



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:01 AM UTC

PDB ID : 5XA0 / pdb_00005xa0
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor cytosolic domain
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2017-03-10
Resolution : 5.81 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
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

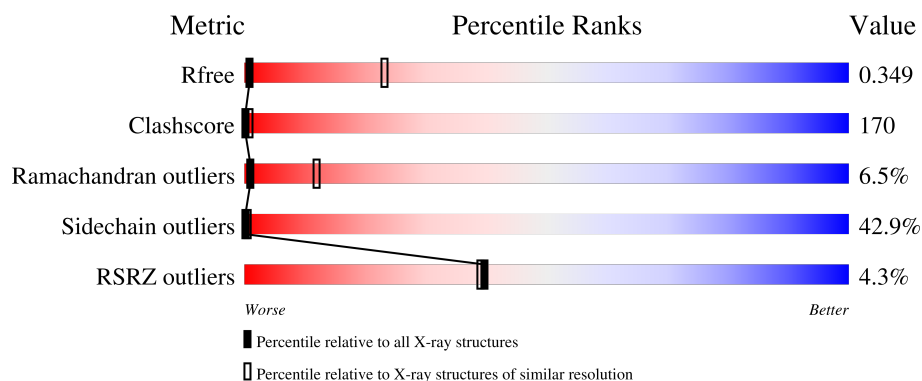
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.81 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	1126 (7.64-4.00)
Clashscore	190562	1191 (7.64-4.00)
Ramachandran outliers	187476	1019 (7.60-4.00)
Sidechain outliers	187428	1009 (7.60-3.98)
RSRZ outliers	180081	1119 (7.64-4.00)

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	1581	 3% 35% 31% 12% • 21%
1	B	1581	 4% 35% 30% 12% • 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17919 atoms, of which 2970 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.

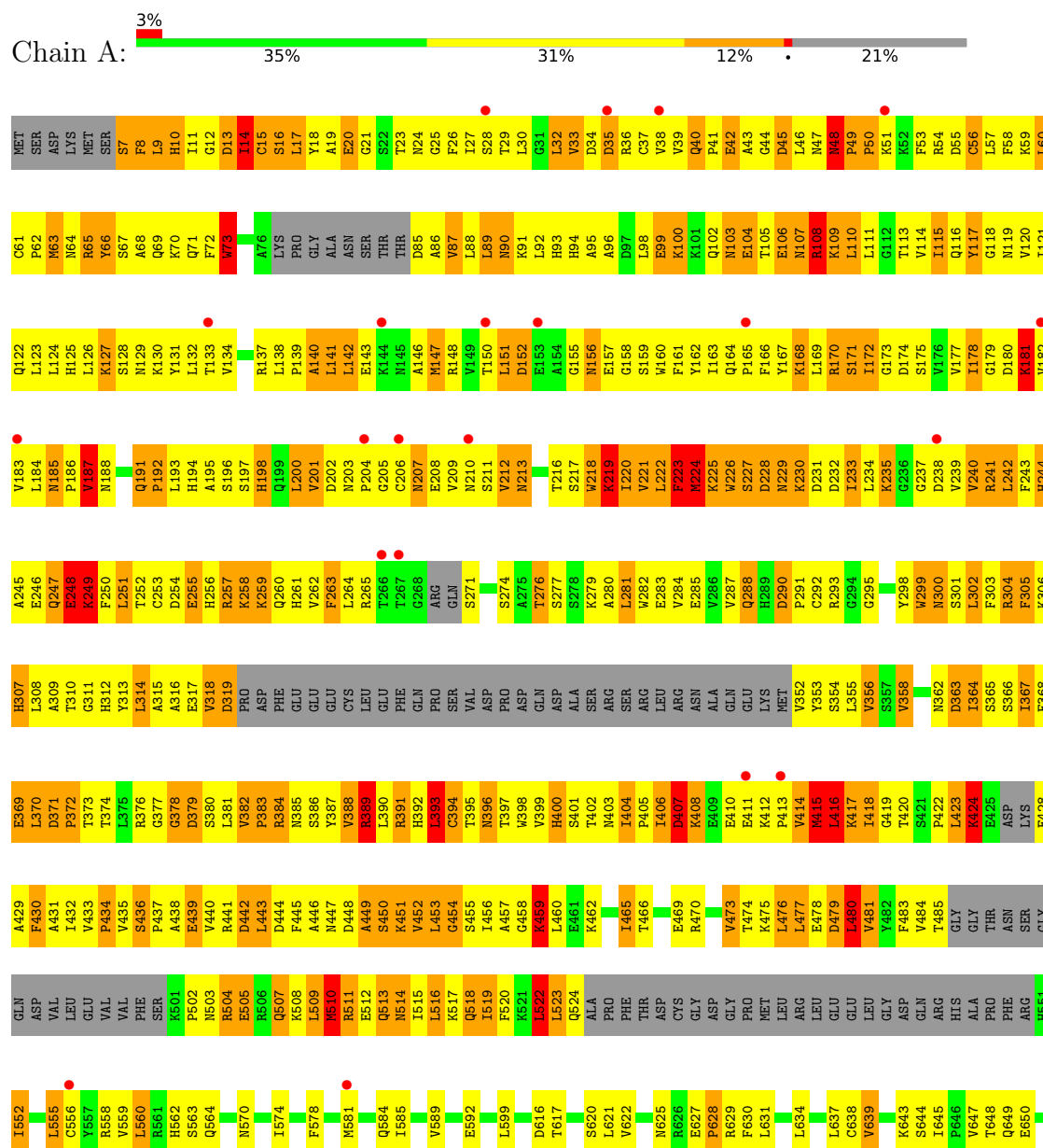
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

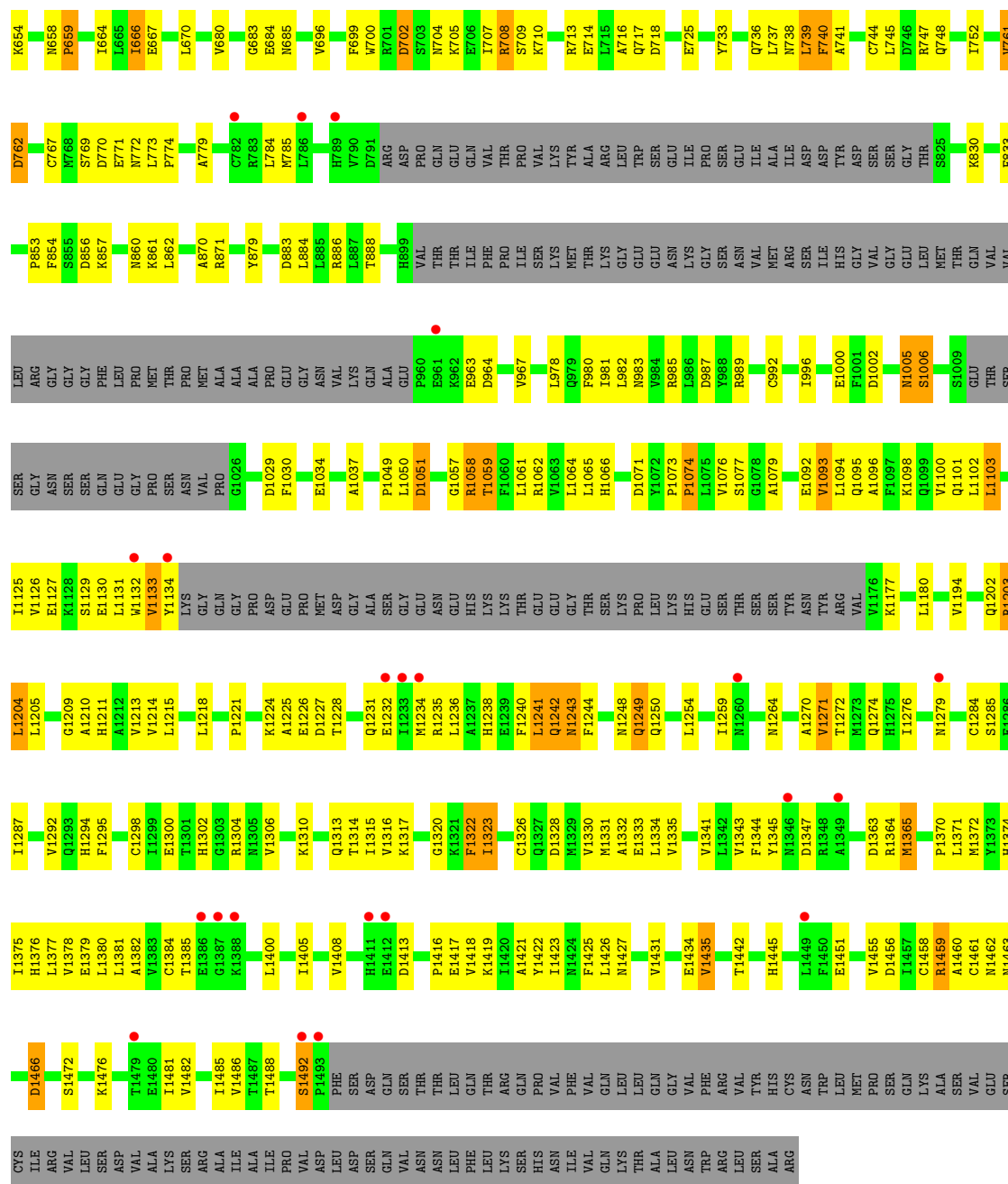
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1252	Total	C	H	N	O	S	0	0	0
			8949	4595	1485	1410	1444	15			
1	B	1252	Total	C	H	N	O	S	0	0	0
			8970	4610	1485	1412	1447	16			

3 Residue-property plots

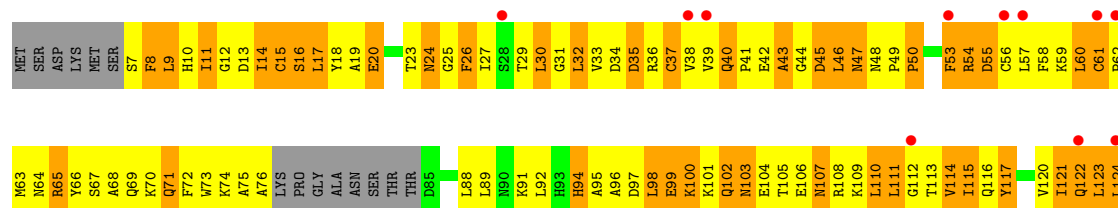
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Inositol 1,4,5-trisphosphate receptor type 1





• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1





SER	GLN	LYS	ALA	VAL	GLU	SER	CYS	ILE	ARG	VAL	LEU	SER	ASP	VAL	LYS	SER	ARG	ALA	ILE	ALA	ILE	PRO	VAL	ASP	LEU	ASP	SER	GLN	VAL	ASN	ASN	THR	THR	LEU	GLN	THR	LEU	LYS	SER	HIS	ASN	ILE	VAL	GLN	LYS	THR	ALA	LEU	ASN	TRP	ARG	LEU	ALA	ARG	
F1453	L1454	C1458	R1459	A1460	C1461	N1462	N1463	T1464	S1472	I1473	L1474	E1475	K1476	Y1477	V1478	T1481	T1488	F1489	F1490	S1491	S1492	P1493	PHE	SER	ASP	SER	GLN	VAL	ASN	ASN	THR	THR	LEU	GLN	THR	LEU	LYS	SER	HIS	ASN	ILE	VAL	GLN	LYS	THR	ALA	LEU	ASN	TRP	ARG	LEU	ALA	ARG		
Q1356	M1357	S1360	E1361	R1364	S1369	P1370	L1371	I1375	H1376	L1377	V1378	E1379	L1380	L1381	A1382	V1383	C1384	T1385	K1395	G1396	N1397	L1400	P1401	L1402	D1403	D1404	D1413	T1420	A1421	N1424	F1425	H1428	C1429	Y1430	V1431	D1432	T1433	E1434	V1435	K1438	E1439	I1440	Y1441	T1442	S1443	N1444	N1452								
L1183	S1184	C1187	V1188	S1191	A1192	S1193	V1194	R1195	K1196	S1197	R1198	R1203	L1204	L1205	R1206	N1207	M1208	G1209	A1210	H1211	A1212	V1213	V1214	L1215	E1216	L1217	L1218	Q1219	I1220	P1221	Y1222	K1223	K1224	A1225	E1226	D1227	T1228	K1229	M1230	Q1231	E1232	I1233	M1234	R1235	L1236	A1237	H1238	E1239	Q1242	N1243	F1244	C1245	A1246	G1247	N1248
Q1249	Q1250	M1251	L1255	H1256	K1257	H1258	I1259	N1260	L1261	A1270	Q1274	H1275	M1278	N1279	N1280	F1281	Q1282	L1283	C1284	S1285	E1286	I1287	N1288	V1292	Q1293	T1301	I1309	I1315	V1316	K1317	A1318	E1319	I1323	M1329	V1330	E1339	D1340	V1341	L1342	V1343	F1344	Y1345	N1346	D1347	S1350	I1355									

4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	128.16Å 128.16Å 369.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 5.81 48.81 – 5.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.81-5.81) 99.9 (48.81-5.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 5.73Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.278 , 0.342 0.281 , 0.349	Depositor DCC
R_{free} test set	818 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 389.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.368 for h,-k,-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	17919	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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	0.72	4/7527 (0.1%)	1.02	24/10362 (0.2%)
1	B	0.73	5/7549 (0.1%)	1.01	17/10390 (0.2%)
All	All	0.73	9/15076 (0.1%)	1.02	41/20752 (0.2%)

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	A	0	7
1	B	0	11
All	All	0	18

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	ARG	C-N	5.79	1.45	1.33
1	B	288	GLN	CG-CD	-5.74	1.37	1.52
1	A	430	PHE	CD1-CE1	5.63	1.55	1.38
1	B	462	LYS	CD-CE	5.55	1.69	1.52
1	B	385	ASN	CB-CG	-5.53	1.38	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	GLY	N-CA-C	12.29	142.31	113.18
1	B	376	ARG	CA-C-N	10.13	141.26	121.41
1	B	376	ARG	C-N-CA	10.13	141.26	121.41
1	A	108	ARG	CG-CD-NE	-9.50	91.10	112.00
1	B	243	PHE	CA-C-N	-9.39	103.20	122.07

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ILE	Peptide
1	A	213	ASN	Peptide
1	A	226	TRP	Peptide
1	A	248	GLU	Peptide
1	A	393	LEU	Peptide

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	7464	1485	5141	2123	2
1	B	7485	1485	5190	2173	2
All	All	14949	2970	10331	4296	4

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 170.

The worst 5 of 4296 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:263:PHE:HB2	1:A:415:MET:CB	1.50	1.38
1:A:456:ILE:C	1:A:459:LYS:HD3	1.51	1.35
1:B:459:LYS:C	1:B:462:LYS:HE3	1.48	1.35
1:A:32:LEU:CD1	1:A:445:PHE:HA	1.54	1.35
1:B:18:TYR:O	1:B:181:LYS:NZ	1.59	1.32

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ARG:O	1:B:378:GLY:N[2_655]	1.78	0.42
1:A:374:THR:N	1:A:376:ARG:O[2_655]	1.96	0.24
1:B:377:GLY:N	1:B:379:ASP:OD1[2_655]	2.15	0.05
1:A:373:THR:OG1	1:A:376:ARG:O[2_655]	2.16	0.04

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	1230/1581 (78%)	1000 (81%)	155 (13%)	75 (6%)	1	12
1	B	1230/1581 (78%)	980 (80%)	165 (13%)	85 (7%)	1	11
All	All	2460/3162 (78%)	1980 (80%)	320 (13%)	160 (6%)	1	12

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	50	PRO
1	A	104	GLU
1	A	140	ALA
1	A	192	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	376/1427 (26%)	227 (60%)	149 (40%)	0	1
1	B	384/1427 (27%)	207 (54%)	177 (46%)	0	0
All	All	760/2854 (27%)	434 (57%)	326 (43%)	0	0

5 of 326 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	225	LYS

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Mol	Chain	Res	Type
1	B	418	ILE
1	B	242	LEU
1	B	302	LEU
1	B	464	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	215	ASN
1	B	256	HIS
1	B	307	HIS
1	A	247	GLN
1	A	210	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 [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	1252/1581 (79%)	-0.25	43 (3%)	48	43	9, 28, 68, 157	0
1	B	1252/1581 (79%)	-0.24	64 (5%)	33	34	9, 28, 69, 127	0
All	All	2504/3162 (79%)	-0.24	107 (4%)	40	39	9, 28, 69, 157	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	VAL	7.1
1	B	1062	ARG	7.1
1	A	165	PRO	6.8
1	B	1404	ASP	6.6
1	B	1301	THR	6.1

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.