



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:47 PM UTC

PDB ID : 5ZAD / pdb_00005zad
Title : Human topoisomerase II beta in complex with DNA
Authors : Sun, L.Y.; Zhu, L.W.; Tang, Y.J.
Deposited on : 2018-02-07
Resolution : 2.54 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 ⓘ 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
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

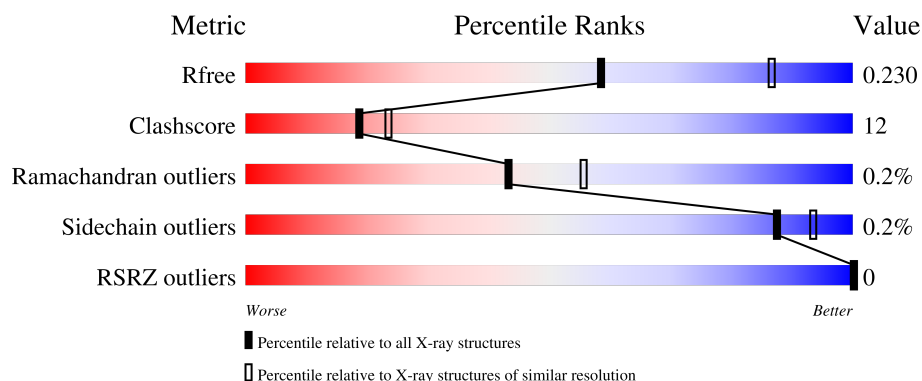
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	803	 70% 20% 9%
1	B	803	 70% 20% 9%
2	C	8	 100%
2	D	8	 88% 12%
3	E	12	 83% 17%

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Mol	Chain	Length	Quality of chain
3	F	12	 83% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12706 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	729	Total	C	N	O	S	0	3	0
			5903	3762	1012	1105	24			
1	B	729	Total	C	N	O	S	0	1	0
			5893	3756	1012	1101	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').

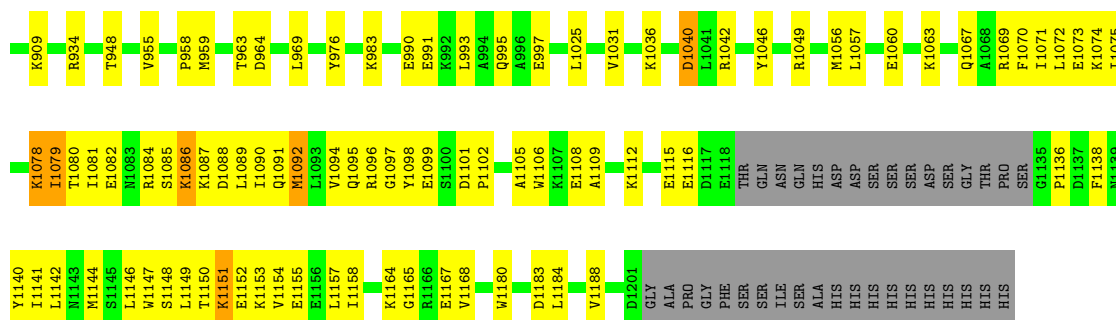
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total 165	C 77	N 34	O 46	P 8	0	0	0
2	D	8	Total 165	C 77	N 34	O 46	P 8	0	0	0

- 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	F	12	Total 245	C 116	N 43	O 74	P 12	0	0	0
3	E	12	Total 245	C 116	N 43	O 74	P 12	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0
4	C	5	Total 5	O 5	0	0
4	F	5	Total 5	O 5	0	0
4	B	31	Total 31	O 31	0	0
4	D	5	Total 5	O 5	0	0
4	E	5	Total 5	O 5	0	0



- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')

Chain C: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')

Chain D: 88% 12%



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

Chain F: 83% 17%



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

Chain E: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	95.01Å 95.01Å 230.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.06 – 2.54 28.06 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.06-2.54) 32.5 (28.06-2.54)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.180 , 0.227 0.184 , 0.230	Depositor DCC
R_{free} test set	6114 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.487 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12706	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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

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	0.41	0/6030	0.66	7/8124 (0.1%)
1	B	0.42	0/6014	0.72	15/8103 (0.2%)
2	C	0.44	0/185	0.67	0/283
2	D	0.45	0/185	0.64	0/283
3	E	0.50	0/273	0.65	0/419
3	F	0.53	0/273	0.73	0/419
All	All	0.42	0/12960	0.69	22/17631 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1149	LEU	CB-CG-CD2	-11.62	75.86	110.70
1	A	613	GLU	CA-C-N	-8.47	108.96	122.76
1	A	613	GLU	C-N-CA	-8.47	108.96	122.76
1	B	1149	LEU	CB-CG-CD1	7.75	133.94	110.70
1	B	1149	LEU	CD1-CG-CD2	-7.40	94.53	110.80
1	B	1086	LYS	CD-CE-NZ	-7.21	88.81	111.90
1	B	692	ARG	CA-CB-CG	6.88	127.87	114.10
1	A	613	GLU	CB-CA-C	-6.86	100.96	112.00
1	B	1151	LYS	CA-CB-CG	-6.65	100.80	114.10
1	A	613	GLU	N-CA-CB	6.36	120.20	110.60
1	B	1078	LYS	CA-C-N	5.93	132.12	122.69
1	B	1078	LYS	C-N-CA	5.93	132.12	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	ARG	N-CA-CB	-5.92	101.17	110.46
1	A	551	LYS	CG-CD-CE	5.91	124.90	111.30
1	B	1086	LYS	CB-CG-CD	-5.86	97.82	111.30
1	B	1079	ILE	CG1-CB-CG2	5.86	128.26	110.70
1	B	1092	MET	CG-SD-CE	-5.50	88.79	100.90
1	B	1151	LYS	CA-C-N	-5.44	113.20	122.56
1	B	1151	LYS	C-N-CA	-5.44	113.20	122.56
1	B	1040	ASP	N-CA-CB	-5.20	102.46	110.16
1	A	993	LEU	CB-CG-CD2	5.16	126.17	110.70
1	A	649	ARG	CA-CB-CG	5.04	124.18	114.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	1079	ILE	CB

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	5903	0	5923	160	0
1	B	5893	0	5909	147	0
2	C	165	0	89	0	0
2	D	165	0	89	2	0
3	E	245	0	136	2	0
3	F	245	0	136	3	0
4	A	39	0	0	1	0
4	B	31	0	0	2	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
All	All	12706	0	12282	297	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 12.

All (297) 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:B:691:ARG:NH2	1:B:698:GLU:OE1	1.85	1.08
1:A:1089:LEU:HA	1:A:1092:MET:HB3	1.43	0.96
1:A:617:HIS:HE1	1:A:624:TRP:CH2	1.84	0.94
1:B:732:PRO:HG2	1:B:869:ALA:HB1	1.50	0.94
1:A:617:HIS:CE1	1:A:624:TRP:CZ3	2.58	0.91
1:A:1084:ARG:HB2	1:A:1089:LEU:HD11	1.55	0.89
1:A:732:PRO:HG2	1:A:869:ALA:HB1	1.54	0.89
1:A:692:ARG:NH2	1:A:696:LEU:O	2.08	0.86
1:A:846:TYR:CZ	1:A:851:ARG:HG3	2.12	0.84
1:A:617:HIS:HE1	1:A:624:TRP:CZ3	1.96	0.83
1:A:959:MET:HE2	1:A:969:LEU:HD22	1.61	0.83
1:A:551:LYS:HZ3	1:A:587:GLU:HG3	1.45	0.81
1:A:1083:ASN:HB2	1:B:1075:ILE:HD11	1.60	0.81
1:A:551:LYS:NZ	1:A:587:GLU:CG	2.44	0.81
1:A:1152:GLU:OE1	1:B:1087:LYS:NZ	2.13	0.81
1:B:555:MET:HG3	1:B:589:PHE:HB3	1.68	0.76
1:A:613:GLU:OE2	1:A:700:PHE:HE1	1.69	0.75
1:B:1073:GLU:OE1	1:B:1079:ILE:HD11	1.86	0.75
1:B:551:LYS:NZ	1:B:587:GLU:OE1	2.17	0.74
1:B:1151:LYS:HA	1:B:1154:VAL:HG22	1.68	0.74
1:A:1149:LEU:HD12	1:B:1081:ILE:HD11	1.70	0.73
1:A:551:LYS:HZ3	1:A:587:GLU:CG	2.02	0.73
1:A:1099:GLU:O	1:A:1140:TYR:OH	2.07	0.72
1:B:805:GLN:HE22	1:B:808:THR:HG23	1.55	0.72
1:B:457:LEU:HD22	1:B:529:ILE:HG12	1.70	0.71
1:A:1112:LYS:HA	1:A:1115:GLU:HB3	1.73	0.71
1:B:1072:LEU:O	1:B:1075:ILE:HG22	1.91	0.70
1:A:555:MET:HG3	1:A:589:PHE:HB3	1.73	0.70
1:A:1141:ILE:O	1:A:1144:MET:HB2	1.91	0.70
1:A:617:HIS:CE1	1:A:624:TRP:HZ3	2.07	0.70
1:B:1087:LYS:H	1:B:1087:LYS:HD3	1.56	0.70
1:A:1150:THR:HB	1:A:1153:LYS:HG2	1.73	0.69
1:B:1069:ARG:O	1:B:1073:GLU:HB2	1.93	0.69
1:B:1112:LYS:HA	1:B:1115:GLU:HB3	1.76	0.68
1:A:1102:PRO:HA	1:A:1105:ALA:HB3	1.75	0.67
1:B:1057:LEU:HB3	1:B:1168:VAL:HG12	1.76	0.67
1:A:617:HIS:HD1	1:A:618:ILE:H	1.43	0.67
1:A:551:LYS:HE2	1:A:584:GLY:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:SER:O	1:A:1089:LEU:HD12	1.96	0.66
1:B:1096:ARG:HG3	1:B:1097:GLY:N	2.11	0.66
1:A:1096:ARG:HG2	1:A:1097:GLY:N	2.11	0.66
1:A:617:HIS:HD1	1:A:618:ILE:N	1.93	0.65
1:A:1091:GLN:HA	1:A:1094:VAL:HG12	1.78	0.65
1:A:1096:ARG:HG2	1:A:1097:GLY:H	1.62	0.65
1:A:1142:LEU:HB3	1:B:1147:TRP:CE3	2.33	0.64
1:B:1074:LYS:HE2	1:B:1080:THR:HA	1.77	0.64
1:B:594:VAL:HG12	1:B:605:PHE:HB2	1.79	0.64
1:B:692:ARG:HH22	1:B:698:GLU:HB2	1.62	0.64
1:B:1071:ILE:HD11	1:B:1148:SER:C	2.24	0.63
1:B:858:ILE:HG13	1:B:1042:ARG:HD2	1.80	0.63
1:B:485:ALA:HB2	1:B:555:MET:HE1	1.80	0.63
1:B:739:LYS:NZ	1:B:870:GLU:O	2.31	0.63
1:B:1141:ILE:O	1:B:1144:MET:HB2	1.98	0.63
1:A:485:ALA:HB2	1:A:555:MET:HE1	1.80	0.63
1:A:1063:LYS:O	1:A:1067:GLN:HG3	1.98	0.63
1:B:538:TYR:OH	4:B:1301:HOH:O	2.16	0.62
1:B:1116:GLU:CD	1:B:1116:GLU:O	2.41	0.62
1:B:1086:LYS:HB3	1:B:1087:LYS:HZ2	1.65	0.62
1:A:1157:LEU:HD23	1:A:1157:LEU:O	1.99	0.62
1:B:1063:LYS:O	1:B:1067:GLN:HG3	2.00	0.62
1:A:694:HIS:HB2	1:A:696:LEU:HD13	1.82	0.61
1:A:551:LYS:NZ	1:A:587:GLU:HG3	2.10	0.61
1:B:651:ARG:O	1:B:707:LYS:HE3	2.00	0.61
1:A:1083:ASN:N	1:B:1075:ILE:HD11	2.15	0.60
1:A:1096:ARG:HD3	1:A:1098:TYR:CE2	2.37	0.60
1:B:594:VAL:HG11	1:B:611:PHE:CG	2.36	0.60
1:B:1079:ILE:HG13	1:B:1096:ARG:HH11	1.67	0.60
1:A:928:GLU:HG3	1:A:930:PHE:CZ	2.37	0.59
1:A:1106:TRP:CE2	1:A:1110:GLN:NE2	2.71	0.59
1:A:1056:MET:HE2	1:A:1106:TRP:CZ3	2.38	0.59
1:B:598:LYS:HZ3	1:B:624:TRP:N	2.01	0.58
1:B:1089:LEU:HA	1:B:1092:MET:HB3	1.84	0.58
1:A:1152:GLU:N	1:A:1152:GLU:OE2	2.36	0.58
1:B:839:ASP:HA	1:B:842:LEU:CD2	2.33	0.58
1:A:1069:ARG:O	1:A:1073:GLU:HG3	2.03	0.58
1:B:752:ARG:HD3	1:B:754:ASP:OD2	2.03	0.58
1:A:1096:ARG:HD3	1:A:1098:TYR:HE2	1.68	0.58
1:B:1141:ILE:HA	1:B:1144:MET:HE3	1.86	0.58
1:A:1085:SER:OG	1:B:1152:GLU:OE2	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ARG:O	1:A:707:LYS:HE3	2.04	0.57
1:B:1090:ILE:O	1:B:1094:VAL:HG13	2.04	0.57
1:A:1155:GLU:O	1:A:1159:LYS:HG3	2.05	0.57
1:B:1147:TRP:O	1:B:1150:THR:HG22	2.05	0.57
1:A:846:TYR:CE1	1:A:851:ARG:HG3	2.39	0.57
1:A:1057:LEU:HB3	1:A:1168:VAL:HG12	1.86	0.57
1:B:909:LYS:NZ	4:B:1302:HOH:O	2.37	0.57
1:B:610:GLU:HB2	1:B:700:PHE:CD2	2.40	0.56
1:A:1085:SER:OG	1:A:1087:LYS:HG2	2.06	0.56
1:B:613:GLU:O	1:B:616:LYS:HB3	2.05	0.56
1:B:934:ARG:HB2	1:B:990:GLU:HG3	1.88	0.56
1:B:1090:ILE:HG13	1:B:1091:GLN:N	2.21	0.56
1:A:1071:ILE:O	1:A:1075:ILE:HG12	2.05	0.56
1:B:1080:THR:O	1:B:1084:ARG:NH2	2.38	0.56
1:A:617:HIS:CE1	1:A:624:TRP:CH2	2.75	0.55
1:B:1071:ILE:HD11	1:B:1148:SER:O	2.07	0.55
1:A:1152:GLU:HA	1:A:1155:GLU:OE1	2.06	0.55
1:B:1087:LYS:HD3	1:B:1087:LYS:N	2.20	0.55
1:A:551:LYS:HZ2	1:A:587:GLU:CG	2.18	0.55
1:B:1087:LYS:H	1:B:1087:LYS:CD	2.13	0.55
1:B:1150:THR:CG2	1:B:1153:LYS:HG2	2.36	0.55
1:B:1155:GLU:OE1	1:B:1155:GLU:N	2.39	0.55
1:A:1147:TRP:CE2	1:B:1142:LEU:HB3	2.42	0.54
1:B:746:LEU:HD21	1:B:750:PHE:CE2	2.41	0.54
1:A:457:LEU:HD22	1:A:529:ILE:HG12	1.88	0.54
1:A:648:GLU:H	1:A:648:GLU:CD	2.15	0.54
1:B:1155:GLU:O	1:B:1158:ILE:HG13	2.07	0.54
1:A:610:GLU:HB2	1:A:700:PHE:CD2	2.43	0.54
1:A:1106:TRP:CZ2	1:A:1110:GLN:NE2	2.76	0.54
1:B:1056:MET:HB2	1:B:1106:TRP:CZ3	2.43	0.54
1:A:617:HIS:ND1	1:A:618:ILE:O	2.39	0.54
1:A:1073:GLU:OE2	1:A:1079:ILE:HD11	2.08	0.54
1:A:1083:ASN:CB	1:B:1075:ILE:HD11	2.35	0.53
1:B:839:ASP:HA	1:B:842:LEU:HD23	1.90	0.53
1:B:1147:TRP:CD1	1:B:1150:THR:HG21	2.44	0.53
1:A:938:GLU:OE1	1:A:983:LYS:NZ	2.32	0.53
1:B:648:GLU:HA	1:B:707:LYS:NZ	2.23	0.53
1:A:593:ILE:HG23	1:A:594:VAL:HG23	1.89	0.53
1:A:651:ARG:NH1	4:A:1301:HOH:O	2.40	0.53
1:A:883:TYR:OH	1:A:1031:VAL:HG21	2.09	0.53
1:A:1155:GLU:O	1:A:1158:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1071:ILE:HG21	1:B:1157:LEU:HD13	1.90	0.52
1:B:1151:LYS:HA	1:B:1154:VAL:CG2	2.38	0.52
1:B:550:GLY:O	1:B:551:LYS:HG3	2.09	0.52
1:A:1091:GLN:O	1:A:1095:GLN:HB2	2.10	0.52
1:B:1036:LYS:O	1:B:1040:ASP:HB2	2.09	0.52
1:A:1082:GLU:HB3	1:B:1075:ILE:HD12	1.91	0.51
1:A:1141:ILE:HA	1:A:1144:MET:HE3	1.93	0.51
1:B:529:ILE:O	1:B:548:ARG:HD3	2.11	0.51
1:A:1079:ILE:HG13	1:A:1096:ARG:NH2	2.24	0.51
1:A:1136:PRO:HB2	1:A:1138:PHE:CE1	2.46	0.51
1:B:1116:GLU:O	1:B:1116:GLU:OE1	2.28	0.51
1:B:1094:VAL:HG12	1:B:1138:PHE:HZ	1.75	0.51
1:B:1074:LYS:HD2	1:B:1079:ILE:O	2.11	0.50
1:B:704:THR:HG22	1:B:705:ALA:N	2.26	0.50
1:B:466:LYS:HE2	1:B:466:LYS:H	1.77	0.50
1:A:1074:LYS:O	1:B:1082:GLU:HG2	2.11	0.50
1:A:1170:ASP:OD1	1:A:1173:ARG:NH2	2.44	0.50
1:A:844:PHE:HA	1:A:854:PRO:HA	1.93	0.50
1:A:1083:ASN:HB2	1:B:1075:ILE:CD1	2.35	0.50
1:B:595:LYS:HD2	1:B:629:TYR:CZ	2.46	0.50
1:A:615:LYS:HD3	1:A:615:LYS:H	1.77	0.50
1:B:1099:GLU:O	1:B:1140:TYR:OH	2.23	0.50
1:A:503:ARG:HG2	3:F:11:DC:N3	2.27	0.49
1:A:1079:ILE:HG23	1:A:1092:MET:HE1	1.94	0.49
1:A:1074:LYS:NZ	1:A:1082:GLU:OE2	2.45	0.49
1:A:617:HIS:HE1	1:A:624:TRP:HH2	1.50	0.49
1:A:1108:GLU:OE2	1:A:1109:ALA:N	2.45	0.49
1:B:1060:GLU:OE1	1:B:1164:LYS:NZ	2.44	0.49
1:A:529:ILE:O	1:A:548:ARG:HD3	2.13	0.49
1:A:704:THR:HG22	1:A:705:ALA:N	2.28	0.48
1:A:551:LYS:NZ	1:A:587:GLU:HG2	2.26	0.48
1:A:858:ILE:HG23	1:A:858:ILE:O	2.13	0.48
1:A:1050:LYS:NZ	1:A:1174:LYS:O	2.36	0.48
1:A:1155:GLU:HA	1:A:1158:ILE:HG12	1.95	0.48
1:A:636:THR:OG1	1:A:639:GLU:HG3	2.13	0.48
1:A:560:GLN:HB3	1:A:722:PHE:HA	1.96	0.48
1:B:595:LYS:HD2	1:B:629:TYR:CE1	2.49	0.48
1:A:1165:GLY:O	1:A:1168:VAL:HG22	2.14	0.48
1:B:570:ILE:HG12	1:B:711:TYR:HE1	1.79	0.48
1:A:692:ARG:NH1	1:A:698:GLU:HB2	2.29	0.48
1:A:573:ILE:HG22	1:A:581:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:HG23	1:A:609:PRO:HD3	1.96	0.47
1:A:1073:GLU:HB3	1:A:1079:ILE:CD1	2.44	0.47
3:E:11:DC:H2"	3:E:12:DA:H5'	1.96	0.47
1:A:692:ARG:HH22	1:A:697:PRO:HA	1.79	0.47
1:B:810:LEU:HD12	1:B:948:THR:HB	1.95	0.47
2:D:1:DA:H8	2:D:1:DA:P	2.38	0.47
1:A:503:ARG:HG2	3:F:11:DC:C2	2.49	0.47
1:A:739:LYS:NZ	1:A:870:GLU:O	2.43	0.47
1:B:1079:ILE:CG1	1:B:1096:ARG:HH11	2.27	0.47
1:B:1141:ILE:HD12	1:B:1141:ILE:H	1.79	0.47
1:A:551:LYS:HZ2	1:A:587:GLU:HG2	1.80	0.47
1:A:1056:MET:HE2	1:A:1106:TRP:CE3	2.50	0.47
1:A:756:ARG:NH2	1:B:769:GLU:OE2	2.45	0.47
1:B:503:ARG:HG2	3:E:11:DC:N3	2.30	0.47
1:B:730:SER:O	1:B:871:GLY:HA3	2.15	0.47
1:B:805:GLN:HE22	1:B:808:THR:CG2	2.26	0.47
1:B:1091:GLN:O	1:B:1095:GLN:HB2	2.15	0.47
3:F:11:DC:H2"	3:F:12:DA:H5'	1.97	0.47
1:B:1075:ILE:HD12	1:B:1075:ILE:HA	1.60	0.47
1:A:595:LYS:NZ	1:A:639:GLU:OE1	2.48	0.46
1:A:1154:VAL:O	1:A:1158:ILE:HG23	2.15	0.46
1:A:1152:GLU:C	1:A:1153:LYS:HD2	2.41	0.46
1:B:768:ALA:HA	1:B:773:TYR:HB3	1.96	0.46
1:A:1146:LEU:HD12	1:B:1146:LEU:HD12	1.97	0.46
1:B:606:TYR:HB2	1:B:702:TYR:HB2	1.98	0.46
1:B:1073:GLU:O	1:B:1078:LYS:HD3	2.15	0.46
1:B:1102:PRO:HA	1:B:1105:ALA:HB3	1.96	0.46
1:A:687:ASP:HB3	1:A:691:ARG:HH12	1.80	0.46
1:B:991:GLU:OE1	1:B:995:GLN:NE2	2.47	0.46
1:B:692:ARG:NH2	1:B:698:GLU:HB2	2.29	0.45
1:B:959:MET:HE2	1:B:969:LEU:HD23	1.98	0.45
1:A:1145:SER:O	1:A:1148:SER:OG	2.27	0.45
1:B:1165:GLY:O	1:B:1168:VAL:HG22	2.17	0.45
1:B:696:LEU:HD23	1:B:697:PRO:HD2	1.99	0.45
1:B:1147:TRP:HD1	1:B:1150:THR:HG21	1.82	0.45
1:A:773:TYR:CZ	1:A:775:HIS:HB2	2.52	0.45
1:A:1075:ILE:HD13	1:A:1075:ILE:HA	1.78	0.45
1:B:844:PHE:HA	1:B:854:PRO:HA	1.98	0.45
1:A:1050:LYS:NZ	1:A:1172:LYS:O	2.50	0.45
1:B:955:VAL:C	1:B:958:PRO:HD2	2.42	0.45
1:A:513:SER:OG	1:A:516:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:HIS:ND1	1:A:618:ILE:N	2.58	0.44
1:B:551:LYS:CE	1:B:587:GLU:OE1	2.64	0.44
1:A:1070:PHE:HA	1:A:1098:TYR:OH	2.17	0.44
1:A:660:GLU:H	1:A:660:GLU:CD	2.24	0.44
1:A:691:ARG:NE	1:A:698:GLU:OE1	2.42	0.44
1:B:759:LYS:HD3	1:B:820:ARG:O	2.17	0.44
1:A:595:LYS:HD2	1:A:629:TYR:CE1	2.52	0.44
1:B:993:LEU:O	1:B:997:GLU:HG2	2.18	0.44
1:B:1049:ARG:NH2	1:B:1183:ASP:OD2	2.41	0.44
1:B:1056:MET:HE2	1:B:1106:TRP:CE3	2.52	0.44
1:B:1070:PHE:HA	1:B:1098:TYR:OH	2.17	0.44
1:A:768:ALA:HA	1:A:773:TYR:HB3	2.00	0.44
1:A:1079:ILE:HG23	1:A:1092:MET:CE	2.48	0.44
1:A:1150:THR:O	1:A:1154:VAL:HG22	2.18	0.44
1:B:649:ARG:O	1:B:649:ARG:NH2	2.51	0.44
1:A:648:GLU:HA	1:A:707:LYS:NZ	2.33	0.43
1:A:595:LYS:HD2	1:A:629:TYR:CZ	2.53	0.43
1:A:1068:ALA:HA	1:A:1157:LEU:HD13	2.00	0.43
1:B:482:LYS:O	1:B:486:VAL:HG13	2.18	0.43
1:B:1094:VAL:HG12	1:B:1138:PHE:CZ	2.53	0.43
1:B:976:TYR:HB2	1:B:983:LYS:HB3	2.00	0.43
1:B:1046:TYR:CE2	1:B:1180:TRP:CG	3.06	0.43
1:B:1101:ASP:HA	1:B:1140:TYR:CE1	2.53	0.43
1:A:693:LEU:HD23	1:A:694:HIS:CE1	2.53	0.43
1:A:551:LYS:NZ	1:A:587:GLU:CD	2.76	0.43
1:B:805:GLN:OE1	1:B:805:GLN:HA	2.18	0.43
1:B:1063:LYS:HA	1:B:1102:PRO:HG2	2.01	0.43
1:B:1084:ARG:NH1	1:B:1088:ASP:OD2	2.52	0.43
1:B:1096:ARG:HG2	1:B:1098:TYR:CE1	2.53	0.43
1:A:1087:LYS:HE2	1:B:1152:GLU:OE2	2.19	0.43
1:B:780:LEU:HD12	1:B:780:LEU:HA	1.74	0.43
1:B:770:MET:HE3	1:B:770:MET:HB2	1.88	0.43
1:B:1071:ILE:CD1	1:B:1148:SER:HB3	2.49	0.43
1:A:482:LYS:O	1:A:486:VAL:HG13	2.19	0.43
1:A:1025:LEU:HD23	1:A:1025:LEU:HA	1.87	0.43
1:A:999:ALA:O	1:A:1003:LYS:HE2	2.19	0.42
1:A:1046:TYR:CE2	1:A:1180:TRP:CG	3.06	0.42
1:A:1161:ARG:HE	1:A:1161:ARG:HB3	1.49	0.42
1:B:492:ILE:HD12	1:B:492:ILE:HA	1.83	0.42
1:A:1074:LYS:HB2	1:A:1074:LYS:HE3	1.60	0.42
1:B:560:GLN:HB3	1:B:722:PHE:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1085:SER:OG	1:B:1087:LYS:HG2	2.19	0.42
1:B:1108:GLU:OE1	1:B:1109:ALA:N	2.51	0.42
2:D:1:DA:H2'	2:D:1:DA:OP2	2.19	0.42
1:B:594:VAL:HG11	1:B:611:PHE:CB	2.49	0.42
1:B:807:GLY:HA3	1:B:813:GLY:HA2	2.01	0.42
1:B:1136:PRO:HB2	1:B:1138:PHE:CE1	2.54	0.42
1:B:883:TYR:CZ	1:B:1031:VAL:HG11	2.54	0.42
1:B:552:ILE:HB	1:B:586:LEU:HD23	2.00	0.42
1:A:1063:LYS:HB2	1:A:1102:PRO:HG2	2.01	0.42
1:B:520:ASN:OD1	1:B:523:ILE:HG12	2.19	0.42
1:B:1025:LEU:HD12	1:B:1025:LEU:HA	1.91	0.42
1:B:1073:GLU:HG2	1:B:1078:LYS:HB2	2.01	0.42
1:A:637:ALA:O	1:A:641:LYS:HG3	2.20	0.42
1:B:1079:ILE:HG23	1:B:1092:MET:HE1	2.01	0.42
1:A:993:LEU:O	1:A:997:GLU:HG2	2.20	0.42
1:B:773:TYR:CZ	1:B:775:HIS:HB2	2.55	0.42
1:A:833:LEU:HD21	1:A:1187:PHE:CZ	2.55	0.41
1:B:746:LEU:CD2	1:B:750:PHE:CE2	3.03	0.41
1:A:1088:ASP:OD2	1:A:1089:LEU:HG	2.20	0.41
1:A:1142:LEU:HA	1:A:1142:LEU:HD23	1.68	0.41
1:B:1070:PHE:CG	1:B:1141:ILE:HG21	2.55	0.41
1:A:560:GLN:OE1	1:A:560:GLN:N	2.46	0.41
1:A:1164:LYS:HA	1:A:1164:LYS:HD3	1.81	0.41
1:A:807:GLY:HA3	1:A:813:GLY:HA2	2.02	0.41
1:A:833:LEU:HD21	1:A:1187:PHE:CE1	2.56	0.41
1:A:883:TYR:CZ	1:A:1031:VAL:HG21	2.56	0.41
1:A:1087:LYS:O	1:A:1090:ILE:HG13	2.21	0.41
1:A:536:LYS:HD3	1:A:538:TYR:CE1	2.56	0.41
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.94	0.41
1:A:655:ARG:O	1:A:710:THR:HA	2.20	0.41
1:A:730:SER:O	1:A:871:GLY:HA3	2.21	0.41
1:A:1117:ASP:HB3	1:A:1118:GLU:H	1.71	0.41
1:B:746:LEU:HD21	1:B:750:PHE:CZ	2.56	0.41
1:A:780:LEU:HD12	1:A:780:LEU:HA	1.80	0.41
1:A:1070:PHE:CG	1:A:1141:ILE:HG21	2.56	0.41
1:A:1101:ASP:HA	1:A:1140:TYR:CE1	2.56	0.41
1:A:1136:PRO:HB2	1:A:1138:PHE:HE1	1.84	0.41
1:B:595:LYS:HD2	1:B:629:TYR:OH	2.21	0.41
1:B:1152:GLU:O	1:B:1153:LYS:HD2	2.20	0.41
1:B:1184:LEU:O	1:B:1188:VAL:HG13	2.21	0.41
1:A:1141:ILE:H	1:A:1141:ILE:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:GLU:O	1:A:1153:LYS:HD2	2.21	0.41
1:B:825:MET:HE3	1:B:825:MET:HB2	1.92	0.41
1:A:1109:ALA:HA	1:A:1112:LYS:HE3	2.03	0.40
1:B:594:VAL:HG11	1:B:611:PHE:HB2	2.03	0.40
1:B:1056:MET:HE2	1:B:1106:TRP:CZ3	2.55	0.40
1:A:691:ARG:NH2	1:A:698:GLU:OE1	2.53	0.40
1:B:594:VAL:CG1	1:B:605:PHE:HB2	2.50	0.40
1:A:606:TYR:HB2	1:A:702:TYR:HB2	2.03	0.40
1:B:452:LYS:HB2	1:B:453:GLY:H	1.62	0.40
1:B:963:THR:OG1	1:B:964:ASP:N	2.52	0.40
1:A:785:VAL:O	1:A:789:GLN:HG3	2.22	0.40
1:A:834:PHE:HD2	1:A:857:TYR:HB3	1.85	0.40
1:A:1073:GLU:CB	1:A:1079:ILE:CD1	3.00	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	726/803 (90%)	687 (95%)	38 (5%)	1 (0%)	48	61
1	B	724/803 (90%)	684 (94%)	38 (5%)	2 (0%)	36	45
All	All	1450/1606 (90%)	1371 (95%)	76 (5%)	3 (0%)	43	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	616	LYS
1	B	616	LYS
1	B	455	PRO

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	642/704 (91%)	641 (100%)	1 (0%)	87	93
1	B	639/704 (91%)	638 (100%)	1 (0%)	87	93
All	All	1281/1408 (91%)	1279 (100%)	2 (0%)	87	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1156	GLU
1	B	1167	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	514	HIS
1	A	533	GLN
1	A	617	HIS
1	A	694	HIS
1	A	1110	GLN
1	B	514	HIS
1	B	650	HIS
1	B	753	ASN
1	B	840	ASN
1	B	935	ASN
1	B	961	ASN
1	B	1083	ASN
1	B	1139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	729/803 (90%)	-1.16	0 100 100	35, 65, 131, 173	9 (1%)
1	B	729/803 (90%)	-1.17	0 100 100	38, 66, 130, 172	5 (0%)
2	C	8/8 (100%)	-1.45	0 100 100	47, 49, 74, 107	0
2	D	8/8 (100%)	-1.32	0 100 100	47, 50, 73, 106	0
3	E	12/12 (100%)	-1.38	0 100 100	49, 59, 106, 146	0
3	F	12/12 (100%)	-1.36	0 100 100	48, 59, 111, 136	0
All	All	1498/1646 (91%)	-1.17	0 100 100	35, 65, 131, 173	14 (0%)

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.