



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 08:13 AM EST

PDB ID : 4I43
Title : Crystal structure of Prp8:Aar2 complex
Authors : Galej, W.P.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on : 2012-11-27
Resolution : 2.00 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

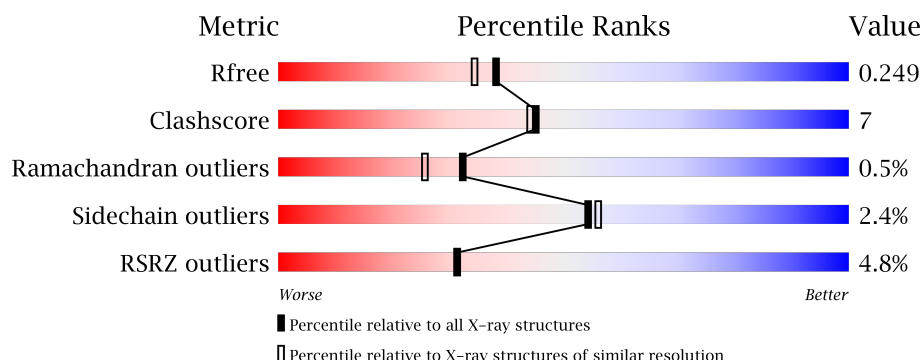
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 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	384	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	1564	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14902 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 A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2751	1754	447	533	17			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	ALA	-	EXPRESSION TAG	UNP P32357
A	357	ALA	-	EXPRESSION TAG	UNP P32357
A	358	GLY	-	EXPRESSION TAG	UNP P32357
A	359	LYS	-	EXPRESSION TAG	UNP P32357
A	360	VAL	-	EXPRESSION TAG	UNP P32357
A	361	ALA	-	EXPRESSION TAG	UNP P32357
A	362	ARG	-	EXPRESSION TAG	UNP P32357
A	363	GLY	-	EXPRESSION TAG	UNP P32357
A	364	SER	-	EXPRESSION TAG	UNP P32357
A	365	ARG	-	EXPRESSION TAG	UNP P32357
A	366	SER	-	EXPRESSION TAG	UNP P32357
A	367	GLY	-	EXPRESSION TAG	UNP P32357
A	368	SER	-	EXPRESSION TAG	UNP P32357
A	369	GLU	-	EXPRESSION TAG	UNP P32357
A	370	ASN	-	EXPRESSION TAG	UNP P32357
A	371	LEU	-	EXPRESSION TAG	UNP P32357
A	372	TYR	-	EXPRESSION TAG	UNP P32357
A	373	PHE	-	EXPRESSION TAG	UNP P32357
A	374	GLN	-	EXPRESSION TAG	UNP P32357
A	375	GLY	-	EXPRESSION TAG	UNP P32357
A	376	SER	-	EXPRESSION TAG	UNP P32357
A	377	HIS	-	EXPRESSION TAG	UNP P32357
A	378	HIS	-	EXPRESSION TAG	UNP P32357
A	379	HIS	-	EXPRESSION TAG	UNP P32357
A	380	HIS	-	EXPRESSION TAG	UNP P32357
A	381	HIS	-	EXPRESSION TAG	UNP P32357
A	382	HIS	-	EXPRESSION TAG	UNP P32357

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Chain	Residue	Modelled	Actual	Comment	Reference
A	383	HIS	-	EXPRESSION TAG	UNP P32357
A	384	HIS	-	EXPRESSION TAG	UNP P32357

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1407	Total	C	N	O	S	0	0	0
			11481	7384	1936	2124	37			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	850	MET	-	EXPRESSION TAG	UNP P33334
B	851	ALA	-	EXPRESSION TAG	UNP P33334
B	852	ARG	-	EXPRESSION TAG	UNP P33334
B	853	ALA	-	EXPRESSION TAG	UNP P33334
B	854	LYS	-	EXPRESSION TAG	UNP P33334
B	855	ARG	-	EXPRESSION TAG	UNP P33334
B	856	ARG	-	EXPRESSION TAG	UNP P33334
B	857	TRP	-	EXPRESSION TAG	UNP P33334
B	858	LYS	-	EXPRESSION TAG	UNP P33334
B	859	LYS	-	EXPRESSION TAG	UNP P33334
B	860	ASN	-	EXPRESSION TAG	UNP P33334
B	861	PHE	-	EXPRESSION TAG	UNP P33334
B	862	ILE	-	EXPRESSION TAG	UNP P33334
B	863	ALA	-	EXPRESSION TAG	UNP P33334
B	864	VAL	-	EXPRESSION TAG	UNP P33334
B	865	SER	-	EXPRESSION TAG	UNP P33334
B	866	ALA	-	EXPRESSION TAG	UNP P33334
B	867	ALA	-	EXPRESSION TAG	UNP P33334
B	868	ASN	-	EXPRESSION TAG	UNP P33334
B	869	ARG	-	EXPRESSION TAG	UNP P33334
B	870	PHE	-	EXPRESSION TAG	UNP P33334
B	871	LYS	-	EXPRESSION TAG	UNP P33334
B	872	LYS	-	EXPRESSION TAG	UNP P33334
B	873	ILE	-	EXPRESSION TAG	UNP P33334
B	874	SER	-	EXPRESSION TAG	UNP P33334
B	875	SER	-	EXPRESSION TAG	UNP P33334
B	876	SER	-	EXPRESSION TAG	UNP P33334
B	877	GLY	-	EXPRESSION TAG	UNP P33334
B	878	ALA	-	EXPRESSION TAG	UNP P33334
B	879	LEU	-	EXPRESSION TAG	UNP P33334

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Chain	Residue	Modelled	Actual	Comment	Reference
B	880	GLY	-	EXPRESSION TAG	UNP P33334
B	881	SER	-	EXPRESSION TAG	UNP P33334
B	882	GLY	-	EXPRESSION TAG	UNP P33334
B	883	SER	-	EXPRESSION TAG	UNP P33334
B	884	GLY	-	EXPRESSION TAG	UNP P33334

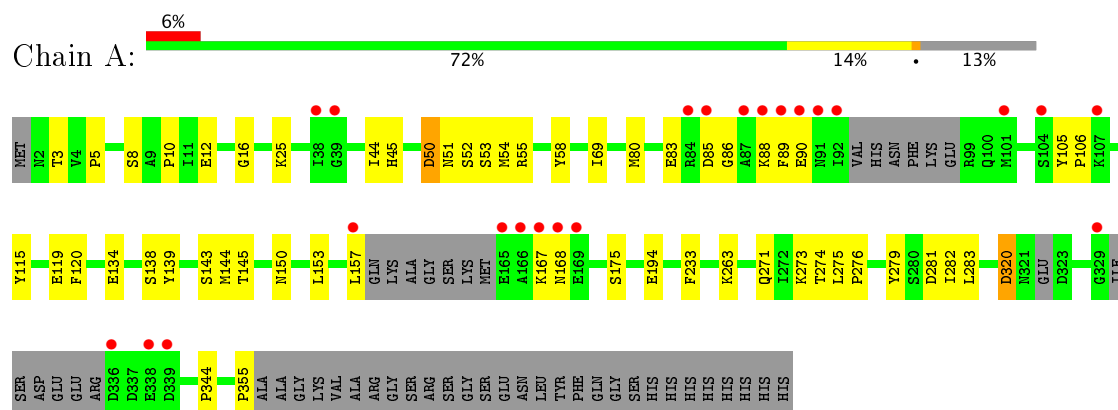
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total	O	0	0
			156	156		
3	B	514	Total	O	0	0
			514	514		

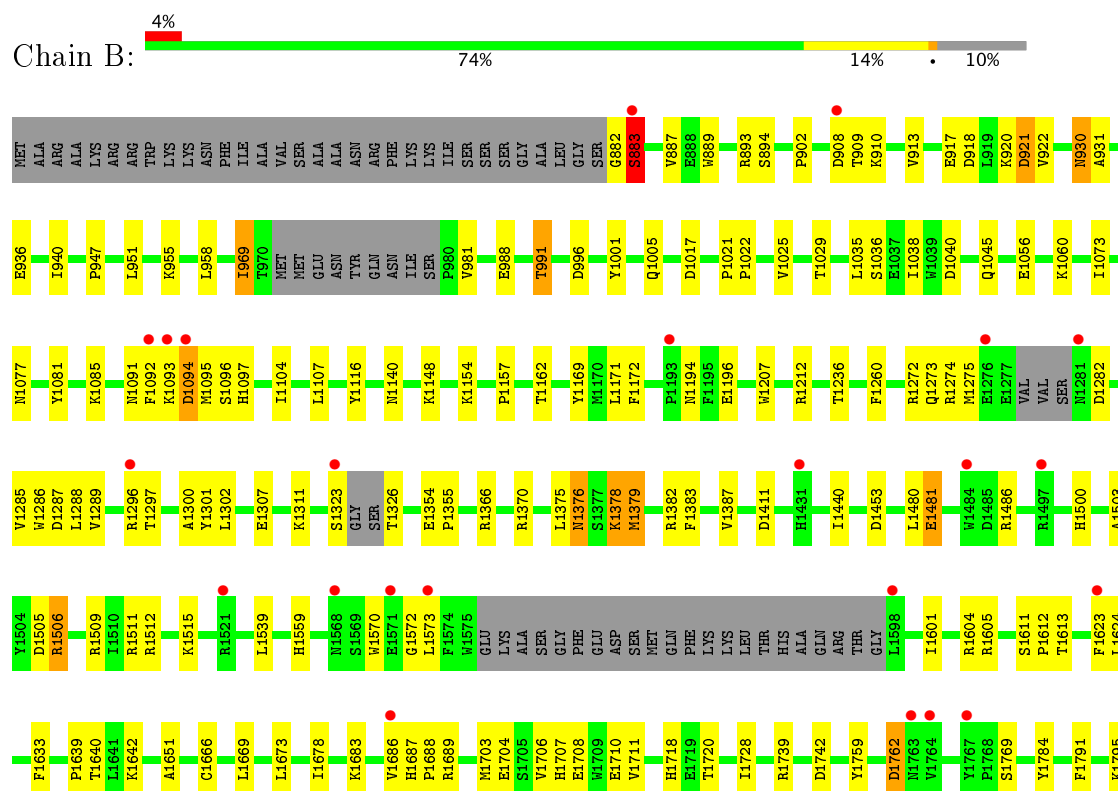
3 Residue-property plots

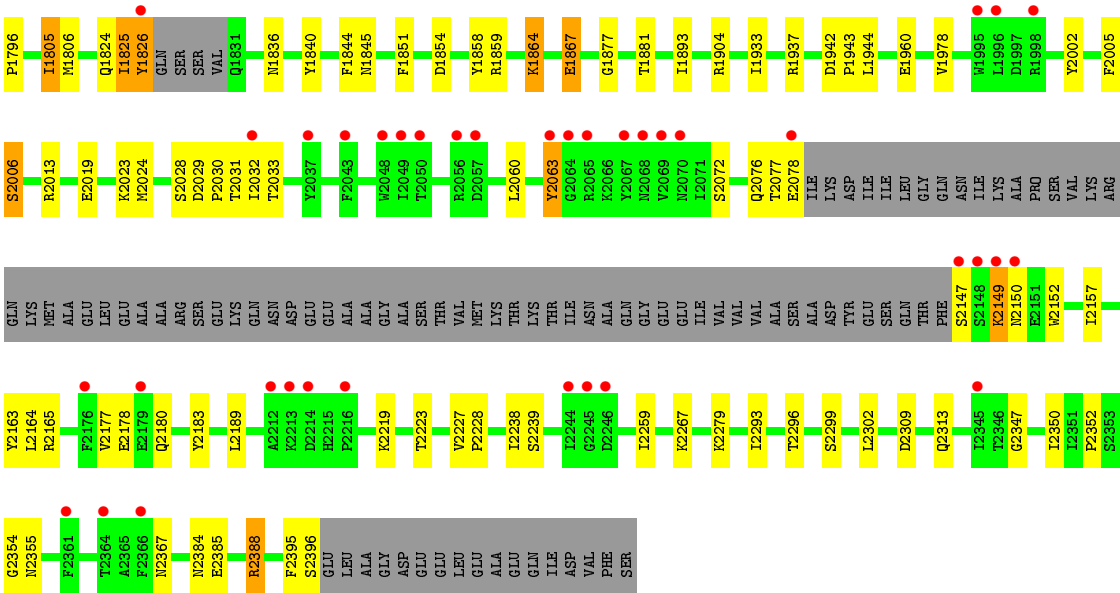
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: A1 cistron-splicing factor AAR2



• Molecule 2: Pre-mRNA-splicing factor 8





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.86Å 158.59Å 220.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.00 48.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.30-2.00) 100.0 (48.30-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.198 , 0.249 0.202 , 0.249	Depositor DCC
R_{free} test set	7044 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14902	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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](#)

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	0.39	0/2818	0.50	0/3806
2	B	0.35	0/11756	0.51	0/15941
All	All	0.36	0/14574	0.51	0/19747

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1825	ILE	Peptide

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	2751	0	2597	41	0
2	B	11481	0	11410	177	0
3	A	156	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	514	0	0	22	1
All	All	14902	0	14007	209	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 7.

All (209) 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)
2:B:1207:TRP:O	2:B:1212:ARG:NH1	2.06	0.89
1:A:282:ILE:HG13	2:B:1604:ARG:HD3	1.56	0.87
2:B:918:ASP:OD1	2:B:1515:LYS:NZ	2.12	0.83
2:B:1091:ASN:OD1	2:B:1096:SER:HB3	1.78	0.82
2:B:1383:PHE:HE2	2:B:1387:VAL:HG21	1.45	0.82
2:B:1017:ASP:HA	2:B:1509:ARG:HG3	1.65	0.79
2:B:1759:TYR:O	2:B:1762:ASP:HB2	1.83	0.78
2:B:1854:ASP:OD1	2:B:1937:ARG:HD3	1.87	0.75
2:B:1383:PHE:CE2	2:B:1387:VAL:HG21	2.21	0.74
2:B:882:GLY:O	2:B:883:SER:HB3	1.86	0.74
1:A:282:ILE:HG13	2:B:1604:ARG:CD	2.17	0.73
2:B:1687:HIS:HD2	2:B:1689:ARG:H	1.39	0.71
2:B:2385:GLU:HG3	2:B:2388:ARG:NH2	2.06	0.70
2:B:2227:VAL:CG1	2:B:2239:SER:OG	2.41	0.69
1:A:145:THR:HG23	2:B:1651:ALA:HB2	1.77	0.66
2:B:1453:ASP:OD2	2:B:1486:ARG:HD2	1.95	0.66
2:B:1718:HIS:CE1	3:B:3002:HOH:O	2.48	0.65
2:B:2149:LYS:HG3	2:B:2150:ASN:N	2.12	0.63
2:B:1025:VAL:O	2:B:1029:THR:HG23	1.99	0.63
2:B:908:ASP:OD1	2:B:951:LEU:HD22	1.99	0.63
2:B:1825:ILE:O	2:B:1826:TYR:CD1	2.52	0.63
2:B:1375:LEU:O	2:B:1376:ASN:HB2	1.98	0.62
2:B:1060:LYS:HG3	3:B:2579:HOH:O	1.99	0.61
2:B:1383:PHE:HE2	2:B:1387:VAL:CG2	2.12	0.61
3:A:551:HOH:O	2:B:1864:LYS:HE2	2.00	0.61
2:B:2077:THR:O	2:B:2078:GLU:CB	2.49	0.60
2:B:913:VAL:O	2:B:917:GLU:HG2	2.02	0.59
2:B:908:ASP:OD2	2:B:951:LEU:HD13	2.03	0.59
2:B:1687:HIS:CD2	2:B:1688:PRO:HD2	2.38	0.58
2:B:2227:VAL:HG13	2:B:2239:SER:OG	2.03	0.58
2:B:889:TRP:O	2:B:893:ARG:HG2	2.03	0.58
1:A:105:TYR:CD1	1:A:106:PRO:HD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:CG2	2:B:1651:ALA:HB2	2.34	0.57
2:B:1669:LEU:HD13	2:B:1703:MET:HE3	1.87	0.57
2:B:2019:GLU:HG2	2:B:2023:LYS:HD2	1.87	0.57
1:A:8:SER:OG	1:A:10:PRO:HD3	2.04	0.57
1:A:139:TYR:CD2	1:A:144:MET:HE1	2.41	0.56
2:B:1505:ASP:OD1	2:B:1511:ARG:NH2	2.38	0.56
1:A:120:PHE:O	3:A:542:HOH:O	2.17	0.56
2:B:883:SER:O	2:B:887:VAL:HG23	2.06	0.56
2:B:1287:ASP:HB3	2:B:1296:ARG:HD2	1.87	0.56
2:B:2077:THR:O	2:B:2078:GLU:HB2	2.05	0.56
2:B:1085:LYS:CE	3:B:2749:HOH:O	2.54	0.56
1:A:115:TYR:O	1:A:119:GLU:N	2.38	0.56
1:A:273:LYS:NZ	3:A:536:HOH:O	2.39	0.55
1:A:355:PRO:HB2	2:B:2267:LYS:HD3	1.89	0.55
1:A:69:ILE:HD13	1:A:80:MET:HA	1.88	0.55
2:B:1370:ARG:NH1	3:B:2966:HOH:O	2.40	0.55
2:B:1559:HIS:HD2	2:B:1613:THR:OG1	1.89	0.55
2:B:1311:LYS:NZ	3:B:2818:HOH:O	2.38	0.54
2:B:2076:GLN:OE1	2:B:2076:GLN:N	2.40	0.54
2:B:1378:LYS:HE2	2:B:1623:PHE:HE2	1.73	0.54
2:B:1687:HIS:CD2	2:B:1689:ARG:H	2.23	0.54
2:B:2013:ARG:HE	2:B:2078:GLU:HG2	1.73	0.54
1:A:275:LEU:HD11	1:A:283:LEU:HD22	1.89	0.54
2:B:2302:LEU:N	2:B:2302:LEU:HD12	2.21	0.54
2:B:1056:GLU:O	2:B:1060:LYS:HG2	2.08	0.54
1:A:282:ILE:HD11	2:B:1640:THR:HB	1.89	0.54
2:B:2028:SER:O	2:B:2030:PRO:HD3	2.09	0.53
2:B:1711:VAL:HG12	2:B:1791:PHE:HB3	1.90	0.53
1:A:153:LEU:HD12	1:A:157:LEU:HD13	1.91	0.52
2:B:2259:ILE:HD11	2:B:2293:ILE:HD11	1.91	0.52
2:B:1669:LEU:HD22	2:B:1703:MET:CE	2.40	0.52
2:B:2163:TYR:CE2	2:B:2164:LEU:HD23	2.45	0.52
1:A:50:ASP:O	1:A:52:SER:N	2.41	0.52
2:B:1382:ARG:NH1	3:B:3013:HOH:O	2.43	0.51
2:B:1624:LEU:C	2:B:1624:LEU:HD23	2.31	0.51
1:A:276:PRO:HG2	1:A:279:TYR:CD2	2.46	0.51
2:B:1500:HIS:NE2	2:B:2267:LYS:HE2	2.25	0.51
2:B:1273:GLN:HG2	3:B:2670:HOH:O	2.10	0.50
2:B:1854:ASP:OD1	2:B:1937:ARG:CD	2.59	0.50
1:A:12:GLU:HG3	1:A:25:LYS:HA	1.93	0.50
1:A:16:GLY:HA3	1:A:45:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1867:GLU:N	2:B:1867:GLU:CD	2.64	0.50
2:B:1669:LEU:HD22	2:B:1703:MET:HE3	1.93	0.50
2:B:1704:GLU:HG2	3:B:2570:HOH:O	2.11	0.50
2:B:2152:TRP:CZ3	2:B:2388:ARG:HD3	2.47	0.50
1:A:50:ASP:C	1:A:52:SER:H	2.15	0.50
2:B:1795:LYS:HB3	2:B:1796:PRO:HD3	1.94	0.50
2:B:1605:ARG:NE	2:B:1824:GLN:OE1	2.43	0.50
2:B:2077:THR:O	2:B:2078:GLU:CG	2.60	0.49
2:B:902:PRO:O	2:B:955:LYS:NZ	2.44	0.49
2:B:2395:PHE:O	2:B:2396:SER:C	2.50	0.49
2:B:1960:GLU:HA	2:B:1960:GLU:OE1	2.11	0.49
2:B:1570:TRP:CZ2	2:B:1572:GLY:HA2	2.47	0.49
2:B:1942:ASP:HB2	2:B:1943:PRO:HD3	1.94	0.49
2:B:1104:ILE:HG22	2:B:1107:LEU:HD13	1.94	0.49
2:B:909:THR:HG23	2:B:910:LYS:N	2.27	0.49
2:B:1140:ASN:OD1	2:B:1148:LYS:NZ	2.28	0.49
2:B:1378:LYS:O	2:B:1379:MET:HB3	2.13	0.48
2:B:1651:ALA:HB3	3:B:2621:HOH:O	2.12	0.48
2:B:2354:GLY:O	2:B:2355:ASN:HB2	2.14	0.48
1:A:53:SER:O	2:B:1642:LYS:NZ	2.46	0.48
2:B:1286:TRP:CE2	2:B:1302:LEU:HD11	2.48	0.48
2:B:1104:ILE:CG2	2:B:1107:LEU:HD13	2.43	0.48
1:A:3:THR:HG22	1:A:5:PRO:HD3	1.95	0.48
2:B:2024:MET:SD	2:B:2157:ILE:HG22	2.53	0.48
2:B:2183:TYR:CE2	2:B:2219:LYS:HD3	2.49	0.47
2:B:1666:CYS:SG	2:B:1683:LYS:HE3	2.55	0.47
2:B:2309:ASP:O	2:B:2313:GLN:HG2	2.15	0.47
2:B:2063:TYR:CD1	2:B:2063:TYR:C	2.87	0.47
1:A:344:PRO:HB3	2:B:1858:TYR:CE2	2.50	0.47
2:B:1503:ALA:O	2:B:1506:ARG:NH1	2.45	0.47
1:A:320:ASP:OD1	1:A:320:ASP:N	2.47	0.47
2:B:1867:GLU:H	2:B:1867:GLU:CD	2.18	0.47
2:B:920:LYS:O	2:B:921:ASP:C	2.53	0.47
1:A:86:GLY:O	1:A:90:GLU:HG3	2.15	0.47
2:B:2177:VAL:CG2	2:B:2180:GLN:HB2	2.44	0.47
2:B:2189:LEU:HD11	2:B:2347:GLY:HA3	1.97	0.47
2:B:2228:PRO:HD3	2:B:2352:PRO:HG3	1.97	0.46
2:B:1091:ASN:OD1	2:B:1096:SER:CB	2.57	0.46
2:B:2019:GLU:CG	2:B:2023:LYS:HD2	2.45	0.46
1:A:194:GLU:OE1	3:A:506:HOH:O	2.20	0.46
2:B:1005:GLN:OE1	2:B:1506:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:ASP:OD2	2:B:1511:ARG:HD3	2.14	0.46
2:B:1687:HIS:CD2	2:B:1688:PRO:CD	2.98	0.46
2:B:1021:PRO:HB2	2:B:1022:PRO:HD3	1.98	0.46
2:B:920:LYS:HG3	2:B:940:ILE:HG21	1.96	0.46
2:B:958:LEU:HA	2:B:1081:TYR:CD2	2.50	0.46
2:B:1706:VAL:HG12	2:B:1707:HIS:N	2.31	0.46
2:B:2060:LEU:HA	2:B:2063:TYR:HB3	1.98	0.46
2:B:988:GLU:O	2:B:991:THR:CG2	2.63	0.46
2:B:1035:LEU:CD1	2:B:1171:LEU:CD2	2.94	0.45
2:B:1286:TRP:HB2	2:B:1300:ALA:HB3	1.97	0.45
2:B:1739:ARG:HD3	3:B:2501:HOH:O	2.15	0.45
1:A:16:GLY:O	1:A:44:ILE:HA	2.17	0.45
2:B:1673:LEU:HA	2:B:1678:ILE:HB	1.99	0.45
2:B:1639:PRO:C	2:B:1640:THR:HG23	2.36	0.45
1:A:150:ASN:ND2	1:A:175:SER:OG	2.49	0.45
2:B:2177:VAL:HG23	2:B:2180:GLN:HB2	1.98	0.45
2:B:2223:THR:HG21	2:B:2350:ILE:CG1	2.47	0.45
2:B:920:LYS:O	2:B:922:VAL:N	2.51	0.44
1:A:54:MET:SD	1:A:143:SER:HB3	2.57	0.44
2:B:1720:THR:HA	3:B:2897:HOH:O	2.18	0.44
1:A:83:GLU:CG	1:A:89:PHE:HB2	2.48	0.44
2:B:1092:PHE:HE1	2:B:1093:LYS:HE3	1.82	0.44
2:B:2149:LYS:HA	2:B:2149:LYS:HZ3	1.83	0.44
2:B:988:GLU:OE1	3:B:2695:HOH:O	2.21	0.44
2:B:1840:TYR:HH	2:B:2005:PHE:HD2	1.63	0.44
2:B:930:ASN:CG	2:B:931:ALA:N	2.71	0.44
1:A:134:GLU:N	1:A:134:GLU:OE1	2.34	0.44
2:B:1366:ARG:HD2	3:B:2885:HOH:O	2.16	0.44
2:B:1904:ARG:HH11	2:B:1904:ARG:HG2	1.83	0.44
2:B:1036:SER:OG	2:B:1154:LYS:CE	2.66	0.44
2:B:1035:LEU:HB2	2:B:1038:ILE:HB	1.99	0.44
2:B:1272:ARG:O	2:B:1274:ARG:N	2.50	0.44
2:B:1687:HIS:CD2	2:B:1688:PRO:N	2.86	0.44
2:B:909:THR:HG23	2:B:910:LYS:H	1.81	0.44
2:B:2165:ARG:O	2:B:2299:SER:HA	2.18	0.43
2:B:1085:LYS:HE2	3:B:2749:HOH:O	2.18	0.43
2:B:1157:PRO:O	2:B:1172:PHE:HA	2.18	0.43
1:A:355:PRO:CB	2:B:2267:LYS:HD3	2.48	0.43
2:B:1077:ASN:ND2	3:B:3010:HOH:O	2.28	0.43
2:B:1708:GLU:O	3:B:2962:HOH:O	2.21	0.43
2:B:1093:LYS:HB3	2:B:1094:ASP:H	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1666:CYS:SG	2:B:1683:LYS:CE	3.06	0.43
2:B:1307:GLU:O	2:B:1311:LYS:HG3	2.18	0.43
2:B:1383:PHE:CE2	2:B:1387:VAL:CG2	2.94	0.43
2:B:1480:LEU:O	2:B:1481:GLU:C	2.56	0.43
2:B:969:ILE:HA	2:B:981:VAL:O	2.18	0.43
1:A:50:ASP:O	1:A:50:ASP:CG	2.56	0.43
2:B:1029:THR:HG22	2:B:1260:PHE:HZ	1.84	0.42
1:A:55:ARG:HD2	1:A:233:PHE:O	2.19	0.42
1:A:271:GLN:O	1:A:274:THR:HG22	2.18	0.42
2:B:2002:TYR:O	2:B:2006:SER:OG	2.38	0.42
2:B:1060:LYS:HE2	2:B:1060:LYS:HB3	1.84	0.42
2:B:1710:GLU:HG2	2:B:1728:ILE:HD13	2.01	0.42
2:B:1836:ASN:O	2:B:1840:TYR:N	2.53	0.42
2:B:1851:PHE:O	2:B:1881:THR:HA	2.20	0.42
2:B:1236:THR:HG22	2:B:1236:THR:O	2.20	0.42
2:B:1411:ASP:O	2:B:1559:HIS:HE1	2.01	0.42
2:B:1805:ILE:N	2:B:1805:ILE:HD13	2.34	0.42
2:B:2033:THR:OG1	3:B:2979:HOH:O	2.22	0.42
2:B:1859:ARG:HD2	2:B:1877:GLY:HA2	2.01	0.42
2:B:1844:PHE:CE1	2:B:2002:TYR:HA	2.54	0.42
2:B:1040:ASP:OD2	2:B:1045:GLN:NE2	2.48	0.42
2:B:1073:ILE:HD13	2:B:1116:TYR:CE1	2.54	0.42
2:B:1601:ILE:HG23	2:B:1605:ARG:HD2	2.01	0.42
2:B:988:GLU:O	2:B:991:THR:HG23	2.20	0.42
2:B:1354:GLU:N	2:B:1355:PRO:CD	2.83	0.42
1:A:85:ASP:HB3	1:A:88:LYS:HB3	2.02	0.41
2:B:1512:ARG:HG3	3:B:2868:HOH:O	2.19	0.41
2:B:2238:ILE:HG22	2:B:2239:SER:O	2.20	0.41
2:B:1624:LEU:HD21	2:B:1633:PHE:CD1	2.55	0.41
1:A:120:PHE:CE2	1:A:263:LYS:HE3	2.55	0.41
2:B:1285:VAL:HG12	2:B:1301:TYR:CD2	2.56	0.41
2:B:1001:TYR:HA	2:B:1506:ARG:HG3	2.02	0.41
2:B:2157:ILE:CD1	3:B:2943:HOH:O	2.68	0.41
2:B:1092:PHE:CE1	2:B:1093:LYS:HG3	2.56	0.41
2:B:1194:ASN:HB2	2:B:1196:GLU:HG3	2.03	0.41
2:B:1784:TYR:CD1	2:B:1806:MET:HG3	2.55	0.41
1:A:275:LEU:CD1	1:A:283:LEU:HD22	2.49	0.41
2:B:1611:SER:N	2:B:1612:PRO:CD	2.84	0.41
2:B:1933:ILE:HG21	2:B:1944:LEU:HD21	2.03	0.41
1:A:167:LYS:O	1:A:168:ASN:C	2.59	0.41
2:B:1162:THR:HG22	2:B:1169:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1440:ILE:HD11	2:B:1539:LEU:HD21	2.02	0.41
2:B:2157:ILE:HD13	3:B:2943:HOH:O	2.21	0.41
2:B:2029:ASP:HB3	2:B:2032:ILE:HD12	2.03	0.41
2:B:1893:ILE:HD12	2:B:1978:VAL:HG22	2.03	0.41
1:A:105:TYR:CD1	1:A:106:PRO:CD	3.03	0.40
2:B:1289:VAL:HG22	2:B:1296:ARG:HH11	1.86	0.40
2:B:1378:LYS:O	2:B:1379:MET:CB	2.69	0.40
2:B:2177:VAL:O	2:B:2177:VAL:HG23	2.20	0.40
2:B:2279:LYS:HE2	3:B:2931:HOH:O	2.22	0.40
2:B:1376:ASN:HB3	3:B:3014:HOH:O	2.21	0.40
2:B:1710:GLU:HG2	2:B:1728:ILE:CD1	2.51	0.40
2:B:1742:ASP:C	2:B:1742:ASP:OD1	2.60	0.40
1:A:58:TYR:HA	1:A:138:SER:O	2.22	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)
3:B:2720:HOH:O	3:B:2814:HOH:O[3_655]	2.10	0.10

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	324/384 (84%)	306 (94%)	16 (5%)	2 (1%)	28	21
2	B	1393/1564 (89%)	1336 (96%)	50 (4%)	7 (0%)	32	26
All	All	1717/1948 (88%)	1642 (96%)	66 (4%)	9 (0%)	32	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	320	ASP
2	B	921	ASP
2	B	1376	ASN
2	B	883	SER
2	B	2384	ASN
2	B	1379	MET
2	B	1845	ASN
2	B	947	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	305/348 (88%)	303 (99%)	2 (1%)	87	90
2	B	1265/1397 (91%)	1229 (97%)	36 (3%)	49	49
All	All	1570/1745 (90%)	1532 (98%)	38 (2%)	54	56

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	281	ASP
2	B	883	SER
2	B	894	SER
2	B	930	ASN
2	B	936	GLU
2	B	969	ILE
2	B	991	THR
2	B	1094	ASP
2	B	1095	MET
2	B	1097	HIS
2	B	1275	MET
2	B	1282	ASP
2	B	1288	LEU
2	B	1297	THR

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Mol	Chain	Res	Type
2	B	1323	SER
2	B	1326	THR
2	B	1378	LYS
2	B	1481	GLU
2	B	1506	ARG
2	B	1573	LEU
2	B	1686	VAL
2	B	1762	ASP
2	B	1769	SER
2	B	1805	ILE
2	B	1826	TYR
2	B	1864	LYS
2	B	1867	GLU
2	B	2006	SER
2	B	2031	THR
2	B	2063	TYR
2	B	2072	SER
2	B	2147	SER
2	B	2149	LYS
2	B	2178	GLU
2	B	2296	THR
2	B	2367	ASN
2	B	2388	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	45	HIS
1	A	150	ASN
2	B	1516	GLN
2	B	1559	HIS
2	B	1687	HIS
2	B	2018	ASN
2	B	2070	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 carbohydrates 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	334/384 (86%)	0.35	23 (6%)	18 18	24, 45, 105, 133	0
2	B	1407/1564 (89%)	0.24	60 (4%)	36 36	23, 49, 85, 127	0
All	All	1741/1948 (89%)	0.26	83 (4%)	31 31	23, 48, 90, 133	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	ASN	6.3
2	B	1598	LEU	5.3
1	A	87	ALA	5.1
2	B	2147	SER	4.9
1	A	90	GLU	4.6
1	A	165	GLU	4.6
2	B	2148	SER	4.5
2	B	1092	PHE	4.3
1	A	336	ASP	4.2
2	B	2069	VAL	4.2
1	A	84	ARG	4.2
1	A	38	ILE	4.1
1	A	169	GLU	4.0
2	B	908	ASP	3.9
1	A	167	LYS	3.8
1	A	92	ILE	3.8
2	B	2068	ASN	3.7
1	A	166	ALA	3.7
2	B	1568	ASN	3.7
2	B	2070	ASN	3.7
2	B	2179	GLU	3.7
2	B	2213	LYS	3.6
1	A	157	LEU	3.6
2	B	2212	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	2043	PHE	3.5
1	A	338	GLU	3.5
2	B	1484	TRP	3.5
1	A	89	PHE	3.5
2	B	2064	GLY	3.5
2	B	1763	ASN	3.4
2	B	2057	ASP	3.3
2	B	2063	TYR	3.3
2	B	2150	ASN	3.2
1	A	101	MET	3.2
2	B	1826	TYR	3.2
1	A	329	GLY	3.1
1	A	168	ASN	3.1
2	B	2214	ASP	3.1
2	B	883	SER	3.1
2	B	1323	SER	3.0
2	B	1571	GLU	2.9
1	A	39	GLY	2.8
2	B	1193	PRO	2.7
2	B	2065	ARG	2.7
2	B	1296	ARG	2.7
2	B	2245	GLY	2.6
2	B	2361	PHE	2.5
2	B	2176	PHE	2.5
2	B	1995	TRP	2.5
2	B	1276	GLU	2.4
1	A	88	LYS	2.4
1	A	85	ASP	2.4
2	B	2067	TYR	2.4
2	B	2056	ARG	2.4
2	B	2078	GLU	2.4
2	B	1093	LYS	2.4
2	B	2049	ILE	2.4
2	B	2048	TRP	2.4
2	B	1998	ARG	2.3
2	B	2050	THR	2.3
2	B	1996	LEU	2.3
2	B	2345	ILE	2.3
2	B	1764	VAL	2.3
2	B	2216	PRO	2.3
2	B	1281	ASN	2.3
2	B	2037	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1094	ASP	2.2
2	B	1431	HIS	2.2
2	B	2366	PHE	2.2
2	B	2244	ILE	2.2
1	A	107	LYS	2.2
2	B	2032	ILE	2.1
1	A	104	SER	2.1
2	B	1497	ARG	2.1
2	B	1686	VAL	2.1
2	B	2246	ASP	2.1
2	B	1767	TYR	2.1
2	B	2149	LYS	2.1
2	B	2364	THR	2.1
2	B	1521	ARG	2.1
2	B	1623	PHE	2.1
1	A	339	ASP	2.1
2	B	1573	LEU	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.