



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:00 AM EDT

PDB ID : 5M5P / pdb_00005m5p
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

<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

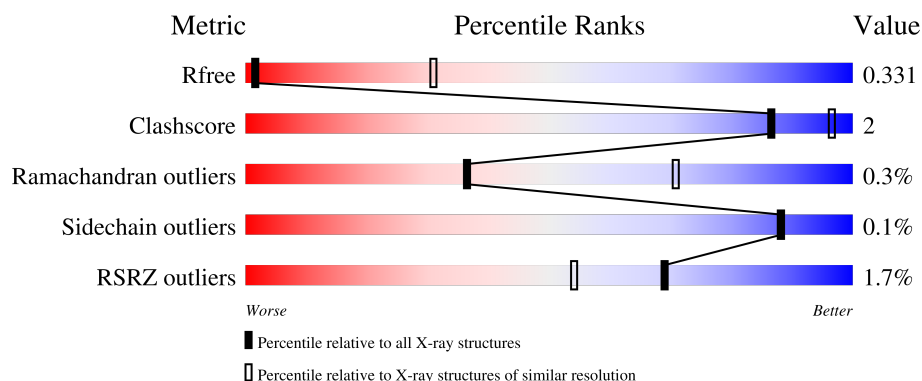
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	1897	0% 92% 5%
1	C	1897	2% 92% 5%
2	B	270	88% 8%
2	D	270	2% 84% 7% 8%

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

Continued on next page...

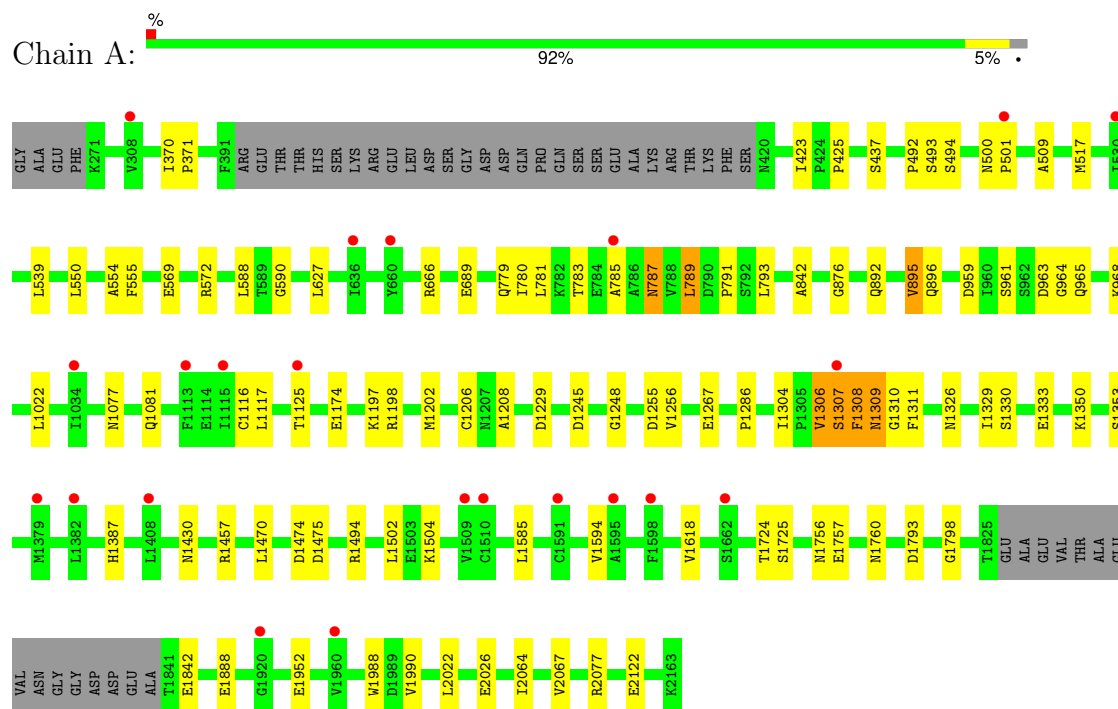
Continued from previous page...

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

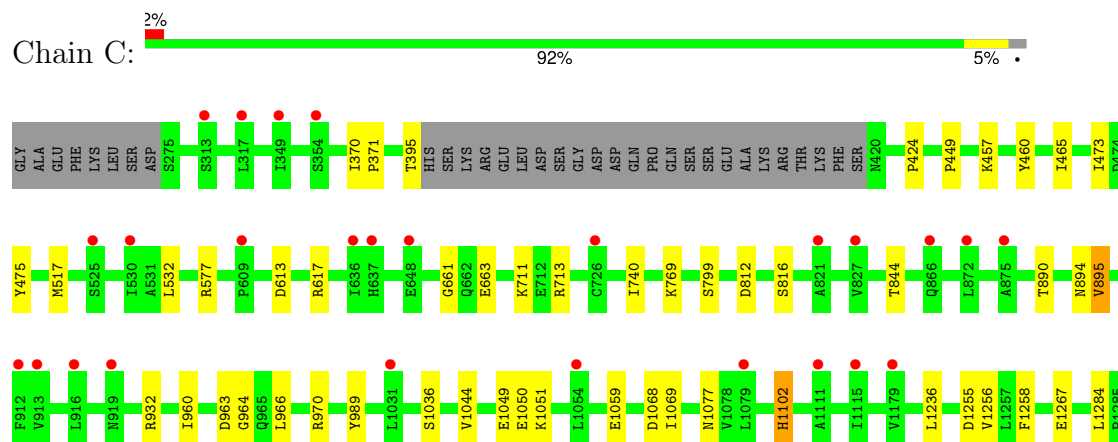
3 Residue-property plots [i](#)

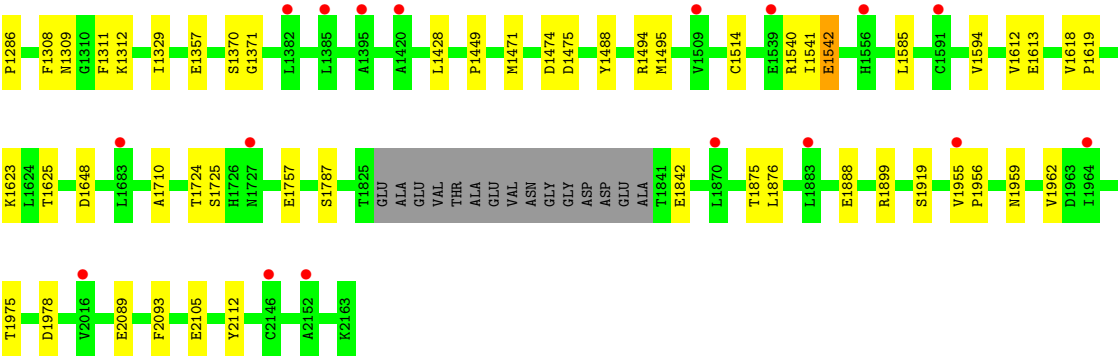
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pre-mRNA-splicing helicase BRR2

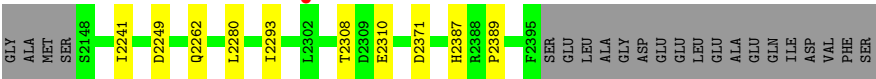
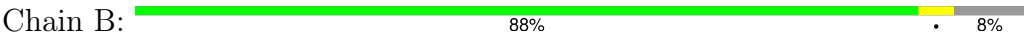


• Molecule 1: Pre-mRNA-splicing helicase BRR2

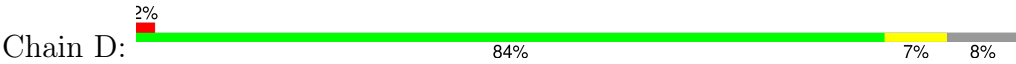




● Molecule 2: Pre-mRNA-splicing factor 8



● 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 95.50 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.50-4.20) 99.8 (95.50-4.20)	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 1.9_1692	Depositor
R, R_{free}	0.307 , 0.335 0.309 , 0.331	Depositor DCC
R_{free} test set	2667 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	147.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 117.7	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	0.86	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	0.30	0/15149	0.70	4/20529 (0.0%)
1	C	0.31	0/15152	0.70	1/20534 (0.0%)
2	B	0.28	0/2038	0.65	0/2764
2	D	0.28	0/2038	0.67	0/2764
All	All	0.30	0/34377	0.70	5/46591 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	517	MET	N-CA-C	5.44	116.54	108.60
1	A	787	ASN	N-CA-C	5.38	118.31	109.76
1	A	1618	VAL	CB-CA-C	-5.32	108.71	114.35
1	A	437	SER	CB-CA-C	-5.12	110.69	116.63
1	A	517	MET	N-CA-C	5.02	115.93	108.60

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	67	0
1	C	14838	14878	14875	57	1
2	B	1989	1952	1951	7	0
2	D	1989	1952	1951	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33651	33658	33651	141	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 (141) 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:890:THR:OG1	1:C:894:ASN:OD1	2.17	0.61
1:C:1050:GLU:N	1:C:1050:GLU:OE1	2.33	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:1309:ASN:OD1	2:B:2249:ASP:CG	2.46	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:O	1:C:395:THR:HG22	2.04	0.57
1:A:492:PRO:O	1:A:494:SER:N	2.37	0.57
1:A:1330:SER:OG	1:A:1333:GLU:OE1	2.19	0.56
1:C:2089:GLU:N	1:C:2089:GLU:OE1	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1888:GLU:OE1	1:A:1888:GLU:N	2.38	0.56
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
2:D:2272:SER:OG	2:D:2273:GLU:OE1	2.25	0.55
1:C:1888:GLU:N	1:C:1888:GLU:OE1	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:C:1267:GLU:N	1:C:1267:GLU:OE1	2.41	0.54
1:A:1308:PHE:C	1:A:1310:GLY:H	2.12	0.54
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
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:689:GLU:OE1	1:A:689:GLU:N	2.44	0.51
1:A:1842:GLU:OE1	1:A:1842:GLU:N	2.42	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: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
2:D:2269:MET:HE2	2:D:2269:MET:HA	1.97	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
2:D:2269:MET:HE3	2:D:2305:TYR:CD2	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:509:ALA:O	1:A:666:ARG:NH2	2.50	0.44
1:A:1202:MET:SD	1:A:1202:MET:N	2.90	0.44
1:C:812:ASP:O	1:C:816:SER:N	2.50	0.44
1:C:1585:LEU:HD21	1:C:1594:VAL:HG21	1.99	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:OE1	1:C:1049:GLU:N	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:OE1	1:C:1842:GLU:N	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:C:1102:HIS:ND1	1:C:1102:HIS:C	2.77	0.42
1:A:500:ASN:HB2	1:A:501:PRO:HD2	2.02	0.42
1:A:1326:ASN:ND2	1:A:1353:SER:OG	2.52	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:2105:GLU:OE1	1:C:2112:TYR:OH	2.33	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:787:ASN:CG	1:A:789:LEU:HG	2.45	0.41
1:A:1387:HIS:HB2	1:A:1470:LEU:HD22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:2387:HIS:C	2:B:2389:PRO:HD3	2.46	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
2:B:2262:GLN:N	2:B:2293:ILE:O	2.53	0.41
1:C:613:ASP:OD2	1:C:617:ARG:NH2	2.54	0.41
1:C:661:GLY:C	1:C:663:GLU:H	2.29	0.41
1:C:894:ASN:O	1:C:895:VAL:C	2.64	0.41
1:C:1236:LEU:HD11	1:C:1258:PHE:HB3	2.02	0.41
1:C:1312:LYS:H	1:C:1787:SER:HG	1.63	0.41
1:C:1428:LEU:HD21	1:C:2093:PHE:HB3	2.02	0.41
1:C:1471:MET:SD	1:C:1495:MET:HG3	2.61	0.41
1:C:1618:VAL:HB	1:C:1619:PRO:HD3	2.03	0.41
1:C:1959:ASN:HA	1:C:1962:VAL:HG12	2.03	0.41
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:963:ASP:OD2	1:A:968:LYS:N	2.54	0.40
1:A:2022:LEU:HG	1:A:2026:GLU:HB2	2.02	0.40
2:D:2166:LEU:HD13	2:D:2191:LYS:HA	2.02	0.40
1:A:1988:TRP:C	1:A:1990:VAL:H	2.29	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%)	30	66
1	C	1844/1897 (97%)	1698 (92%)	141 (8%)	5 (0%)	36	71
2	B	246/270 (91%)	229 (93%)	17 (7%)	0	100	100
2	D	246/270 (91%)	225 (92%)	20 (8%)	1 (0%)	30	66
All	All	4180/4334 (96%)	3856 (92%)	310 (7%)	14 (0%)	36	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	SER
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%)	1668 (100%)	3 (0%)	87	85
1	C	1671/1709 (98%)	1669 (100%)	2 (0%)	88	88
2	B	220/237 (93%)	220 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	220/237 (93%)	220 (100%)	0	100	100
All	All	3782/3892 (97%)	3777 (100%)	5 (0%)	88	88

All (5) 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	C	1102	HIS
1	C	1542	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	905	GLN
1	A	1349	ASN
1	A	1352	GLN
1	A	1435	ASN
1	A	1565	GLN
1	A	1864	GLN
1	A	1931	GLN
2	B	2150	ASN
2	B	2237	GLN
1	C	326	ASN
1	C	620	ASN
1	C	804	HIS
1	C	903	ASN
1	C	911	GLN
1	C	1143	ASN
1	C	1363	ASN
1	C	1386	ASN
1	C	1387	HIS
1	C	1390	GLN
1	C	1517	ASN
1	C	1547	ASN
1	C	1556	HIS
1	C	1931	GLN
2	D	2237	GLN
2	D	2313	GLN

5.3.3 RNA [i](#)

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 ⓘ

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%)	0.16	22 (1%) 76 61	140, 157, 168, 177	0
1	C	1850/1897 (97%)	0.28	43 (2%) 61 47	143, 158, 169, 179	0
2	B	248/270 (91%)	0.11	1 (0%) 88 77	148, 159, 168, 174	0
2	D	248/270 (91%)	0.22	5 (2%) 65 50	147, 160, 168, 177	0
All	All	4196/4334 (96%)	0.22	71 (1%) 69 54	140, 157, 168, 179	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1115	ILE	5.0
1	C	1382	LEU	4.8
1	C	1509	VAL	4.4
2	D	2164	LEU	4.4
1	C	1111	ALA	3.8
1	C	1179	VAL	3.7
1	C	872	LEU	3.6
1	C	916	LEU	3.5
1	A	1510	CYS	3.3
1	A	1595	ALA	3.2
1	C	636	ILE	3.1
1	C	354	SER	3.0
1	A	1382	LEU	3.0
1	A	785	ALA	2.9
1	C	637	HIS	2.8
1	C	1955	VAL	2.8
1	C	2152	ALA	2.7
1	C	919	ASN	2.6
1	A	1662	SER	2.6
1	C	317	LEU	2.5
1	C	1031	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1539	GLU	2.5
1	C	912	PHE	2.5
1	C	1883	LEU	2.5
2	D	2244	ILE	2.5
1	C	525	SER	2.5
1	C	1395	ALA	2.5
1	C	866	GLN	2.5
2	D	2302	LEU	2.5
1	C	2016	VAL	2.5
2	D	2239	SER	2.5
1	C	1385	LEU	2.5
1	C	609	PRO	2.5
1	A	660	TYR	2.4
1	A	1598	PHE	2.4
1	C	530	ILE	2.4
1	C	1870	LEU	2.4
1	A	636	ILE	2.4
1	A	1509	VAL	2.3
1	A	1591	CYS	2.3
1	A	1920	GLY	2.3
1	A	530	ILE	2.3
1	C	648	GLU	2.3
1	C	913	VAL	2.3
1	A	1115	ILE	2.3
1	C	1683	LEU	2.2
1	C	1556	HIS	2.2
1	C	821	ALA	2.2
1	C	875	ALA	2.2
1	A	501	PRO	2.2
1	C	1727	ASN	2.2
1	C	313	SER	2.2
1	C	1964	ILE	2.2
1	C	1591	CYS	2.2
1	A	1307	SER	2.2
1	A	308	VAL	2.1
2	D	2236	VAL	2.1
1	C	1079	LEU	2.1
1	A	1960	VAL	2.1
1	C	827	VAL	2.1
1	A	1034	ILE	2.1
1	A	1408	LEU	2.1
1	A	1125	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1054	LEU	2.1
2	B	2302	LEU	2.1
1	A	1113	PHE	2.1
1	C	726	CYS	2.0
1	C	349	ILE	2.0
1	A	1379	MET	2.0
1	C	1420	ALA	2.0
1	C	2146	CYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.