



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2017 – 08:32 AM EST

PDB ID : 5M5P
Title : S. cerevisiae spliceosomal helicase Brr2 (271-end) in complex with the Jab/MPN domain of S. cerevisiae Prp8
Authors : Becke, C.; Absmeier, E.; Wollenhaupt, J.; Santos, K.F.; Wahl, M.C.
Deposited on : 2016-10-22
Resolution : 4.20 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

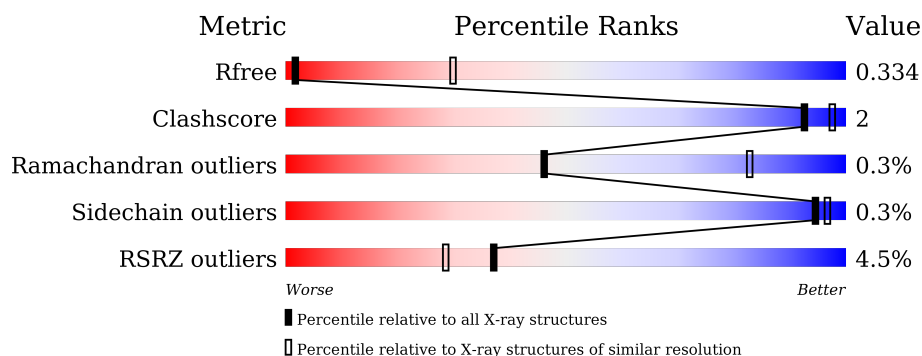
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	1897	<div> <div>3%</div> <div>92%</div> <div>5%</div> </div>
1	C	1897	<div> <div>5%</div> <div>92%</div> <div>5%</div> </div>
2	B	270	<div> <div>8%</div> <div>89%</div> <div>8%</div> </div>
2	D	270	<div> <div>8%</div> <div>85%</div> <div>7%</div> <div>8%</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 67309 atoms, of which 33658 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 Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1850	Total	C	H	N	O	S	0	0	0
			29711	9505	14876	2465	2808	57			
1	C	1850	Total	C	H	N	O	S	0	0	0
			29716	9505	14878	2467	2809	57			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLY	-	expression tag	UNP P32639
A	268	ALA	-	expression tag	UNP P32639
A	269	GLU	-	expression tag	UNP P32639
A	270	PHE	-	expression tag	UNP P32639
C	267	GLY	-	expression tag	UNP P32639
C	268	ALA	-	expression tag	UNP P32639
C	269	GLU	-	expression tag	UNP P32639
C	270	PHE	-	expression tag	UNP P32639

- Molecule 2 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	248	Total	C	H	N	O	S	0	0	0
			3941	1284	1952	322	377	6			
2	D	248	Total	C	H	N	O	S	0	0	0
			3941	1284	1952	322	377	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2144	GLY	-	expression tag	UNP P33334
B	2145	ALA	-	expression tag	UNP P33334
B	2146	MET	-	expression tag	UNP P33334
D	2144	GLY	-	expression tag	UNP P33334

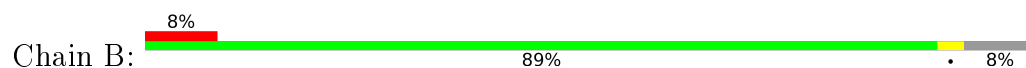
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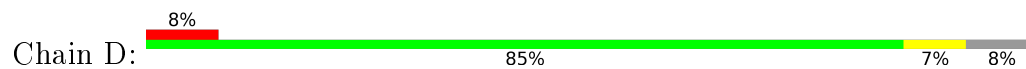
Chain	Residue	Modelled	Actual	Comment	Reference
D	2145	ALA	-	expression tag	UNP P33334
D	2146	MET	-	expression tag	UNP P33334



• Molecule 2: Pre-mRNA-splicing factor 8



• Molecule 2: Pre-mRNA-splicing factor 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	185.97Å 196.87Å 191.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.50 – 4.20 95.52 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.50-4.20) 99.9 (95.52-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.32	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 4.15Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.307 , 0.335 0.307 , 0.334	Depositor DCC
R_{free} test set	2665 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	147.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 94.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	67309	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.23	0/15149	0.43	1/20529 (0.0%)
1	C	0.24	0/15152	0.42	0/20534
2	B	0.22	0/2038	0.40	0/2764
2	D	0.23	0/2038	0.41	0/2764
All	All	0.23	0/34377	0.42	1/46591 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	789	LEU	CA-CB-CG	5.17	127.20	115.30

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	14835	14876	14874	65	0
1	C	14838	14878	14875	52	1
2	B	1989	1952	1951	6	0
2	D	1989	1952	1951	13	0
All	All	33651	33658	33651	131	1

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 2.

All (131) 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:1208:ALA:CB	1:A:1307:SER:OG	1.67	1.38
1:A:1208:ALA:HB3	1:A:1307:SER:OG	1.02	1.17
1:A:1286:PRO:O	1:A:1308:PHE:CD1	2.06	0.99
1:A:1309:ASN:OD1	2:B:2249:ASP:OD1	1.81	0.96
1:A:1208:ALA:HB2	1:A:1307:SER:OG	1.72	0.88
1:A:1307:SER:HB3	1:A:1311:PHE:CE2	2.13	0.82
1:C:1540:ARG:NH2	1:C:1710:ALA:O	2.13	0.82
1:A:963:ASP:O	1:A:965:GLN:N	2.11	0.82
1:A:1206:CYS:SG	1:A:1306:VAL:HG13	2.23	0.79
1:A:1286:PRO:O	1:A:1308:PHE:CG	2.36	0.78
1:A:1308:PHE:O	1:A:1310:GLY:N	2.16	0.78
1:A:787:ASN:OD1	1:A:789:LEU:N	2.20	0.74
1:A:1307:SER:HB3	1:A:1311:PHE:HE2	1.54	0.72
1:A:1077:ASN:OD1	1:A:1081:GLN:NE2	2.25	0.69
2:D:2165:ARG:NH1	2:D:2295:SER:O	2.25	0.69
1:C:1059:GLU:O	2:D:2153:ARG:NH2	2.26	0.68
1:C:769:LYS:NZ	1:C:799:SER:O	2.27	0.67
1:A:1174:GLU:OE1	1:A:1197:LYS:NZ	2.31	0.64
1:C:963:ASP:O	1:C:966:LEU:N	2.27	0.64
1:A:1307:SER:CB	1:A:1311:PHE:CE2	2.80	0.63
1:A:959:ASP:OD1	1:A:961:SER:OG	2.16	0.63
1:C:1625:THR:OG1	1:C:1648:ASP:OD1	2.15	0.63
1:C:1050:GLU:N	1:C:1050:GLU:OE1	2.33	0.61
1:C:890:THR:OG1	1:C:894:ASN:OD1	2.17	0.61
1:A:1307:SER:CB	1:A:1311:PHE:HE2	2.15	0.60
2:D:2273:GLU:N	2:D:2273:GLU:OE1	2.35	0.59
1:A:779:GLN:O	1:A:783:THR:N	2.35	0.58
1:A:1494:ARG:NH1	1:A:1757:GLU:OE2	2.37	0.58
1:C:395:THR:HG22	1:C:395:THR:O	2.04	0.57
1:A:492:PRO:O	1:A:494:SER:N	2.37	0.57
1:C:2089:GLU:OE1	1:C:2089:GLU:N	2.37	0.56
1:A:1888:GLU:N	1:A:1888:GLU:OE1	2.38	0.56
1:A:1330:SER:OG	1:A:1333:GLU:OE1	2.19	0.55
1:A:1326:ASN:ND2	1:A:1350:LYS:O	2.39	0.55
1:A:1286:PRO:O	1:A:1308:PHE:HA	2.07	0.55
1:C:1888:GLU:OE1	1:C:1888:GLU:N	2.38	0.55
1:A:1198:ARG:NH1	1:A:1229:ASP:OD2	2.40	0.54
1:C:960:ILE:O	1:C:964:GLY:N	2.40	0.54
1:A:1309:ASN:OD1	2:B:2249:ASP:CG	2.46	0.54
1:C:1267:GLU:N	1:C:1267:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1036:SER:OG	1:C:1077:ASN:OD1	2.27	0.53
1:A:370:ILE:HB	1:A:371:PRO:HD3	1.92	0.52
2:D:2272:SER:OG	2:D:2273:GLU:OE1	2.25	0.52
1:A:781:LEU:HA	1:A:785:ALA:HB3	1.90	0.52
2:D:2310:GLU:OE1	2:D:2313:GLN:NE2	2.43	0.52
1:A:1842:GLU:OE1	1:A:1842:GLU:N	2.42	0.51
1:A:689:GLU:N	1:A:689:GLU:OE1	2.44	0.51
1:C:1312:LYS:N	1:C:1787:SER:OG	2.36	0.51
2:B:2371:ASP:OD2	2:D:2319:LYS:NZ	2.42	0.51
1:C:960:ILE:HA	1:C:963:ASP:HB3	1.93	0.51
1:C:1284:LEU:HD11	1:C:1308:PHE:HB3	1.94	0.50
1:A:539:LEU:HD22	1:A:550:LEU:HD21	1.94	0.50
1:A:892:GLN:HA	1:A:895:VAL:HG23	1.94	0.49
1:C:966:LEU:O	1:C:970:ARG:NE	2.39	0.49
1:A:1308:PHE:C	1:A:1310:GLY:H	2.12	0.49
1:A:1255:ASP:OD1	1:A:1256:VAL:N	2.44	0.49
1:C:1449:PRO:HG3	1:C:1488:TYR:HD2	1.78	0.48
1:C:370:ILE:HB	1:C:371:PRO:HD3	1.96	0.47
1:C:1068:ASP:OD1	1:C:1069:ILE:N	2.47	0.47
2:D:2165:ARG:HB3	2:D:2300:VAL:HG13	1.97	0.47
1:C:1474:ASP:OD1	1:C:1475:ASP:N	2.47	0.47
1:C:740:ILE:HG22	1:C:844:THR:HB	1.96	0.46
1:A:780:ILE:O	1:A:785:ALA:N	2.46	0.46
1:A:1267:GLU:OE1	1:A:1267:GLU:N	2.44	0.46
1:C:532:LEU:HD22	1:C:577:ARG:HD3	1.98	0.46
1:A:1022:LEU:HD21	1:A:1116:CYS:SG	2.56	0.45
1:C:1724:THR:OG1	1:C:1725:SER:N	2.49	0.45
1:A:1474:ASP:OD1	1:A:1475:ASP:N	2.49	0.45
1:A:1724:THR:OG1	1:A:1725:SER:N	2.48	0.45
1:C:1370:SER:O	1:C:1514:CYS:N	2.49	0.45
1:A:1502:LEU:O	1:A:1504:LYS:N	2.43	0.45
1:C:1255:ASP:OD1	1:C:1256:VAL:N	2.47	0.45
1:C:1875:THR:OG1	1:C:1876:LEU:N	2.48	0.45
2:D:2262:GLN:N	2:D:2293:ILE:O	2.50	0.45
1:C:1612:VAL:HG22	1:C:1613:GLU:N	2.31	0.44
1:C:473:ILE:HG12	1:C:475:TYR:H	1.82	0.44
1:C:932:ARG:NH2	1:C:989:TYR:OH	2.50	0.44
1:A:842:ALA:O	1:A:876:GLY:N	2.49	0.44
1:A:1202:MET:N	1:A:1202:MET:SD	2.90	0.44
1:A:509:ALA:O	1:A:666:ARG:NH2	2.50	0.44
1:C:1585:LEU:HD21	1:C:1594:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:812:ASP:O	1:C:816:SER:N	2.50	0.44
1:C:1623:LYS:O	1:C:1625:THR:N	2.48	0.44
1:A:588:LEU:O	1:A:590:GLY:N	2.51	0.44
1:A:787:ASN:ND2	1:A:789:LEU:HG	2.32	0.44
1:C:1049:GLU:N	1:C:1049:GLU:OE1	2.45	0.44
1:A:1245:ASP:OD1	1:A:1248:GLY:N	2.47	0.43
1:C:1311:PHE:HD1	1:C:1787:SER:HB3	1.83	0.43
1:C:1541:ILE:HG23	1:C:1542:GLU:HG2	2.01	0.43
1:C:1975:THR:O	1:C:1978:ASP:N	2.52	0.43
2:B:2308:THR:OG1	2:B:2310:GLU:OE1	2.23	0.43
1:A:539:LEU:HD23	1:A:555:PHE:CE2	2.54	0.43
2:D:2279:LYS:HE3	2:D:2319:LYS:HA	2.01	0.43
1:C:1494:ARG:NH1	1:C:1757:GLU:OE2	2.51	0.42
1:C:1842:GLU:N	1:C:1842:GLU:OE1	2.43	0.42
1:C:1899:ARG:NH2	1:C:1919:SER:OG	2.47	0.42
1:A:423:ILE:O	1:A:425:PRO:HD3	2.19	0.42
1:A:569:GLU:OE1	1:A:572:ARG:NH2	2.47	0.42
1:C:711:LYS:O	1:C:713:ARG:NH1	2.52	0.42
1:A:1326:ASN:ND2	1:A:1353:SER:OG	2.52	0.42
1:A:500:ASN:HB2	1:A:501:PRO:HD2	2.02	0.42
2:D:2192:LYS:HA	2:D:2195:GLU:HG2	2.01	0.42
1:A:789:LEU:HD11	1:A:793:LEU:HD12	2.01	0.42
1:A:1793:ASP:HB2	1:A:1798:GLY:HA3	2.02	0.42
1:C:457:LYS:HD2	1:C:460:TYR:CE1	2.55	0.42
2:B:2241:ILE:HG13	2:B:2280:LEU:HD21	2.02	0.42
1:C:449:PRO:HG2	1:C:465:ILE:HG23	2.00	0.42
1:A:1457:ARG:O	1:A:1760:ASN:ND2	2.42	0.41
1:C:1370:SER:OG	1:C:1371:GLY:N	2.53	0.41
1:A:1387:HIS:HB2	1:A:1470:LEU:HD22	2.01	0.41
1:A:1585:LEU:HD21	1:A:1594:VAL:HG21	2.01	0.41
1:A:1117:LEU:HA	1:A:1125:THR:HG21	2.03	0.41
1:C:1286:PRO:HD3	2:D:2346:THR:HB	2.02	0.41
1:A:554:ALA:HA	1:A:627:LEU:HD22	2.03	0.41
1:A:895:VAL:HG12	1:A:896:GLN:N	2.36	0.41
1:C:1236:LEU:HD11	1:C:1258:PHE:HB3	2.02	0.41
1:C:1618:VAL:HB	1:C:1619:PRO:HD3	2.03	0.41
1:C:1428:LEU:HD21	1:C:2093:PHE:HB3	2.02	0.41
2:B:2262:GLN:N	2:B:2293:ILE:O	2.53	0.41
1:C:1471:MET:SD	1:C:1495:MET:HG3	2.61	0.41
1:C:1959:ASN:HA	1:C:1962:VAL:HG12	2.03	0.41
1:C:613:ASP:OD2	1:C:617:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2295:SER:HA	2:D:2300:VAL:HG12	2.03	0.41
1:A:2077:ARG:N	1:A:2122:GLU:O	2.46	0.41
1:A:2022:LEU:HG	1:A:2026:GLU:HB2	2.02	0.40
1:A:963:ASP:OD2	1:A:968:LYS:N	2.54	0.40
2:D:2166:LEU:HD13	2:D:2191:LYS:HA	2.02	0.40
1:C:1955:VAL:HB	1:C:1956:PRO:HD3	2.03	0.40
1:A:1494:ARG:NH2	1:A:1756:ASN:OD1	2.54	0.40
1:A:2064:ILE:HB	1:A:2067:VAL:HB	2.03	0.40
1:A:1430:ASN:ND2	1:A:1952:GLU:O	2.54	0.40

All (1) 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:C:1051:LYS:NZ	1:C:1357:GLU:OE1[3_444]	2.17	0.03

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	1844/1897 (97%)	1704 (92%)	132 (7%)	8 (0%)	39	80
1	C	1844/1897 (97%)	1698 (92%)	141 (8%)	5 (0%)	46	83
2	B	246/270 (91%)	229 (93%)	17 (7%)	0	100	100
2	D	246/270 (91%)	225 (92%)	20 (8%)	1 (0%)	39	80
All	All	4180/4334 (96%)	3856 (92%)	310 (7%)	14 (0%)	46	83

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	SER

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Mol	Chain	Res	Type
1	A	895	VAL
1	A	964	GLY
1	A	1307	SER
1	A	1308	PHE
1	A	1309	ASN
1	C	895	VAL
1	C	1309	ASN
1	C	1329	ILE
1	A	1329	ILE
2	D	2280	LEU
1	C	424	PRO
1	A	791	PRO
1	C	1044	VAL

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	1671/1709 (98%)	1667 (100%)	4 (0%)	95	97
1	C	1671/1709 (98%)	1667 (100%)	4 (0%)	95	97
2	B	220/237 (93%)	219 (100%)	1 (0%)	92	96
2	D	220/237 (93%)	219 (100%)	1 (0%)	92	96
All	All	3782/3892 (97%)	3772 (100%)	10 (0%)	94	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	789	LEU
1	A	1304	ILE
1	A	1306	VAL
1	A	1488	TYR
2	B	2258	TRP
1	C	953	MET
1	C	1102	HIS
1	C	1348	PHE

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Mol	Chain	Res	Type
1	C	1542	GLU
2	D	2258	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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

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	1850/1897 (97%)	0.40	57 (3%)	52	41	141, 156, 170, 178	0
1	C	1850/1897 (97%)	0.44	87 (4%)	35	27	143, 158, 169, 180	0
2	B	248/270 (91%)	0.63	22 (8%)	12	9	148, 159, 168, 175	0
2	D	248/270 (91%)	0.62	21 (8%)	13	10	148, 160, 169, 177	0
All	All	4196/4334 (96%)	0.45	187 (4%)	37	28	141, 157, 169, 180	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	LEU	8.1
1	C	438	SER	5.7
1	C	437	SER	4.9
1	A	1825	THR	4.7
2	D	2239	SER	4.6
1	A	1662	SER	4.3
1	A	303	TYR	4.2
1	A	1616	GLN	4.1
1	A	442	THR	4.1
1	A	769	LYS	4.0
1	C	590	GLY	3.9
1	C	821	ALA	3.9
1	A	768	HIS	3.9
1	C	394	THR	3.8
1	C	525	SER	3.8
1	C	439	LYS	3.8
1	A	362	LEU	3.7
1	C	875	ALA	3.7
1	C	442	THR	3.7
1	A	440	LEU	3.7
1	C	1145	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1179	VAL	3.6
1	C	823	GLY	3.6
1	C	1535	PHE	3.5
1	C	1356	PHE	3.5
1	A	660	TYR	3.4
1	C	841	PRO	3.3
2	B	2258	TRP	3.3
1	C	1382	LEU	3.3
1	A	285	ILE	3.2
2	B	2334	SER	3.2
2	B	2280	LEU	3.2
1	C	636	ILE	3.2
1	C	840	LEU	3.2
1	A	1173	LEU	3.2
1	A	278	SER	3.1
2	D	2200	LYS	3.1
1	C	317	LEU	3.1
1	C	1509	VAL	3.1
2	D	2395	PHE	3.1
2	B	2284	LYS	3.0
2	D	2362	MET	3.0
1	C	637	HIS	3.0
1	A	273	SER	3.0
2	D	2369	GLU	3.0
1	C	1395	ALA	2.9
1	C	609	PRO	2.9
1	A	308	VAL	2.9
1	A	826	GLN	2.9
1	C	275	SER	2.9
1	C	2097	GLU	2.9
1	C	1607	TRP	2.9
2	D	2368	GLN	2.9
2	D	2164	LEU	2.9
1	C	1991	ASP	2.9
1	A	391	PHE	2.9
1	C	303	TYR	2.9
2	B	2242	PRO	2.9
1	C	522	PRO	2.9
2	B	2192	LYS	2.8
2	B	2204	ALA	2.8
1	A	1661	VAL	2.8
1	C	1366	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	785	ALA	2.8
1	A	281	GLU	2.8
1	A	1307	SER	2.8
1	C	745	HIS	2.7
1	C	468	PRO	2.7
2	B	2269	MET	2.7
1	A	1125	THR	2.7
2	D	2240	ASN	2.7
1	C	783	THR	2.7
2	B	2236	VAL	2.7
1	C	1115	ILE	2.7
2	D	2242	PRO	2.7
1	C	1683	LEU	2.7
1	C	660	TYR	2.6
2	B	2282	ALA	2.6
1	A	290	GLU	2.6
2	D	2148	SER	2.6
1	C	530	ILE	2.6
1	C	285	ILE	2.6
1	C	919	ASN	2.6
1	A	694	PHE	2.6
1	C	803	THR	2.6
1	C	1297	TRP	2.6
2	D	2167	LYS	2.5
1	C	707	PHE	2.5
2	B	2273	GLU	2.5
1	A	727	TYR	2.5
1	A	357	PHE	2.5
1	A	279	ASN	2.5
1	A	1591	CYS	2.5
1	A	848	LYS	2.5
1	C	294	GLN	2.5
1	C	754	ALA	2.5
1	C	1539	GLU	2.5
1	A	1510	CYS	2.5
1	C	822	ASP	2.5
1	C	885	GLU	2.5
1	C	781	LEU	2.5
1	C	1985	GLN	2.5
1	C	824	LEU	2.5
1	C	313	SER	2.5
1	A	770	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1472	ILE	2.4
1	A	1519	ARG	2.4
1	C	708	CYS	2.4
1	C	866	GLN	2.4
1	C	283	VAL	2.4
1	C	827	VAL	2.4
1	C	836	TRP	2.4
1	A	803	THR	2.4
1	A	1297	TRP	2.4
1	A	1208	ALA	2.3
1	A	309	ILE	2.3
1	A	1379	MET	2.3
1	A	292	PHE	2.3
2	D	2238	ILE	2.3
2	B	2241	ILE	2.3
1	A	1534	ASN	2.3
1	C	366	THR	2.3
2	B	2183	TYR	2.3
1	C	872	LEU	2.3
2	D	2374	PHE	2.3
2	D	2392	PHE	2.3
1	C	393	GLU	2.3
1	A	358	TRP	2.3
2	B	2202	GLN	2.3
1	A	743	PHE	2.3
2	B	2349	PHE	2.2
1	C	593	ARG	2.2
1	A	2119	LEU	2.2
1	A	928	ASN	2.2
1	C	334	LEU	2.2
1	A	1149	PHE	2.2
1	C	591	ASP	2.2
2	B	2193	PHE	2.2
1	C	912	PHE	2.2
1	C	882	THR	2.2
1	A	1445	LEU	2.2
1	C	441	MET	2.2
1	A	1416	PHE	2.2
1	A	1323	LEU	2.2
1	C	1396	VAL	2.2
1	C	1634	LYS	2.2
1	C	304	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	903	ASN	2.2
1	C	634	ASP	2.2
1	A	313	SER	2.2
1	A	741	ILE	2.2
2	D	2231	GLY	2.1
1	C	1111	ALA	2.1
1	C	1298	TRP	2.1
1	C	562	PRO	2.1
1	C	293	LEU	2.1
1	C	367	GLU	2.1
1	C	1415	ARG	2.1
1	C	1031	LEU	2.1
2	D	2293	ILE	2.1
1	C	1606	GLU	2.1
2	B	2194	ILE	2.1
2	B	2173	ALA	2.1
2	B	2380	LEU	2.1
2	D	2228	PRO	2.1
1	A	1368	VAL	2.1
1	C	1089	PHE	2.1
1	A	1791	VAL	2.1
1	C	617	ARG	2.1
2	B	2206	PHE	2.1
1	A	1183	ILE	2.1
1	C	1686	ASN	2.1
2	B	2283	ASP	2.1
2	B	2228	PRO	2.0
2	D	2253	LEU	2.0
1	A	2144	CYS	2.0
1	C	2007	LYS	2.0
2	D	2273	GLU	2.0
2	D	2302	LEU	2.0
1	A	293	LEU	2.0
1	A	1343	PHE	2.0
2	D	2289	ILE	2.0
1	C	738	ASN	2.0
1	A	327	PRO	2.0
1	A	320	ILE	2.0
1	C	828	LEU	2.0
1	C	1444	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.