:A:695:GLY:O	1:A:696:LEU:HD23	2.11	0.49
1:A:1079:ILE:HD11	1:A:1092:MET:CE	2.42	0.49
1:A:1002:HIS:HB3	1:A:1008:GLN:HG3	1.94	0.49
1:A:858:ILE:O	1:A:858:ILE:HG23	2.12	0.49
1:A:769:GLU:HG2	1:A:770:MET:N	2.27	0.49
1:A:1082:GLU:OE2	1:B:1074:LYS:HE3	2.13	0.49
1:B:914:THR:HG22	1:B:916:GLN:HG3	1.95	0.49
1:B:560:GLN:HB3	1:B:722:PHE:HA	1.95	0.48
1:A:1080:THR:O	1:A:1084:ARG:HD2	2.12	0.48
1:A:457:LEU:HD22	1:A:529:ILE:HG12	1.96	0.48
1:B:648:GLU:O	1:B:707:LYS:NZ	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778[B]:GLN:HG2	1:A:779:ALA:N	2.27	0.48
1:B:1193:LYS:HE2	5:B:1738:HOH:O	2.12	0.48
1:B:546:THR:HG23	5:B:1433:HOH:O	2.14	0.48
1:A:560:GLN:HB3	1:A:722:PHE:HA	1.95	0.48
1:B:903:PRO:HA	5:B:1717:HOH:O	2.14	0.47
1:B:461:ASN:HB2	1:B:495:ASP:HA	1.96	0.47
1:A:810[A]:LEU:HD12	1:A:948:THR:HB	1.95	0.47
1:A:727:ASN:ND2	1:A:874:THR:H	2.12	0.47
1:B:820[A]:ARG:NH2	3:D:9:DT:H2'	2.30	0.47
1:A:732:PRO:CG	1:A:869:ALA:HB1	2.44	0.47
1:B:773:TYR:CZ	1:B:775:HIS:HB2	2.49	0.47
1:A:969:LEU:HD12	1:A:992:LYS:HD2	1.97	0.47
1:B:1081:ILE:HG22	1:B:1089:LEU:HD11	1.97	0.46
1:A:957:GLU:HB2	1:A:958:PRO:HD3	1.97	0.46
1:A:1036:LYS:HE3	1:A:1040:ASP:OD2	2.16	0.46
1:A:785:VAL:O	1:A:789:GLN:HG3	2.16	0.46
1:B:796:ASN:H	1:B:867:ASN:HD22	1.63	0.46
3:D:11:DC:H5'	3:D:11:DC:H6	1.80	0.46
1:A:472:THR:HB	1:A:497:TYR:CD2	2.50	0.46
1:A:489:LEU:HD21	1:A:497:TYR:CB	2.46	0.46
1:A:480:SER:HB3	5:A:1593:HOH:O	2.15	0.46
1:A:1146:LEU:HD23	1:B:1146:LEU:HD23	1.98	0.45
1:B:894:ARG:NH2	5:B:1713:HOH:O	2.49	0.45
2:C:1:DA:H8	2:C:1:DA:H5'	1.81	0.45
1:A:1081:ILE:HG22	1:A:1089:LEU:HD11	1.98	0.45
1:A:667:LEU:HD21	1:A:680:TRP:CG	2.52	0.45
1:B:957:GLU:HB2	1:B:958:PRO:HD3	1.97	0.45
1:A:469:LEU:HD11	1:A:544:LEU:O	2.17	0.45
1:A:727:ASN:HD22	1:A:873:GLY:HA3	1.83	0.45
1:A:1091:GLN:O	1:A:1095:GLN:HG3	2.17	0.45
2:C:1:DA:H2''	2:C:2:DG:O5'	2.18	0.44
2:E:1:DA:N7	5:E:120:HOH:O	2.36	0.44
1:A:858:ILE:HG13	1:A:1042:ARG:HD2	1.98	0.44
1:A:1100:SER:O	1:A:1101:ASP:C	2.54	0.44
1:A:844:PHE:HA	1:A:854:PRO:HA	1.99	0.44
1:A:1110:GLN:O	1:A:1111:GLU:CB	2.66	0.44
1:A:1110:GLN:O	1:A:1111:GLU:HB3	2.17	0.44
1:B:1032:GLN:HB2	5:B:1725:HOH:O	2.17	0.44
1:B:1082:GLU:OE1	1:B:1082:GLU:N	2.42	0.44
1:A:555:MET:HE2	1:A:555:MET:HB2	1.84	0.43
1:B:1053:LEU:HB3	1:B:1171:LEU:CD2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:VAL:HG13	1:A:1049:ARG:HD2	1.98	0.43
1:A:525:ASN:O	1:A:529:ILE:HG13	2.19	0.43
1:A:532:LEU:HD13	1:A:577:TRP:CZ3	2.53	0.43
1:A:896:LEU:HD21	1:A:1180:TRP:CE3	2.54	0.43
1:B:1100:SER:O	1:B:1101:ASP:C	2.57	0.43
1:B:991:GLU:O	1:B:995:GLN:HG3	2.19	0.43
1:B:881:PRO:HD3	1:B:1013:CYS:SG	2.58	0.43
1:B:944:VAL:O	1:B:945:ARG:HB2	2.19	0.43
1:B:1104:LYS:HE3	1:B:1104:LYS:HB2	1.91	0.43
1:B:671:LYS:HE3	5:B:1740:HOH:O	2.19	0.43
1:B:861:ILE:HB	1:B:862:PRO:HD2	2.00	0.42
1:A:757:GLU:HB2	1:A:823:PHE:HB3	2.00	0.42
2:C:1:DA:H2	3:F:20:DT:H3	1.57	0.42
1:B:1081:ILE:O	1:B:1084:ARG:HB2	2.20	0.42
1:B:678:LYS:HE3	1:B:876:TRP:CD1	2.53	0.42
1:B:690:GLN:OE1	1:B:690:GLN:HA	2.19	0.42
1:A:554[A]:ILE:HG13	1:A:556:THR:HG23	2.01	0.42
1:A:862:PRO:HD2	1:A:888:ILE:CG2	2.49	0.42
1:B:554[A]:ILE:HG13	1:B:556:THR:HG23	2.02	0.42
1:A:475:LEU:HD12	1:A:569[A]:LEU:HD11	2.01	0.42
1:B:450:LYS:O	1:B:451:ILE:HD13	2.19	0.42
1:B:988:MET:CE	1:B:993:LEU:HD13	2.50	0.42
1:A:1149:LEU:HD12	1:B:1081:ILE:HD11	2.01	0.42
1:A:1106:TRP:O	1:A:1110:GLN:HG2	2.20	0.42
1:A:819:PRO:HA	1:A:822:ILE:HG12	2.01	0.42
1:A:1019:PHE:CZ	1:A:1025:LEU:HD13	2.55	0.42
1:B:536:LYS:HZ3	1:B:546:THR:CG2	2.33	0.42
1:A:538:TYR:CE1	1:A:547:LEU:HD21	2.54	0.42
1:B:757:GLU:HB2	1:B:823:PHE:HB3	2.01	0.42
1:A:1196:SER:O	1:A:1200:GLU:HG3	2.20	0.42
1:A:489:LEU:HD21	1:A:497:TYR:HB2	2.02	0.41
1:B:992:LYS:HE3	5:B:1723:HOH:O	2.20	0.41
1:B:576:ASN:HB2	1:B:577:TRP:CE3	2.55	0.41
1:B:555:MET:HB2	1:B:555:MET:HE3	1.96	0.41
1:B:807:GLY:HA3	1:B:813:GLY:HA2	2.02	0.41
1:A:820[B]:ARG:NH1	1:B:777:GLU:CB	2.81	0.41
1:A:644:PHE:O	1:A:647:MET:HB2	2.21	0.41
1:B:1020:ASP:OD1	1:B:1020:ASP:C	2.59	0.41
1:B:999:ALA:HB1	5:B:1724:HOH:O	2.18	0.41
1:B:996:ALA:O	1:B:999:ALA:O	2.39	0.41
1:B:591:THR:HB	1:B:592:PRO:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ASN:HD22	1:B:873:GLY:HA3	1.86	0.41
1:A:833:LEU:HD21	1:A:1187:PHE:CE1	2.56	0.41
1:A:1158:ILE:HG22	1:A:1159:LYS:N	2.36	0.41
1:A:991[B]:GLU:HG2	1:A:995:GLN:HE21	1.85	0.41
1:A:500:PHE:HA	1:A:501:PRO:HD3	1.87	0.40
1:B:1046:TYR:CZ	1:B:1180:TRP:HA	2.56	0.40
1:B:759:LYS:HE3	1:B:759:LYS:HB2	1.91	0.40
1:B:1046:TYR:CE2	1:B:1180:TRP:CG	3.09	0.40
1:A:778[B]:GLN:CG	5:C:110:HOH:O	2.65	0.40
1:A:778[B]:GLN:HB3	3:D:9:DT:H73	2.03	0.40
1:A:1147:TRP:CZ2	1:B:1142:LEU:HD12	2.57	0.40
1:B:500:PHE:HA	1:B:501:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	676/803 (84%)	654 (97%)	21 (3%)	1 (0%)	56	68
1	B	671/803 (84%)	650 (97%)	19 (3%)	2 (0%)	46	57
All	All	1347/1606 (84%)	1304 (97%)	40 (3%)	3 (0%)	52	64

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%)	78	89
1	B	599/704 (85%)	594 (99%)	5 (1%)	86	94
All	All	1202/1408 (85%)	1190 (99%)	12 (1%)	82	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	551	LYS
1	A	591	THR
1	A	769	GLU
1	A	818	SER
1	A	825	MET
1	A	945	ARG
1	A	971	SER
1	B	551	LYS
1	B	560	GLN
1	B	759	LYS
1	B	945	ARG
1	B	1084	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	467	HIS
1	A	558	GLN
1	A	574	HIS
1	A	576	ASN
1	A	727	ASN
1	A	805	GLN
1	A	882	ASN
1	A	922	GLN
1	A	995	GLN
1	A	1067	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1083	ASN
1	A	1091	GLN
1	A	1139	ASN
1	A	1160	GLN
1	A	1197	GLN
1	B	467	HIS
1	B	560	GLN
1	B	574	HIS
1	B	583	HIS
1	B	694	HIS
1	B	727	ASN
1	B	805	GLN
1	B	867	ASN
1	B	882	ASN
1	B	949	GLN
1	B	1014	ASN
1	B	1021	HIS
1	B	1067	GLN
1	B	1076	GLN
1	B	1095	GLN
1	B	1139	ASN
1	B	1169	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	666/803 (82%)	-0.03	38 (5%) 27 36	24, 44, 81, 112	0
1	B	670/803 (83%)	-0.09	32 (4%) 34 43	25, 40, 72, 96	0
2	C	8/8 (100%)	-0.36	1 (12%) 5 8	37, 40, 62, 82	0
2	E	8/8 (100%)	-0.56	0 100 100	30, 33, 55, 78	0
3	D	12/12 (100%)	-0.24	0 100 100	29, 38, 80, 88	0
3	F	11/12 (91%)	-0.11	1 (9%) 11 17	37, 49, 72, 86	0
All	All	1375/1646 (83%)	-0.07	72 (5%) 31 39	24, 42, 77, 112	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	6.1
1	A	849	ASN	5.2
1	A	490	GLY	4.8
1	A	693	LEU	4.6
1	A	643	TYR	4.5
1	A	542	GLU	4.4
1	B	849	ASN	4.4
1	A	492	ILE	4.4
1	B	592	PRO	4.4
1	B	643	TYR	4.3
1	B	693	LEU	4.2
1	A	848	ASP	4.2
1	B	848	ASP	4.0
1	A	657	ALA	3.8
1	A	466	LYS	3.8
1	A	642	GLU	3.7
1	A	568	LEU	3.7
1	A	543	SER	3.7
1	A	695	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	706	THR	3.6
1	B	568	LEU	3.6
1	B	694	HIS	3.4
1	B	638	LYS	3.3
1	A	552	ILE	3.2
1	B	569[A]	LEU	3.2
1	A	540	ASP	3.1
1	A	645	ALA	3.1
1	B	491	VAL	3.0
1	B	452	LYS	3.0
1	A	541	ALA	2.9
1	B	692	ARG	2.9
1	B	899	LEU	2.9
1	A	696	LEU	2.9
1	B	570	ILE	2.8
1	A	690	GLN	2.8
1	B	466	LYS	2.8
1	A	569[A]	LEU	2.8
1	B	453	GLY	2.7
1	A	570	ILE	2.7
1	B	866	ILE	2.7
1	B	689[A]	ARG	2.7
2	C	1	DA	2.7
1	A	467	HIS	2.5
1	A	462	ASP	2.5
1	A	539	ASP	2.5
1	A	694	HIS	2.5
1	A	465	GLY	2.5
1	B	449	SER	2.5
1	A	644	PHE	2.5
1	B	864	VAL	2.4
1	B	541	ALA	2.4
1	A	1201	ASP	2.4
1	B	490	GLY	2.4
1	A	475	LEU	2.4
1	B	506	ILE	2.4
1	A	572	PHE	2.4
1	B	642	GLU	2.3
1	B	691	ARG	2.3
1	A	641	LYS	2.3
1	B	552	ILE	2.3
1	A	692	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	11	DC	2.2
1	B	492	ILE	2.2
1	A	586	LEU	2.2
1	A	494	ARG	2.2
1	B	567	GLY	2.2
1	A	659	PRO	2.2
1	A	464	GLY	2.1
1	B	565	ILE	2.1
1	B	1201	ASP	2.1
1	B	450	LYS	2.1
1	A	493	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	1302	1/1	0.92	0.51	9.55	67,67,67,67	0
4	MG	A	1303	1/1	0.96	0.13	-0.31	56,56,56,56	0
4	MG	B	1302	1/1	0.94	0.10	-1.30	61,61,61,61	0
4	MG	D	101	1/1	0.90	0.13	-	55,55,55,55	0
4	MG	F	101	1/1	0.71	0.08	-	62,62,62,62	0
4	MG	B	1301	1/1	0.88	0.04	-	38,38,38,38	0
4	MG	A	1301	1/1	0.96	0.04	-	46,46,46,46	0

6.5 Other polymers

There are no such residues in this entry.