



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:17 AM UTC

PDB ID : 4FBQ / pdb_00004fbq
Title : Crystal structure of a covalently fused Nbs1-Mre11 complex with two manganese ions per active site
Authors : Schiller, C.B.; Lammens, K.; Hopfner, K.P.
Deposited on : 2012-05-23
Resolution : 2.50 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

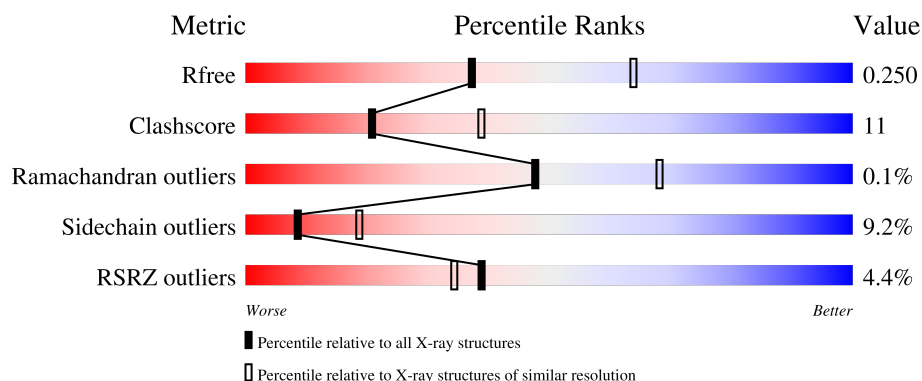
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

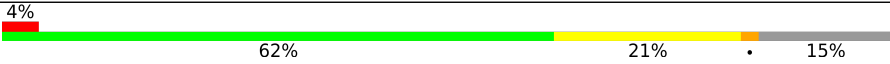
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	472	 4% 62% 24% 11%
1	B	472	 4% 62% 21% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6776 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 repair and telomere maintenance protein nbs1, DNA repair protein rad32 CHIMERIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	87	0	0
			3387	2157	591	631	8			
1	B	402	Total	C	N	O	S	70	0	0
			3240	2065	561	606	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP O43070
A	-3	PRO	-	expression tag	UNP O43070
A	-2	LEU	-	expression tag	UNP O43070
A	-1	GLY	-	expression tag	UNP O43070
A	0	SER	-	expression tag	UNP O43070
A	532	VAL	-	linker	UNP Q09683
A	533	ASP	-	linker	UNP Q09683
A	534	GLY	-	linker	UNP Q09683
A	535	SER	-	linker	UNP Q09683
A	536	ALA	-	linker	UNP Q09683
A	537	GLY	-	linker	UNP Q09683
A	538	SER	-	linker	UNP Q09683
A	539	ALA	-	linker	UNP Q09683
A	540	GLY	-	linker	UNP Q09683
A	541	SER	-	linker	UNP Q09683
B	-4	GLY	-	expression tag	UNP O43070
B	-3	PRO	-	expression tag	UNP O43070
B	-2	LEU	-	expression tag	UNP O43070
B	-1	GLY	-	expression tag	UNP O43070
B	0	SER	-	expression tag	UNP O43070
B	532	VAL	-	linker	UNP Q09683
B	533	ASP	-	linker	UNP Q09683
B	534	GLY	-	linker	UNP Q09683
B	535	SER	-	linker	UNP Q09683

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Chain	Residue	Modelled	Actual	Comment	Reference
B	536	ALA	-	linker	UNP Q09683
B	537	GLY	-	linker	UNP Q09683
B	538	SER	-	linker	UNP Q09683
B	539	ALA	-	linker	UNP Q09683
B	540	GLY	-	linker	UNP Q09683
B	541	SER	-	linker	UNP Q09683

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total 65	O 65	0	0
3	B	80	Total 80	O 80	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.26 Å 79.03 Å 222.97 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.41 – 2.50 47.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.41-2.50) 98.3 (47.41-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.213 , 0.257 0.209 , 0.250	Depositor DCC
R_{free} test set	1994 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6776	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 3.92% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.55	0/3460	0.89	2/4685 (0.0%)
1	B	0.54	0/3313	0.88	3/4497 (0.1%)
All	All	0.54	0/6773	0.88	5/9182 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1368	LYS	CA-C-N	7.24	124.95	119.66
1	B	1368	LYS	C-N-CA	7.24	124.95	119.66
1	A	1115	ASN	N-CA-C	6.38	118.23	111.28
1	B	1115	ASN	N-CA-C	6.02	117.84	111.28
1	A	1378	VAL	N-CA-C	5.09	115.37	107.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3387	0	3358	75	0
1	B	3240	0	3200	69	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	65	0	0	1	0
3	B	80	0	0	1	0
All	All	6776	0	6558	142	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 11.

All (142) 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:1209:ASP:O	1:A:1212:ARG:HG3	1.39	1.19
1:B:1292:LEU:HD21	1:B:1294:ILE:HD11	1.16	1.12
1:B:1292:LEU:CD2	1:B:1294:ILE:HD11	1.88	1.03
1:A:1323:SER:HA	1:A:1325:ILE:H	1.26	0.99
1:B:1164:ASN:HB3	1:B:1193:ARG:HG2	1.52	0.89
1:B:1164:ASN:HB3	1:B:1193:ARG:CG	2.09	0.82
1:B:1016:ASN:O	1:B:1179:THR:HG21	1.79	0.82
1:B:1328:MET:HA	1:B:1383:GLY:HA3	1.63	0.78
1:B:1209:ASP:O	1:B:1212:ARG:HG3	1.83	0.77
1:A:1209:ASP:O	1:A:1212:ARG:CG	2.30	0.73
1:A:1323:SER:HA	1:A:1325:ILE:N	2.02	0.72
1:A:1163:GLU:O	1:A:1164:ASN:ND2	2.22	0.72
1:B:1016:ASN:O	1:B:1179:THR:CG2	2.38	0.71
1:B:1015:GLU:HB3	3:B:1642:HOH:O	1.91	0.69
1:B:1354:TRP:O	1:B:1358:GLN:HG2	1.93	0.69
1:A:1323:SER:OG	1:A:1324:SER:HA	1.93	0.68
1:A:1148:ILE:O	1:A:1152:THR:HG23	1.95	0.67
1:B:495:TYR:CE1	1:B:1212:ARG:HD3	2.31	0.65
1:A:1392:PHE:O	1:A:1395:ARG:HG3	1.97	0.65
1:A:1026:PRO:HG2	1:A:1066:ILE:HA	1.78	0.65
1:A:1164:ASN:O	1:A:1166:ASN:N	2.32	0.63
1:A:1209:ASP:OD1	1:A:1210:LEU:N	2.30	0.63
1:B:487:LEU:O	1:B:1237:SER:HB2	1.99	0.62
1:A:1344:GLU:O	1:A:1348:THR:HG23	2.00	0.62
1:A:1099:LEU:HD21	1:A:1175:GLN:HB2	1.81	0.62
1:B:1180:LYS:HB3	1:B:1215:TRP:CE3	2.35	0.62
1:B:1292:LEU:HD21	1:B:1294:ILE:CD1	2.10	0.62
1:A:1029:GLY:O	1:A:1032:GLU:HG3	1.99	0.62
1:A:1099:LEU:CD2	1:A:1175:GLN:HB2	2.31	0.60
1:B:495:TYR:CD1	1:B:1212:ARG:NE	2.70	0.59
1:B:1216:PHE:CE2	1:B:1294:ILE:HD12	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1171:PRO:HB3	1:B:1184:TYR:CZ	2.37	0.59
1:B:489:ASN:ND2	1:B:1241:ASP:OD2	2.35	0.59
1:B:1164:ASN:CB	1:B:1193:ARG:CG	2.81	0.58
1:B:1210:LEU:HB3	1:B:1211:TYR:CD2	2.38	0.58
1:B:1171:PRO:HB3	1:B:1184:TYR:CE2	2.38	0.58
1:A:496:ILE:HD13	1:A:1206:LEU:HD13	1.85	0.57
1:A:1314:MET:CE	1:A:1375:ARG:HD3	2.34	0.57
1:B:1222:HIS:CD2	1:B:1250:HIS:HB2	2.39	0.57
1:A:521:PHE:CE2	1:A:1097:GLU:HB2	2.40	0.57
1:B:1131:HIS:HD2	1:B:1157:TYR:OH	1.88	0.56
1:B:1368:LYS:HB2	1:B:1369:PRO:HD2	1.86	0.56
1:A:1163:GLU:HG3	1:A:1166:ASN:N	2.20	0.56
1:A:1063:GLY:O	1:A:1222:HIS:HD2	1.89	0.55
1:A:1364:VAL:HG12	1:A:1365:GLU:OE2	2.07	0.55
1:A:1209:ASP:C	1:A:1212:ARG:HG3	2.26	0.55
1:A:1354:TRP:O	1:A:1358:GLN:HG2	2.07	0.54
1:A:1169:VAL:HG12	1:A:1184:TYR:HD1	1.72	0.54
1:A:1316:ASP:OD1	1:A:1377:ARG:HB2	2.07	0.54
1:A:1135:ASP:O	1:A:1136:ASP:C	2.51	0.53
1:A:1148:ILE:HD13	1:B:1077:LEU:HD23	1.89	0.53
1:A:1171:PRO:HB3	1:A:1184:TYR:CZ	2.44	0.53
1:B:1131:HIS:CD2	1:B:1187:SER:HB3	2.43	0.53
1:B:1210:LEU:HB3	1:B:1211:TYR:HD2	1.73	0.53
1:A:1387:GLU:OE2	1:A:1395:ARG:NH1	2.41	0.52
1:A:1213:ASP:O	1:A:1297:LYS:NZ	2.30	0.52
1:A:1375:ARG:HG3	1:A:1375:ARG:HH11	1.74	0.52
1:A:1229:THR:HG22	1:A:1230:PRO:HD2	1.91	0.52
1:A:1097:GLU:HG2	1:A:1099:LEU:HD13	1.93	0.51
1:A:1379:ASP:OD1	1:A:1381:THR:OG1	2.24	0.51
1:A:1131:HIS:CD2	1:A:1187:SER:HB3	2.45	0.51
1:A:1326:PRO:O	1:A:1329:VAL:HG12	2.11	0.51
1:B:1164:ASN:CB	1:B:1193:ARG:HG2	2.33	0.50
1:B:1031:GLY:O	1:B:1038:GLY:HA2	2.10	0.50
1:A:1375:ARG:NH2	1:A:1408:GLN:HB2	2.27	0.50
1:B:1180:LYS:HB3	1:B:1215:TRP:CZ3	2.47	0.50
1:A:520:ASN:OD1	1:A:522:LYS:HG2	2.12	0.50
1:A:1031:GLY:O	1:A:1038:GLY:HA2	2.11	0.50
1:A:1180:LYS:HB3	1:A:1215:TRP:CE3	2.47	0.49
1:A:1133:ASN:ND2	1:A:1134:HIS:HD2	2.10	0.49
1:A:1336:LEU:HD11	1:A:1387:GLU:HB2	1.94	0.49
1:B:1032:GLU:OE2	1:B:1073:SER:OG	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:PRO:HG2	1:A:1238:PHE:CZ	2.48	0.49
1:B:1338:TYR:OH	1:B:1342:LYS:HE2	2.12	0.48
1:A:1375:ARG:NH1	1:A:1405:ASP:O	2.46	0.48
1:B:1375:ARG:NH2	1:B:1408:GLN:OE1	2.46	0.48
1:A:1135:ASP:O	1:A:1136:ASP:O	2.30	0.48
1:A:1312:PHE:C	1:A:1312:PHE:CD1	2.91	0.48
1:A:524:PHE:CD2	1:A:1122:ASN:ND2	2.82	0.48
1:B:1094:CYS:SG	1:B:1096:LEU:HB2	2.54	0.47
1:A:1052:ALA:CB	1:A:1060:ILE:HD11	2.45	0.47
1:A:1131:HIS:C	1:A:1131:HIS:ND1	2.73	0.47
1:B:1196:HIS:O	1:B:1200:GLU:HG2	2.15	0.46
1:B:1332:LYS:O	1:B:1336:LEU:HD13	2.15	0.46
1:A:1284:THR:HG21	1:A:1314:MET:HB3	1.98	0.46
1:A:1303:LYS:HE3	3:A:1618:HOH:O	2.14	0.46
1:A:1261:ASN:O	1:A:1265:LYS:N	2.45	0.46
1:A:1312:PHE:CD1	1:A:1313:ILE:N	2.84	0.46
1:A:1092:LYS:HA	1:A:1093:PRO:HD2	1.80	0.46
1:A:1034:ASP:HA	1:A:1035:PRO:HD3	1.74	0.46
1:B:1026:PRO:HA	1:B:1274:THR:OG1	2.15	0.46
1:B:1238:PHE:N	1:B:1238:PHE:CD1	2.84	0.46
1:B:1019:ARG:NH1	1:B:1055:ARG:O	2.39	0.45
1:A:1180:LYS:HB3	1:A:1215:TRP:CZ3	2.52	0.45
1:B:1243:TYR:O	1:B:1266:PHE:HB3	2.17	0.45
1:B:1146:LEU:HB3	1:B:1157:TYR:CD2	2.52	0.45
1:A:1375:ARG:HG3	1:A:1375:ARG:NH1	2.31	0.45
1:A:1047:GLU:OE1	1:A:1308:THR:HG23	2.16	0.45
1:B:1131:HIS:CD2	1:B:1157:TYR:OH	2.69	0.44
1:A:1146:LEU:HD22	1:A:1146:LEU:HA	1.77	0.44
1:A:1234:LEU:HA	1:A:1235:PRO:HD3	1.81	0.44
1:A:1208:PRO:HG2	1:A:1215:TRP:CD1	2.52	0.44
1:B:1021:LEU:C	1:B:1021:LEU:HD23	2.43	0.44
1:B:1034:ASP:HA	1:B:1035:PRO:HD3	1.78	0.44
1:A:1069:ASP:O	1:A:1072:PRO:HD3	2.18	0.43
1:A:1016:ASN:OD1	1:A:1177:GLY:HA3	2.18	0.43
1:B:1211:TYR:HB3	1:B:1214:GLU:HB2	2.00	0.43
1:B:1264:GLN:O	1:B:1265:LYS:HB2	2.18	0.43
1:B:1161:VAL:HG11	1:B:1189:VAL:CG2	2.48	0.43
1:A:525:GLN:HE21	1:A:525:GLN:HB2	1.64	0.43
1:B:1300:HIS:CD2	1:B:1300:HIS:C	2.96	0.43
1:B:1331:ASN:ND2	1:B:1383:GLY:O	2.49	0.43
1:A:1056:ASP:OD1	1:A:1092:LYS:HE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1051:ILE:O	1:B:1052:ALA:C	2.60	0.42
1:B:1055:ARG:NH2	1:B:1302:GLU:OE1	2.53	0.42
1:A:521:PHE:CZ	1:A:1097:GLU:HB2	2.54	0.42
1:A:1131:HIS:HD2	1:A:1157:TYR:OH	2.01	0.42
1:A:520:ASN:CG	1:A:1093:PRO:HB3	2.44	0.42
1:B:1380:TYR:CD1	1:B:1409:PHE:HB3	2.55	0.42
1:B:1395:ARG:O	1:B:1399:ARG:NH2	2.53	0.42
1:B:1342:LYS:HA	1:B:1342:LYS:HD2	1.60	0.42
1:A:1287:LYS:HB2	1:A:1309:VAL:HG21	2.02	0.41
1:B:1065:ASP:OD1	1:B:1134:HIS:HB2	2.20	0.41
1:A:1071:LYS:HA	1:A:1072:PRO:HD2	1.87	0.41
1:B:1048:ILE:HD13	1:B:1048:ILE:HA	1.80	0.41
1:B:1331:ASN:HD21	1:B:1384:TYR:HA	1.85	0.41
1:B:1328:MET:CA	1:B:1383:GLY:HA3	2.40	0.41
1:A:1278:SER:O	1:A:1283:GLU:HG3	2.21	0.41
1:B:1017:THR:HA	1:B:1294:ILE:O	2.20	0.41
1:B:1026:PRO:HG2	1:B:1066:ILE:HA	2.03	0.41
1:A:1026:PRO:HA	1:A:1274:THR:OG1	2.21	0.41
1:B:1217:ASN:ND2	1:B:1242:PHE:HD2	2.19	0.41
1:B:1299:PHE:O	1:B:1299:PHE:CD2	2.74	0.41
1:B:1328:MET:O	1:B:1328:MET:HG3	2.21	0.41
1:A:1048:ILE:HD11	1:A:1306:LEU:HD21	2.03	0.40
1:B:1178:PHE:CD2	1:B:1179:THR:HG22	2.55	0.40
1:B:1331:ASN:O	1:B:1334:GLU:N	2.51	0.40
1:B:1411:LEU:HA	1:B:1411:LEU:HD23	1.86	0.40
1:B:1189:VAL:O	1:B:1190:ARG:C	2.64	0.40
1:A:1151:VAL:HB	1:B:1078:TYR:CE1	2.57	0.40
1:A:1332:LYS:HE2	1:A:1386:THR:O	2.21	0.40
1:B:1238:PHE:N	1:B:1238:PHE:HD1	2.20	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	406/472 (86%)	386 (95%)	19 (5%)	1 (0%)	43	63
1	B	394/472 (84%)	376 (95%)	18 (5%)	0	100	100
All	All	800/944 (85%)	762 (95%)	37 (5%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1162	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	379/420 (90%)	343 (90%)	36 (10%)	8	17
1	B	362/420 (86%)	330 (91%)	32 (9%)	9	20
All	All	741/840 (88%)	673 (91%)	68 (9%)	8	19

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	LEU
1	A	493	VAL
1	A	496	ILE
1	A	518	ARG
1	A	525	GLN
1	A	1041	SER
1	A	1099	LEU
1	A	1100	SER
1	A	1109	THR
1	A	1111	VAL
1	A	1113	ASN
1	A	1131	HIS
1	A	1142	ARG
1	A	1146	LEU
1	A	1160	ARG

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Mol	Chain	Res	Type
1	A	1163	GLU
1	A	1209	ASP
1	A	1210	LEU
1	A	1213	ASP
1	A	1229	THR
1	A	1259	SER
1	A	1266	PHE
1	A	1267	THR
1	A	1277	THR
1	A	1315	LYS
1	A	1318	ILE
1	A	1319	LEU
1	A	1325	ILE
1	A	1348	THR
1	A	1349	GLU
1	A	1361	VAL
1	A	1365	GLU
1	A	1371	LEU
1	A	1381	THR
1	A	1397	VAL
1	A	1404	THR
1	B	482	GLU
1	B	496	ILE
1	B	1017	THR
1	B	1096	LEU
1	B	1099	LEU
1	B	1112	CYS
1	B	1122	ASN
1	B	1142	ARG
1	B	1146	LEU
1	B	1151	VAL
1	B	1166	ASN
1	B	1179	THR
1	B	1200	GLU
1	B	1209	ASP
1	B	1214	GLU
1	B	1294	ILE
1	B	1295	THR
1	B	1297	LYS
1	B	1298	ASP
1	B	1315	LYS
1	B	1319	LEU

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Mol	Chain	Res	Type
1	B	1329	VAL
1	B	1335	VAL
1	B	1361	VAL
1	B	1367	GLU
1	B	1368	LYS
1	B	1371	LEU
1	B	1381	THR
1	B	1387	GLU
1	B	1393	SER
1	B	1397	VAL
1	B	1404	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	525	GLN
1	A	1039	ASN
1	A	1046	ASN
1	A	1120	ASN
1	A	1122	ASN
1	A	1164	ASN
1	A	1222	HIS
1	A	1300	HIS
1	B	1070	ASN
1	B	1120	ASN
1	B	1131	HIS
1	B	1264	GLN
1	B	1270	GLN
1	B	1300	HIS
1	B	1390	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	418/472 (88%)	0.11	18 (4%) 40 35	21, 42, 77, 109	26 (6%)
1	B	402/472 (85%)	0.09	18 (4%) 38 33	22, 42, 74, 101	18 (4%)
All	All	820/944 (86%)	0.10	36 (4%) 39 34	21, 42, 76, 109	44 (5%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1164	ASN	6.3
1	A	1109	THR	5.3
1	B	1141	GLY	4.3
1	A	1112	CYS	4.0
1	A	541	SER	3.8
1	A	525	GLN	3.7
1	B	1165	ASP	3.7
1	A	1164	ASN	3.7
1	A	1110	ALA	3.5
1	B	496	ILE	3.4
1	A	1111	VAL	3.3
1	A	1211	TYR	3.2
1	A	497	ARG	3.1
1	B	480	ALA	3.0
1	B	1412	LYS	3.0
1	A	1136	ASP	2.9
1	B	1163	GLU	2.6
1	A	1403	ALA	2.6
1	B	1136	ASP	2.6
1	B	1110	ALA	2.5
1	A	520	ASN	2.5
1	A	518	ARG	2.3
1	B	1212	ARG	2.3
1	A	1325	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1213	ASP	2.3
1	B	1297	LYS	2.2
1	B	1295	THR	2.2
1	B	1329	VAL	2.1
1	B	1112	CYS	2.1
1	A	1102	THR	2.1
1	A	526	LYS	2.1
1	B	1093	PRO	2.1
1	A	1196	HIS	2.1
1	B	1328	MET	2.1
1	B	1298	ASP	2.0
1	B	1142	ARG	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 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
2	MN	A	1501	1/1	0.97	0.05	49,49,49,49	0
2	MN	B	1501	1/1	0.97	0.04	36,36,36,36	0
2	MN	B	1502	1/1	0.97	0.05	42,42,42,42	0
2	MN	A	1502	1/1	0.99	0.03	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.