Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 06:26 AM EDT

PDB ID	:	5M52
Title	:	Crystal structure of yeast Brr2 full-lenght in complex with Prp8 Jab1 domain
Authors	:	Wollenhaupt, J.; Absmeier, E.; Becke, C.; Santos, K.F.; Wahl, M.C.
Deposited on	:	2016-10-20
Resolution	:	3.40 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:

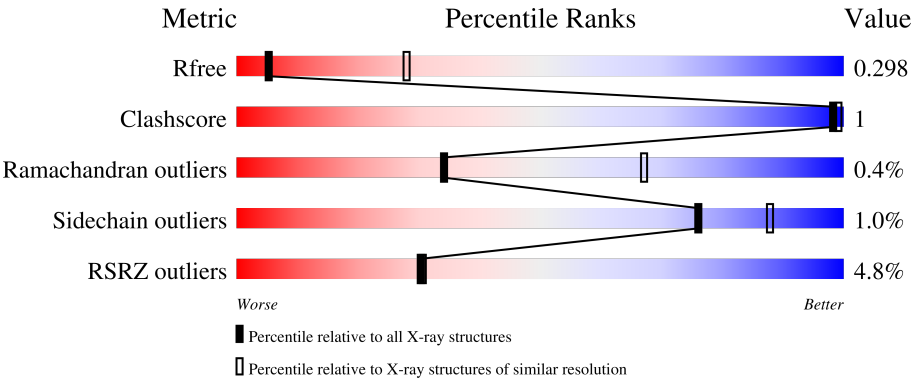
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	2163	4% 86% 12%
1	B	2163	5% 83% 14%
2	C	270	3% 97%
2	D	270	% 96%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34522 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 Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1910	Total	C	N	O	S	0	0	0
			15320	9818	2546	2898	58			
1	B	1862	Total	C	N	O	S	0	0	0
			14927	9563	2476	2832	56			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	266	Total	C	N	O	S	0	0	0
			2127	1368	341	412	6			
2	D	268	Total	C	N	O	S	0	0	0
			2138	1374	343	415	6			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is water.

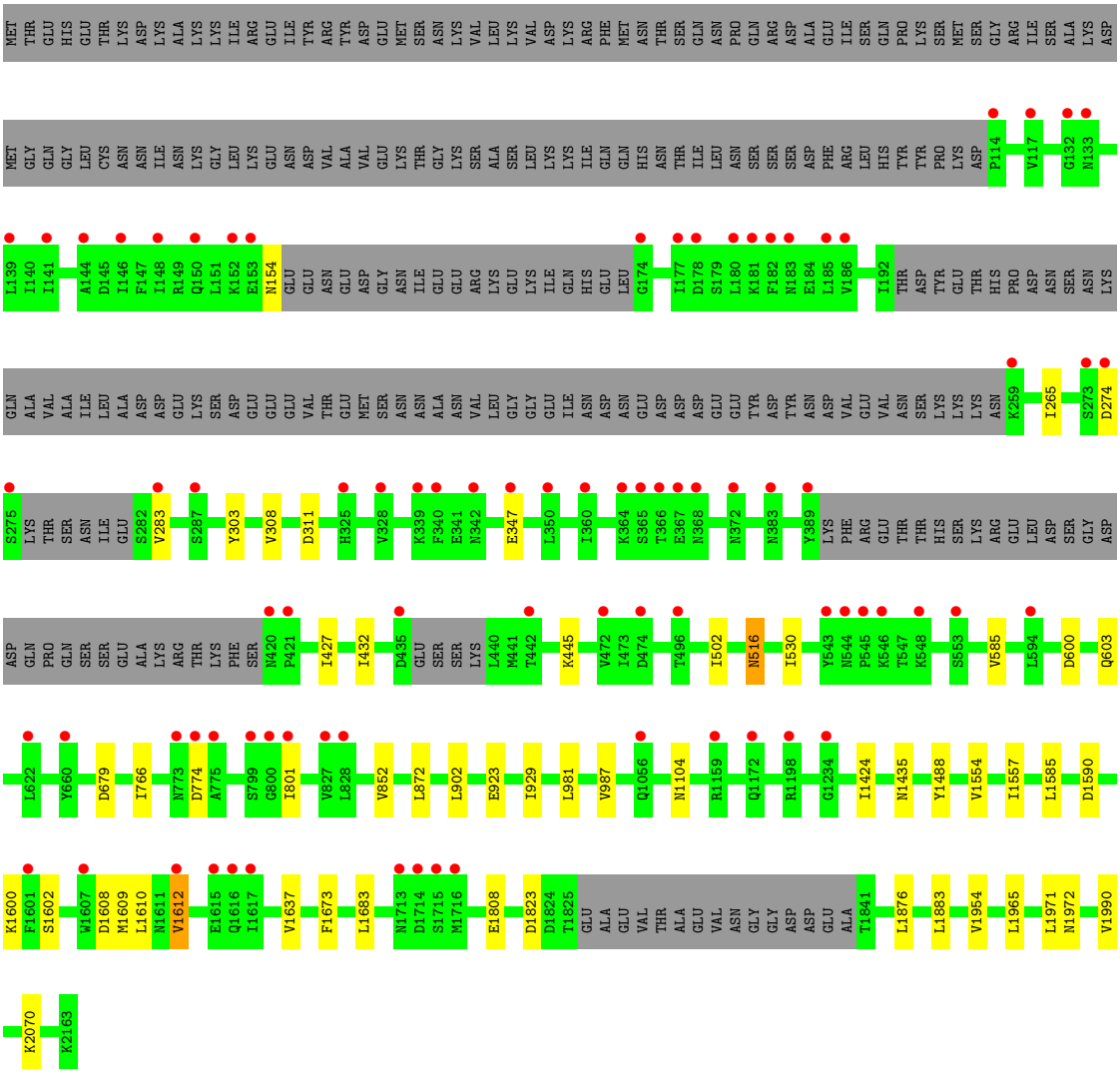
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	4	Total	O	0	0
			4	4		

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.

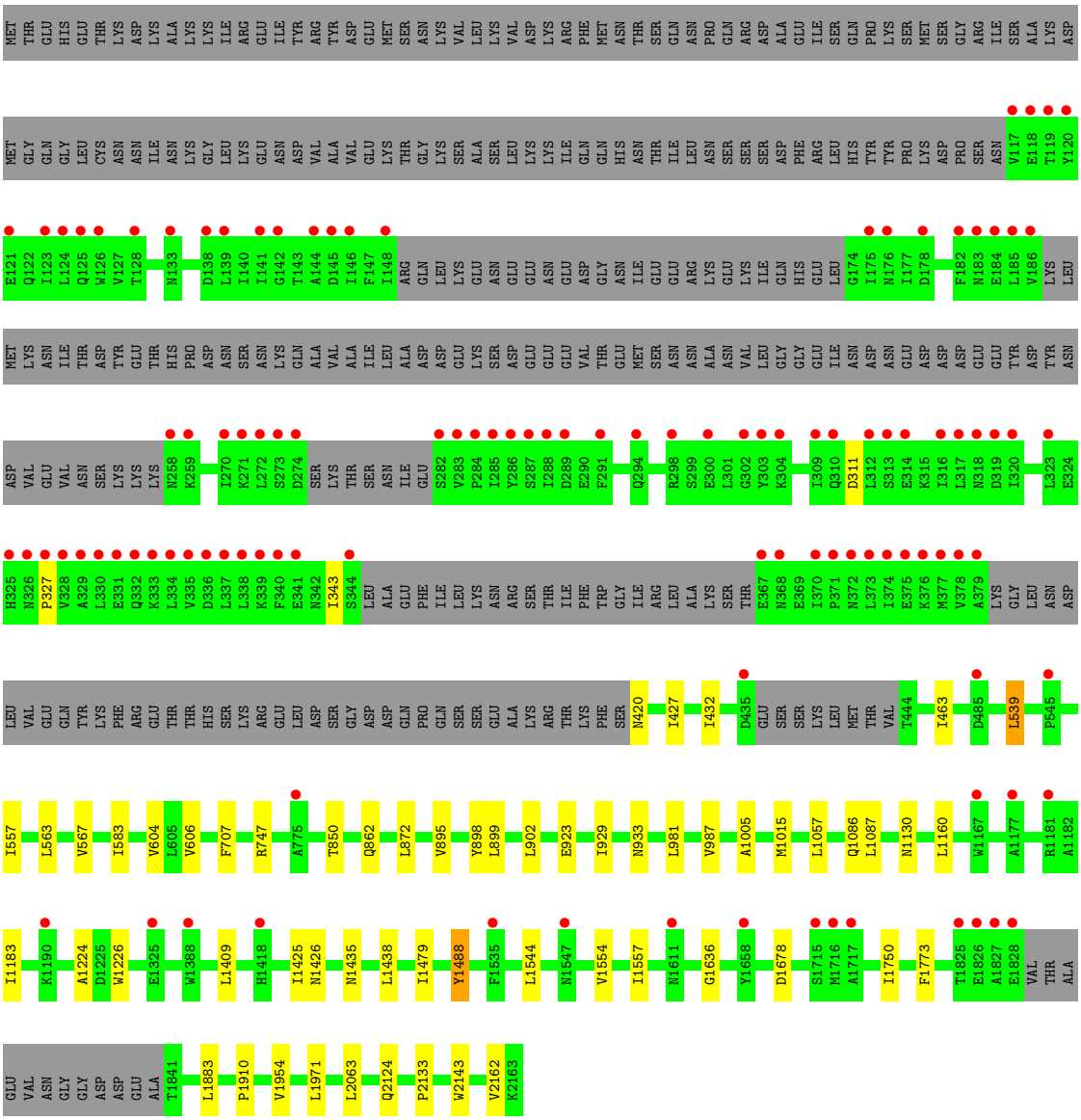
• Molecule 1: Pre-mRNA-splicing helicase BRR2

Chain A:



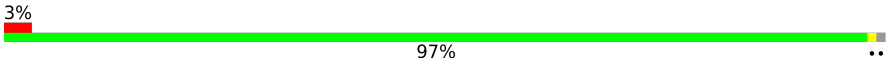
• Molecule 1: Pre-mRNA-splicing helicase BRR2

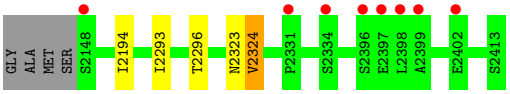
Chain B:



• Molecule 2: Pre-mRNA-splicing factor 8

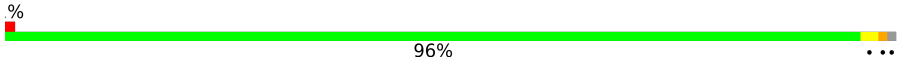
Chain C:

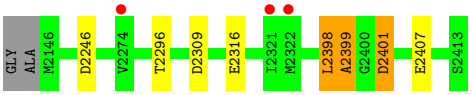




• Molecule 2: Pre-mRNA-splicing factor 8

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	179.34Å 181.16Å 210.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 3.40 48.72 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.72-3.40) 99.7 (48.72-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.33	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.252 , 0.296 0.252 , 0.298	Depositor DCC
R_{free} test set	2100 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å^2)	78.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	34522	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/15638	0.50	0/21190
1	B	0.36	0/15238	0.50	0/20653
2	C	0.35	0/2177	0.47	0/2952
2	D	0.35	0/2188	0.48	1/2966 (0.0%)
All	All	0.36	0/35241	0.49	1/47761 (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
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2398	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2133	PRO	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	15320	0	15372	13	0
1	B	14927	0	14939	25	0
2	C	2127	0	2071	2	0
2	D	2138	0	2075	2	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
All	All	34522	0	34457	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (41) 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:B:1554:VAL:HG23	1:B:1557:ILE:HD11	1.73	0.70
2:C:2194:ILE:HD11	2:C:2293:ILE:HG21	1.74	0.69
1:B:557:ILE:HD11	1:B:604:VAL:HG22	1.81	0.62
1:A:1554:VAL:HG23	1:A:1557:ILE:HD11	1.84	0.59
1:A:1965:LEU:HD22	1:A:1972:ASN:HD22	1.68	0.59
1:B:427:ILE:HD12	1:B:432:ILE:HD11	1.89	0.54
1:B:1971:LEU:HD11	1:B:2143:TRP:CZ3	2.41	0.54
1:B:2063:LEU:HD23	1:B:2162:VAL:HG22	1.89	0.54
1:B:1160:LEU:HD11	1:B:1183:ILE:HG22	1.91	0.53
1:B:1224:ALA:HB1	1:B:1226:TRP:CZ3	2.45	0.52
1:B:1057:LEU:HD11	1:B:1087:LEU:HD11	1.92	0.51
1:B:1883:LEU:HD21	1:B:1954:VAL:HG23	1.94	0.49
1:A:981:LEU:HB3	1:A:987:VAL:HG22	1.94	0.48
2:C:2323:ASN:O	2:C:2324:VAL:HG22	2.13	0.48
1:B:707:PHE:CZ	1:B:902:LEU:HD12	2.49	0.48
1:B:923:GLU:HB2	1:B:929:ILE:HD12	1.96	0.47
1:B:850:THR:HG21	1:B:898:TYR:CE2	2.50	0.47
1:B:1409:LEU:HD22	1:B:1426:ASN:HB3	1.98	0.46
1:A:427:ILE:HD12	1:A:432:ILE:HD11	1.98	0.46
1:B:1479:ILE:HG22	1:B:1488:TYR:HB3	1.98	0.45
1:B:539:LEU:HD11	1:B:583:ILE:HD11	1.98	0.45
1:B:1425:ILE:HG21	1:B:1438:LEU:HD22	1.98	0.45
1:A:502:ILE:HD11	1:A:530:ILE:HD11	1.99	0.44
1:B:981:LEU:HB3	1:B:987:VAL:HG22	1.98	0.44
1:A:516:ASN:HD22	1:A:516:ASN:N	2.16	0.44
1:B:463:ILE:HD12	1:B:895:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:LEU:CD1	1:A:902:LEU:HD21	2.48	0.43
1:A:303:TYR:CD1	1:A:308:VAL:HG11	2.54	0.43
1:A:923:GLU:HB2	1:A:929:ILE:HD12	2.01	0.43
1:B:872:LEU:HD22	1:B:902:LEU:HD21	2.02	0.42
1:B:895:VAL:HG12	1:B:899:LEU:HD13	2.01	0.42
1:A:1435:ASN:N	1:A:1435:ASN:HD22	2.18	0.42
1:B:539:LEU:CD1	1:B:583:ILE:HD11	2.50	0.41
1:A:1585:LEU:HD21	1:A:1683:LEU:HD23	2.01	0.41
1:A:1883:LEU:HD21	1:A:1954:VAL:HG23	2.01	0.41
2:D:2398:LEU:O	2:D:2399:ALA:HB3	2.20	0.41
1:B:563:LEU:HD11	2:D:2407:GLU:HG2	2.02	0.41
1:A:1600:LYS:O	1:A:1602:SER:N	2.53	0.41
1:B:1750:ILE:HD11	1:B:1773:PHE:CZ	2.56	0.41
1:B:567:VAL:HG13	1:B:606:VAL:HG12	2.02	0.40
1:B:1005:ALA:HB2	1:B:1015:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

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	1896/2163 (88%)	1780 (94%)	105 (6%)	11 (1%)	25	57
1	B	1846/2163 (85%)	1740 (94%)	101 (6%)	5 (0%)	41	72
2	C	264/270 (98%)	246 (93%)	17 (6%)	1 (0%)	34	67
2	D	266/270 (98%)	243 (91%)	21 (8%)	2 (1%)	19	51
All	All	4272/4866 (88%)	4009 (94%)	244 (6%)	19 (0%)	34	67

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1612	VAL
2	C	2324	VAL
2	D	2401	ASP
1	A	1424	ILE
1	A	1609	MET
1	B	862	GLN
1	A	603	GLN
1	A	766	ILE
1	A	801	ILE
1	A	283	VAL
1	B	343	ILE
2	D	2399	ALA
1	A	445	LYS
1	A	1673	PHE
1	A	265	ILE
1	B	1636	GLY
1	A	1637	VAL
1	B	1910	PRO
1	B	327	PRO

5.3.2 Protein sidechains (i)

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	1726/1955 (88%)	1704 (99%)	22 (1%)	69 84
1	B	1681/1955 (86%)	1669 (99%)	12 (1%)	84 92
2	C	235/237 (99%)	234 (100%)	1 (0%)	91 95
2	D	235/237 (99%)	230 (98%)	5 (2%)	53 76
All	All	3877/4384 (88%)	3837 (99%)	40 (1%)	76 88

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	274	ASP
1	A	311	ASP

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Mol	Chain	Res	Type
1	A	347	GLU
1	A	516	ASN
1	A	585	VAL
1	A	600	ASP
1	A	679	ASP
1	A	774	ASP
1	A	852	VAL
1	A	1104	ASN
1	A	1488	TYR
1	A	1590	ASP
1	A	1608	ASP
1	A	1610	LEU
1	A	1612	VAL
1	A	1808	GLU
1	A	1823	ASP
1	A	1876	LEU
1	A	1971	LEU
1	A	1990	VAL
1	A	2070	LYS
2	C	2296	THR
1	B	311	ASP
1	B	420	ASN
1	B	539	LEU
1	B	747	ARG
1	B	933	ASN
1	B	1086	GLN
1	B	1130	ASN
1	B	1435	ASN
1	B	1488	TYR
1	B	1544	LEU
1	B	1678	ASP
1	B	2124	GLN
2	D	2246	ASP
2	D	2296	THR
2	D	2309	ASP
2	D	2316	GLU
2	D	2401	ASP

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	154	ASN

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Mol	Chain	Res	Type
1	A	183	ASN
1	A	500	ASN
1	A	516	ASN
1	A	529	ASN
1	A	1104	ASN
1	A	1426	ASN
1	A	1435	ASN
1	A	1972	ASN
1	A	2002	ASN
2	C	2358	ASN
1	B	368	ASN
1	B	676	ASN
1	B	1130	ASN
1	B	1701	ASN
1	B	1755	ASN
1	B	1864	GLN
2	D	2408	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides 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 (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, 95^{th} 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	1910/2163 (88%)	0.28	82 (4%) 35 35	50, 91, 156, 200	0
1	B	1862/2163 (86%)	0.31	112 (6%) 21 23	48, 85, 158, 200	0
2	C	266/270 (98%)	0.26	8 (3%) 50 49	61, 93, 158, 170	0
2	D	268/270 (99%)	0.28	3 (1%) 80 79	63, 95, 137, 162	0
All	All	4306/4866 (88%)	0.29	205 (4%) 30 31	48, 89, 156, 200	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	ILE	6.9
1	B	121	GLU	6.5
1	A	366	THR	6.5
1	B	117	VAL	6.4
1	B	327	PRO	5.9
1	B	325	HIS	5.8
1	B	294	GLN	5.5
1	B	289	ASP	5.3
1	B	1826	GLU	5.3
1	B	326	ASN	5.2
1	B	371	PRO	5.0
1	A	367	GLU	5.0
1	B	338	LEU	5.0
1	B	328	VAL	4.9
1	A	273	SER	4.9
1	B	370	ILE	4.9
1	A	775	ALA	4.8
1	B	1827	ALA	4.8
1	B	125	GLN	4.7
1	B	341	GLU	4.6
1	A	774	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	271	LYS	4.5
1	B	141	ILE	4.4
2	C	2398	LEU	4.4
1	A	365	SER	4.3
1	B	378	VAL	4.3
1	B	1611	ASN	4.3
1	A	372	ASN	4.3
1	B	186	VAL	4.3
1	A	177	ILE	4.2
1	A	1615	GLU	4.2
1	B	337	LEU	4.1
2	C	2397	GLU	4.0
2	D	2321	ILE	4.0
1	B	148	ILE	4.0
1	A	368	ASN	4.0
1	A	420	ASN	4.0
1	A	117	VAL	3.9
1	B	142	GLY	3.9
1	B	1715	SER	3.9
1	B	144	ALA	3.8
1	B	145	ASP	3.8
1	B	182	PHE	3.7
1	A	186	VAL	3.7
2	C	2334	SER	3.7
1	B	335	VAL	3.6
1	A	347	GLU	3.6
1	A	174	GLY	3.6
1	B	368	ASN	3.6
1	A	1714	ASP	3.6
1	B	118	GLU	3.6
1	B	372	ASN	3.6
1	B	375	GLU	3.5
1	B	175	ILE	3.5
1	A	178	ASP	3.5
1	B	545	PRO	3.5
1	B	273	SER	3.4
1	B	282	SER	3.4
1	B	283	VAL	3.4
1	A	185	LEU	3.4
1	B	1658	TYR	3.4
1	A	472	VAL	3.4
1	B	344	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	182	PHE	3.3
1	A	148	ILE	3.3
1	A	180	LEU	3.3
1	A	141	ILE	3.2
1	B	377	MET	3.2
1	A	181	LYS	3.2
2	C	2148	SER	3.2
1	B	298	ARG	3.2
1	A	144	ALA	3.2
1	B	258	ASN	3.2
1	B	285	ILE	3.1
1	B	138	ASP	3.1
1	A	114	PRO	3.1
1	B	287	SER	3.1
1	A	442	THR	3.1
1	B	286	TYR	3.1
1	A	340	PHE	3.1
1	A	1617	ILE	3.1
1	A	274	ASP	3.1
1	A	275	SER	3.1
1	B	274	ASP	3.0
1	B	1167	TRP	3.0
1	A	342	ASN	3.0
1	B	133	ASN	3.0
1	A	259	LYS	3.0
2	C	2399	ALA	3.0
1	B	185	LEU	2.9
1	B	340	PHE	2.9
1	A	132	GLY	2.9
1	A	660	TYR	2.9
1	A	1612	VAL	2.9
2	C	2396	SER	2.9
1	B	259	LYS	2.9
1	B	120	TYR	2.9
1	A	548	LYS	2.9
1	B	183	ASN	2.8
1	B	1325	GLU	2.8
1	A	800	GLY	2.8
1	A	183	ASN	2.8
1	B	373	LEU	2.8
1	B	284	PRO	2.8
1	B	336	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	133	ASN	2.8
1	B	300	GLU	2.8
1	B	320	ILE	2.8
1	A	325	HIS	2.7
1	B	270	ILE	2.7
1	B	1717	ALA	2.7
1	B	178	ASP	2.7
1	B	303	TYR	2.7
1	A	828	LEU	2.7
1	B	184	GLU	2.7
1	B	331	GLU	2.7
1	A	287	SER	2.6
1	B	329	ALA	2.7
1	B	139	LEU	2.6
1	B	128	THR	2.6
1	A	545	PRO	2.6
2	D	2322	MET	2.6
1	A	146	ILE	2.6
1	A	799	SER	2.6
1	A	1172	GLN	2.6
1	A	1713	ASN	2.6
1	A	553	SER	2.6
1	A	435	ASP	2.6
1	B	379	ALA	2.6
1	B	1190	LYS	2.6
1	B	123	ILE	2.6
1	B	126	TRP	2.6
1	A	328	VAL	2.6
1	B	309	ILE	2.6
1	B	310	GLN	2.6
1	B	435	ASP	2.6
1	A	389	TYR	2.5
1	A	1056	GLN	2.5
1	B	367	GLU	2.5
1	A	1716	MET	2.5
1	B	775	ALA	2.5
1	A	546	LYS	2.5
1	B	1716	MET	2.5
1	A	1715	SER	2.5
1	B	317	LEU	2.5
2	D	2274	VAL	2.5
1	B	1825	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	150	GLN	2.5
1	B	318	ASN	2.4
1	A	1616	GLN	2.4
1	B	319	ASP	2.4
1	A	350	LEU	2.4
1	A	1159	ARG	2.4
1	B	1181	ARG	2.4
1	A	474	ASP	2.4
1	A	139	LEU	2.4
1	B	119	THR	2.4
1	B	1388	TRP	2.4
1	B	316	ILE	2.4
1	B	376	LYS	2.4
1	A	283	VAL	2.4
1	A	152	LYS	2.4
1	A	383	ASN	2.4
1	A	622	LEU	2.3
1	A	496	THR	2.3
1	A	1601	PHE	2.3
1	B	1535	PHE	2.3
1	A	801	ILE	2.3
1	B	124	LEU	2.3
1	B	485	ASP	2.3
1	B	314	GLU	2.3
1	A	153	GLU	2.3
1	A	827	VAL	2.3
1	B	288	ILE	2.3
1	A	773	ASN	2.2
1	B	330	LEU	2.2
1	B	291	PHE	2.2
1	A	1234	GLY	2.2
2	C	2402	GLU	2.2
1	A	543	TYR	2.2
1	A	1198	ARG	2.2
1	B	304	LYS	2.2
2	C	2331	PRO	2.2
1	A	421	PRO	2.2
1	A	360	ILE	2.2
1	B	1418	HIS	2.2
1	B	313	SER	2.2
1	B	302	GLY	2.1
1	B	176	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	594	LEU	2.1
1	A	544	ASN	2.1
1	B	272	LEU	2.1
1	B	323	LEU	2.1
1	A	339	LYS	2.1
1	B	1828	GLU	2.1
1	A	364	LYS	2.1
1	A	1607	TRP	2.1
1	B	312	LEU	2.1
1	B	332	GLN	2.1
1	B	1177	ALA	2.1
1	B	333	LYS	2.1
1	B	339	LYS	2.0
1	B	334	LEU	2.0
1	B	374	ILE	2.0
1	B	1547	ASN	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 monosaccharides 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.