



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 AM UTC

PDB ID : 4I43 / pdb_00004i43
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

<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

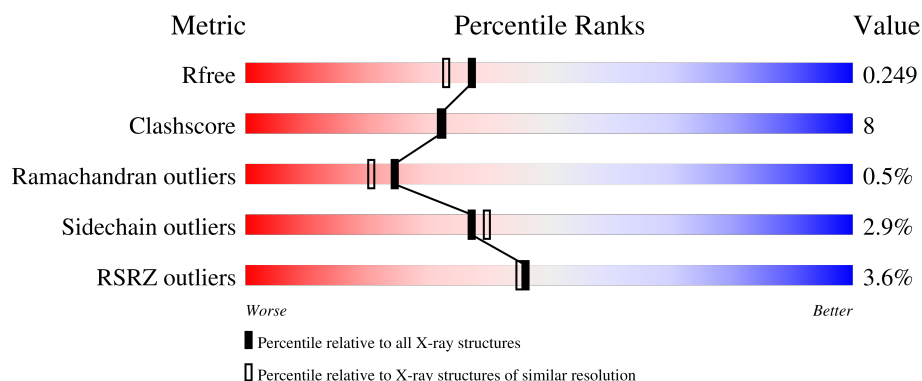
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	384	5% 72% 15% • 13%
2	B	1564	3% 73% 16% • 10%

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

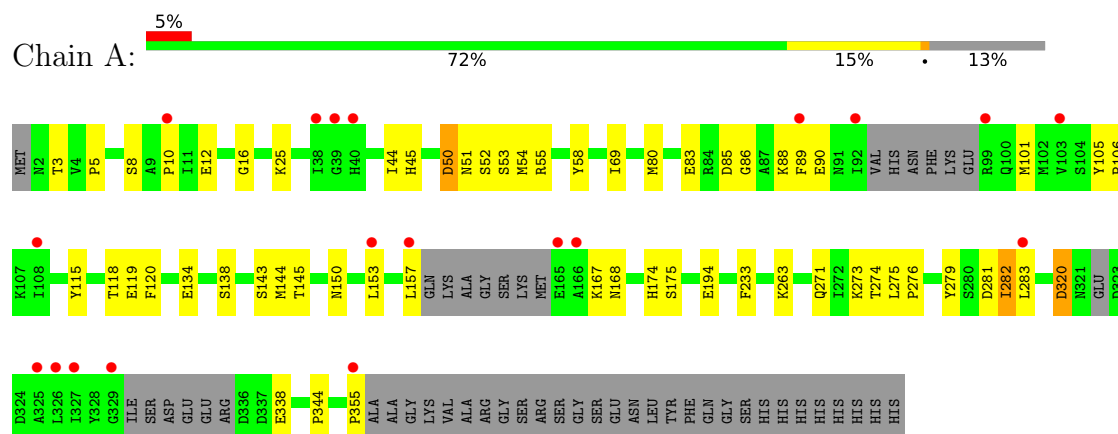
- Molecule 3 is water.

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

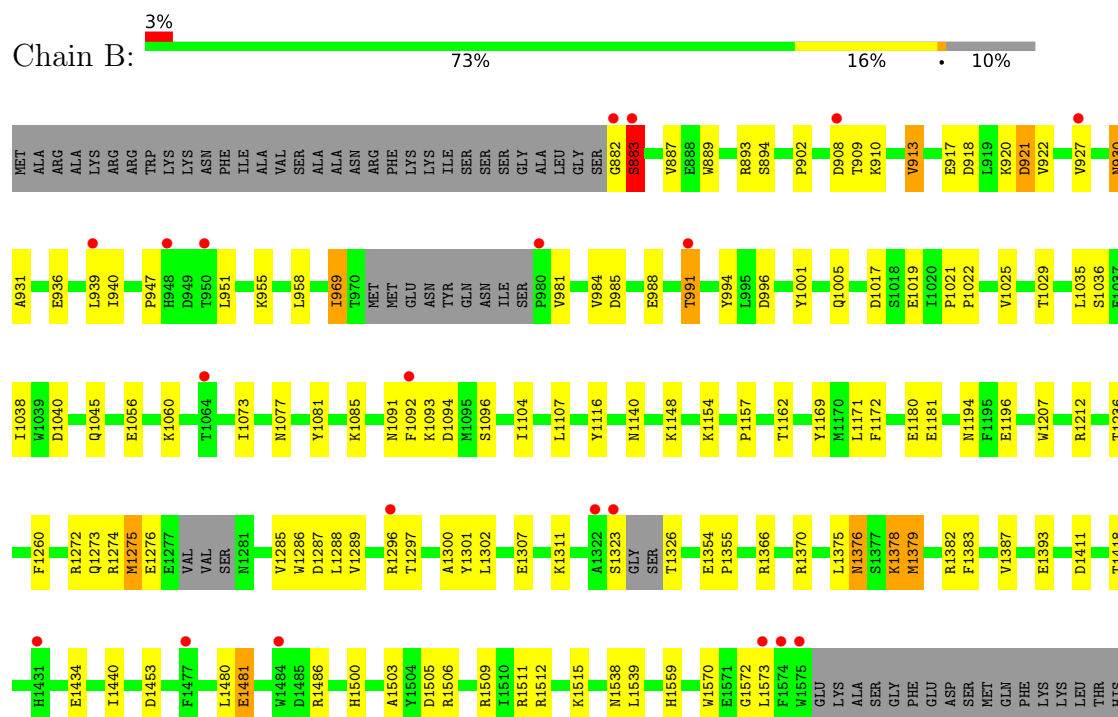
3 Residue-property plots [i](#)

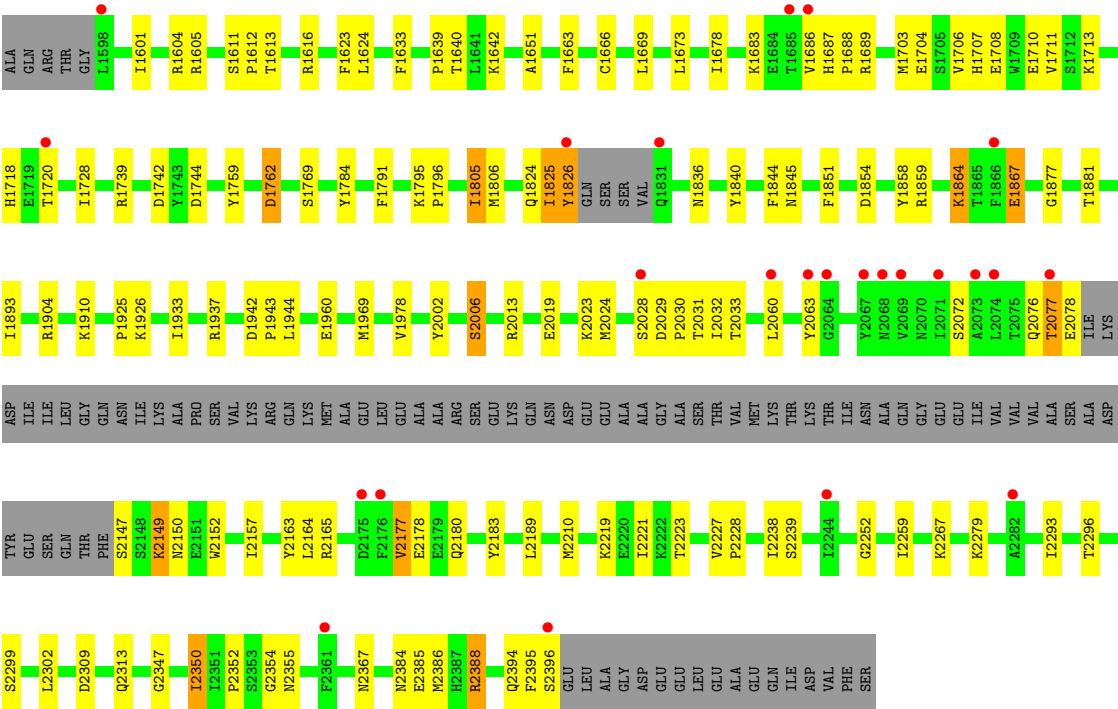
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 2: Pre-mRNA-splicing factor 4





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 (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	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

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	0.52	0/2818	0.72	0/3806
2	B	0.49	0/11756	0.71	1/15941 (0.0%)
All	All	0.49	0/14574	0.71	1/19747 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2077	THR	N-CA-C	5.92	116.36	108.38

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

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	43	0
2	B	11481	0	11410	191	0
3	A	156	0	0	4	0
3	B	514	0	0	21	1
All	All	14902	0	14007	225	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 8.

All (225) 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:1669:LEU:HD22	2:B:1703:MET:HE1	1.68	0.75
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
3:A:551:HOH:O	2:B:1864:LYS:HE2	2.00	0.61
2:B:1383:PHE:HE2	2:B:1387:VAL:CG2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:889:TRP:O	2:B:893:ARG:HG2	2.03	0.58
2:B:2227:VAL:HG13	2:B:2239:SER:OG	2.03	0.58
1:A:105:TYR:CD1	1:A:106:PRO:HD2	2.39	0.57
1:A:145:THR:CG2	2:B:1651:ALA:HB2	2.34	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
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
2:B:1624:LEU:C	2:B:1624:LEU:HD23	2.31	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:1867:GLU:CD	2:B:1867:GLU:N	2.64	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
1:A:50:ASP:C	1:A:52:SER:H	2.15	0.54
2:B:2076:GLN:N	2:B:2076:GLN:OE1	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
2:B:2395:PHE:O	2:B:2396:SER:C	2.50	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:1669:LEU:HD13	2:B:1703:MET:HE3	1.90	0.53
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:101:MET:HE2	1:A:101:MET:HA	1.91	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: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:1669:LEU:HD22	2:B:1703:MET:CE	2.40	0.52
2:B:2063:TYR:CD1	2:B:2063:TYR:C	2.87	0.52
2:B:920:LYS:O	2:B:921:ASP:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1867:GLU:CD	2:B:1867:GLU:H	2.18	0.51
2:B:1382:ARG:NH1	3:B:3013:HOH:O	2.43	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
1:A:144:MET:HE2	1:A:174:HIS:HA	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
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:902:PRO:O	2:B:955:LYS:NZ	2.44	0.49
2:B:1639:PRO:C	2:B:1640:THR:HG23	2.36	0.49
2:B:2077:THR:O	2:B:2078:GLU:CG	2.60	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:909:THR:HG23	2:B:910:LYS:N	2.27	0.49
2:B:1104:ILE:HG22	2:B:1107:LEU:HD13	1.94	0.49
2:B:930:ASN:CG	2:B:931:ALA:N	2.71	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:1480:LEU:O	2:B:1481:GLU:C	2.56	0.47
1:A:50:ASP:O	1:A:50:ASP:CG	2.56	0.47
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:2149:LYS:HA	2:B:2149:LYS:HZ3	1.80	0.47
2:B:2309:ASP:O	2:B:2313:GLN:HG2	2.15	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:N	1:A:320:ASP:OD1	2.47	0.47
1:A:86:GLY:O	1:A:90:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:996:ASP:OD2	2:B:1511:ARG:HD3	2.14	0.46
2:B:1005:GLN:OE1	2:B:1506:ARG:NH2	2.49	0.46
2:B:1687:HIS:CD2	2:B:1688:PRO:CD	2.98	0.46
2:B:920:LYS:HG3	2:B:940:ILE:HG21	1.96	0.46
2:B:1021:PRO:HB2	2:B:1022:PRO:HD3	1.98	0.46
2:B:958:LEU:HA	2:B:1081:TYR:CD2	2.50	0.46
2:B:988:GLU:O	2:B:991:THR:CG2	2.63	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
1:A:167:LYS:O	1:A:168:ASN:C	2.59	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:1742:ASP:C	2:B:1742:ASP:OD1	2.60	0.45
2:B:1969:MET:HE2	2:B:1969:MET:HA	1.98	0.45
2:B:2210:MET:HE2	2:B:2252:GLY:C	2.41	0.45
1:A:118:THR:O	1:A:119:GLU:C	2.60	0.45
1:A:150:ASN:ND2	1:A:175:SER:OG	2.49	0.45
2:B:1538:ASN:OD1	2:B:1538:ASN:C	2.60	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:988:GLU:OE1	3:B:2695:HOH:O	2.21	0.44
2:B:1092:PHE:HE1	2:B:1093:LYS:HE3	1.82	0.44
2:B:1925:PRO:O	2:B:1926:LYS:C	2.60	0.44
1:A:134:GLU:OE1	1:A:134:GLU:N	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:909:THR:HG23	2:B:910:LYS:H	1.81	0.44
2:B:1035:LEU:HB2	2:B:1038:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1036:SER:OG	2:B:1154:LYS:CE	2.66	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:994:TYR:CD1	2:B:994:TYR:C	2.95	0.44
2:B:2394:GLN:O	2:B:2395:PHE:C	2.60	0.44
2:B:1663:PHE:CD1	2:B:1663:PHE:C	2.95	0.44
2:B:2165:ARG:O	2:B:2299:SER:HA	2.18	0.43
1:A:355:PRO:CB	2:B:2267:LYS:HD3	2.48	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
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
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:969:ILE:HA	2:B:981:VAL:O	2.18	0.43
2:B:1678:ILE:HD13	2:B:1703:MET:HE2	2.00	0.43
2:B:1639:PRO:O	2:B:1640:THR:OG1	2.34	0.43
2:B:1029:THR:HG22	2:B:1260:PHE:HZ	1.84	0.42
2:B:1616:ARG:HD2	2:B:1744:ASP:CG	2.43	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:HB3	2:B:1060:LYS:HE2	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:O	2:B:1236:THR:HG22	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:1844:PHE:CE1	2:B:2002:TYR:HA	2.54	0.42
2:B:1859:ARG:HD2	2:B:1877:GLY:HA2	2.01	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:988:GLU:O	2:B:991:THR:HG23	2.20	0.42
2:B:1272:ARG:O	2:B:1273:GLN:C	2.63	0.42
2:B:1601:ILE:HG23	2:B:1605:ARG:HD2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1001:TYR:HA	2:B:1506:ARG:HG3	2.02	0.41
2:B:1285:VAL:HG12	2:B:1301:TYR:CD2	2.56	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
2:B:2002:TYR:CD1	2:B:2002:TYR:C	2.99	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
2:B:2386:MET:HE2	2:B:2386:MET:HB2	1.86	0.41
2:B:1162:THR:HG22	2:B:1169:TYR:HB2	2.02	0.41
2:B:1180:GLU:O	2:B:1181:GLU:C	2.62	0.41
2:B:1440:ILE:HD11	2:B:1539:LEU:HD21	2.02	0.41
2:B:2029:ASP:HB3	2:B:2032:ILE:HD12	2.03	0.41
2:B:2157:ILE:HD13	3:B:2943:HOH:O	2.21	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:HG23	2:B:2177:VAL:O	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
1:A:58:TYR:HA	1:A:138:SER:O	2.22	0.40
2:B:984:VAL:O	2:B:985:ASP:C	2.64	0.40
2:B:1275:MET:O	2:B:1276:GLU:C	2.65	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

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	324/384 (84%)	306 (94%)	16 (5%)	2 (1%)	21	17
2	B	1393/1564 (89%)	1336 (96%)	50 (4%)	7 (0%)	24	21
All	All	1717/1948 (88%)	1642 (96%)	66 (4%)	9 (0%)	24	21

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%)	301 (99%)	4 (1%)	61	68
2	B	1265/1397 (91%)	1223 (97%)	42 (3%)	33	34
All	All	1570/1745 (90%)	1524 (97%)	46 (3%)	37	40

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	281	ASP
1	A	282	ILE
1	A	338	GLU
2	B	883	SER
2	B	894	SER
2	B	913	VAL
2	B	927	VAL
2	B	930	ASN
2	B	936	GLU
2	B	939	LEU
2	B	969	ILE
2	B	991	THR
2	B	1019	GLU
2	B	1275	MET
2	B	1288	LEU
2	B	1297	THR
2	B	1323	SER
2	B	1326	THR
2	B	1378	LYS
2	B	1393	GLU
2	B	1418	THR
2	B	1434	GLU
2	B	1481	GLU
2	B	1573	LEU
2	B	1686	VAL
2	B	1713	LYS
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	1910	LYS
2	B	2006	SER
2	B	2031	THR
2	B	2072	SER
2	B	2147	SER
2	B	2149	LYS
2	B	2177	VAL
2	B	2178	GLU
2	B	2221	ILE

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Mol	Chain	Res	Type
2	B	2296	THR
2	B	2350	ILE
2	B	2367	ASN
2	B	2388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	45	HIS
1	A	136	GLN
1	A	150	ASN
1	A	206	ASN
1	A	300	ASN
1	A	343	ASN
1	A	353	GLN
2	B	907	ASN
2	B	1077	ASN
2	B	1087	ASN
2	B	1404	HIS
2	B	1559	HIS
2	B	1600	GLN
2	B	1687	HIS
2	B	2180	GLN
2	B	2240	ASN
2	B	2336	HIS

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

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	334/384 (86%)	0.30	19 (5%)	29 28	24, 45, 105, 133	0
2	B	1407/1564 (89%)	0.31	44 (3%)	51 50	23, 49, 85, 127	0
All	All	1741/1948 (89%)	0.31	63 (3%)	46 45	23, 48, 90, 133	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1826	TYR	4.3
1	A	157	LEU	4.1
1	A	92	ILE	3.9
2	B	2069	VAL	3.8
2	B	2063	TYR	3.7
1	A	39	GLY	3.7
2	B	1686	VAL	3.7
1	A	38	ILE	3.5
2	B	1598	LEU	3.5
2	B	908	ASP	3.5
2	B	1484	TRP	3.3
2	B	883	SER	3.2
1	A	325	ALA	3.1
2	B	927	VAL	3.1
1	A	89	PHE	3.1
1	A	326	LEU	3.1
2	B	1573	LEU	3.0
2	B	1296	ARG	2.9
2	B	2074	LEU	2.9
2	B	1323	SER	2.9
2	B	980	PRO	2.9
1	A	103	VAL	2.8
2	B	1574	PHE	2.7
1	A	327	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	2.5
2	B	1720	THR	2.5
1	A	99	ARG	2.5
2	B	1866	PHE	2.5
2	B	2077	THR	2.4
2	B	2064	GLY	2.4
2	B	2067	TYR	2.4
2	B	1477	PHE	2.4
1	A	166	ALA	2.3
2	B	2176	PHE	2.3
1	A	108	ILE	2.3
2	B	2244	ILE	2.3
2	B	2028	SER	2.3
2	B	1092	PHE	2.3
2	B	2071	ILE	2.3
1	A	165	GLU	2.2
2	B	2361	PHE	2.2
1	A	355	PRO	2.2
2	B	882	GLY	2.2
2	B	939	LEU	2.2
2	B	2060	LEU	2.2
2	B	2396	SER	2.2
2	B	991	THR	2.2
2	B	1064	THR	2.2
2	B	2073	ALA	2.1
1	A	283	LEU	2.1
2	B	1831	GLN	2.1
2	B	1322	ALA	2.1
2	B	2282	ALA	2.1
1	A	153	LEU	2.1
2	B	948	HIS	2.1
2	B	950	THR	2.1
2	B	1431	HIS	2.1
2	B	2068	ASN	2.0
1	A	40	HIS	2.0
2	B	1575	TRP	2.0
2	B	2175	ASP	2.0
1	A	10	PRO	2.0
2	B	1685	THR	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.