Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 12:01 PM EDT

PDB ID	:	5DCA
Title	:	Crystal structure of yeast full length Brr2 in complex with Prp8 Jab1 domain
Authors	:	Absmeier, E.; Wollenhaupt, J.; Santos, K.F.; Wahl, M.C.
Deposited on	:	2015-08-23
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

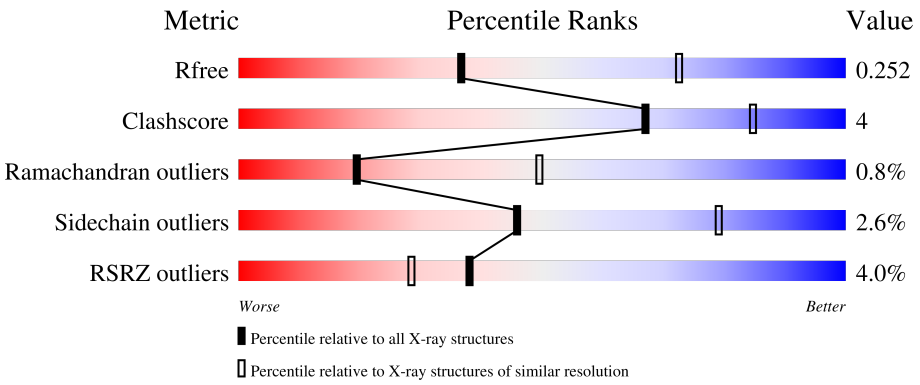
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	1948	4% 88% 11% •
2	J	251	% 90% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17842 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
			Total	C	N	O	S			
1	A	1948	15639	10006	2602	2973	58	0	0	0

There are 103 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	HIS	deletion	UNP P32639
A	?	-	PRO	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ILE	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	MET	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ILE	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	HIS	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P32639
A	?	-	ARG	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	PRO	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	ARG	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	PHE	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	251	2012	1298	325	383	6	0	0	0

- Molecule 3 is water.

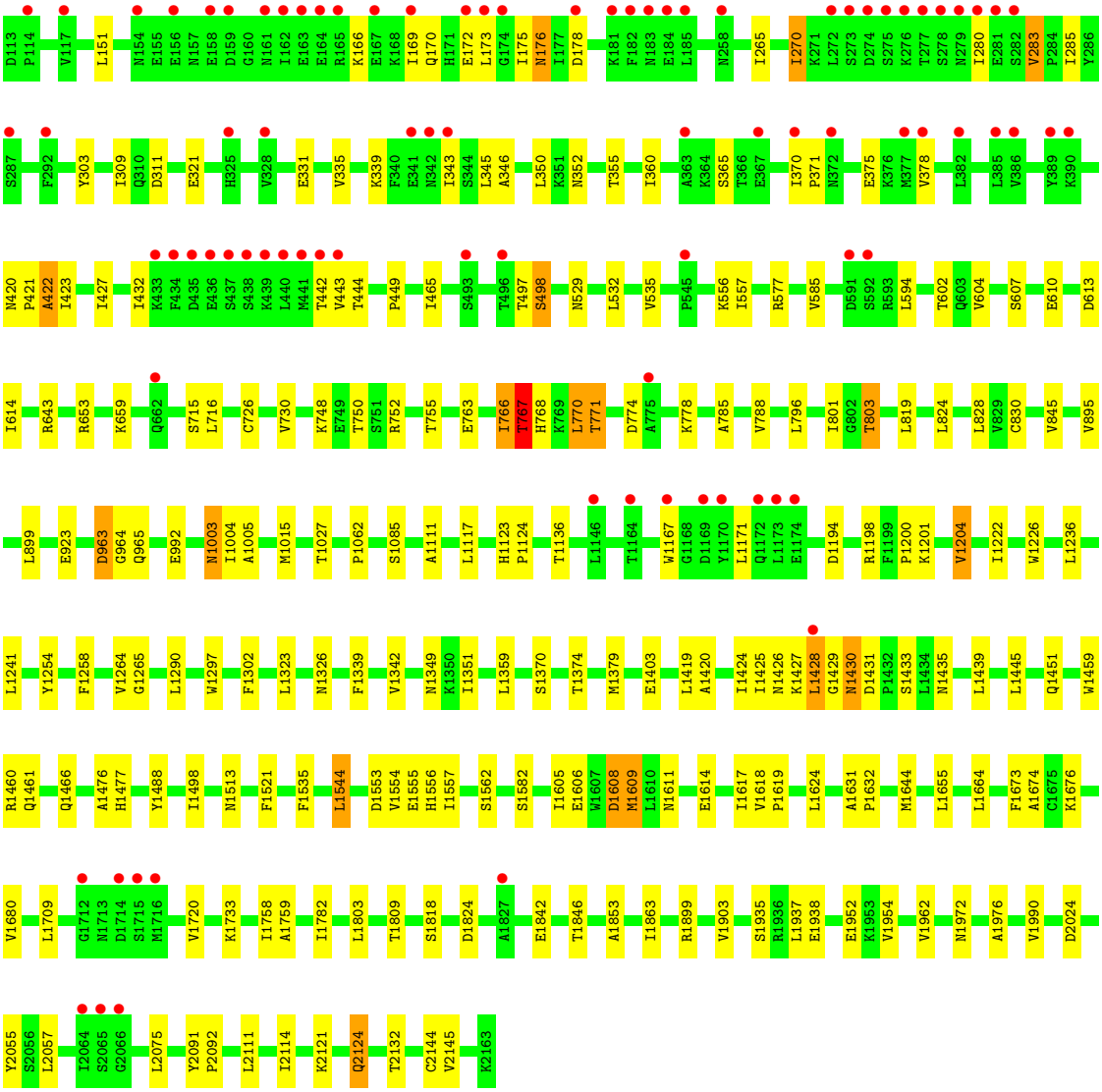
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	169	169	169	0	0
			Total	O		
3	J	22	22	22	0	0

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.

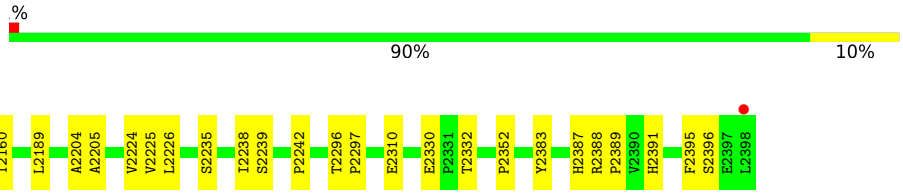
• Molecule 1: Pre-mRNA-splicing helicase BRR2

Chain A: 4% 88% 11%



• Molecule 2: Pre-mRNA-splicing factor 8

Chain J:


%
90%
10%
S2148
W2152
S2155
T2160
L2189
A2204
A2205
V2224
V2225
L2226
S2235
I2238
S2239
P2242
T2296
P2297
E2310
E2330
P2331
T2332
P2352
Y2383
H2387
R2388
P2389
V2390
H2391
F2395
S2396
E2397
L2398

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.85Å 178.85Å 181.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 178.85 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.80) 95.5 (178.85-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.202 , 0.255 0.205 , 0.252	Depositor DCC
R_{free} test set	4481 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	85.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17842	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 (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	0.32	0/15960	0.52	0/21620
2	J	0.32	0/2060	0.51	0/2792
All	All	0.32	0/18020	0.52	0/24412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	15639	0	15665	123	0
2	J	2012	0	1972	17	0
3	A	169	0	0	3	0
3	J	22	0	0	0	0
All	All	17842	0	17637	136	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 4.

All (136) 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:J:2387:HIS:C	2:J:2388:ARG:N	2.05	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:LEU:HA	1:A:1445:LEU:HD11	1.64	0.80
1:A:1555:GLU:C	1:A:1556:HIS:N	2.41	0.74
1:A:767:THR:O	1:A:771:THR:N	2.25	0.70
1:A:2121:LYS:O	1:A:2124:GLN:NE2	2.24	0.69
1:A:1027:THR:HG21	2:J:2160:THR:HG23	1.74	0.69
1:A:557:ILE:HD11	1:A:604:VAL:HG22	1.76	0.68
1:A:1554:VAL:HG23	1:A:1557:ILE:HD11	1.77	0.66
1:A:303:TYR:HB2	1:A:309:ILE:HD11	1.79	0.64
1:A:1609:MET:O	3:A:2201:HOH:O	2.15	0.64
1:A:1339:PHE:O	1:A:1342:VAL:HG22	1.99	0.63
1:A:766:ILE:O	1:A:768:HIS:N	2.32	0.62
1:A:375:GLU:HA	1:A:378:VAL:HG12	1.83	0.61
1:A:343:ILE:O	1:A:343:ILE:HG22	2.01	0.61
1:A:420:ASN:N	1:A:421:PRO:CD	2.65	0.59
1:A:1556:HIS:C	1:A:1557:ILE:N	2.56	0.58
1:A:1556:HIS:N	1:A:1557:ILE:N	2.53	0.57
2:J:2296:THR:O	2:J:2297:PRO:C	2.43	0.57
1:A:175:ILE:HG23	1:A:178:ASP:HB3	1.86	0.56
1:A:1614:GLU:O	1:A:1618:VAL:HG23	2.06	0.56
2:J:2383:TYR:O	2:J:2388:ARG:NH1	2.40	0.55
1:A:283:VAL:HG11	1:A:355:THR:OG1	2.07	0.54
1:A:442:THR:O	1:A:444:THR:N	2.40	0.54
1:A:1617:ILE:HD11	1:A:1655:LEU:HD22	1.89	0.54
1:A:427:ILE:HD12	1:A:432:ILE:HD11	1.88	0.54
1:A:1990:VAL:HG12	1:A:1990:VAL:O	2.07	0.54
1:A:1680:VAL:CG1	1:A:1720:VAL:HG22	2.38	0.54
1:A:166:LYS:O	1:A:170:GLN:N	2.37	0.53
1:A:1618:VAL:N	1:A:1619:PRO:HD2	2.25	0.52
2:J:2225:VAL:HG11	2:J:2242:PRO:HG3	1.92	0.52
1:A:423:ILE:HD11	1:A:992:GLU:HA	1.92	0.52
1:A:1005:ALA:HB2	1:A:1015:MET:HG3	1.92	0.52
1:A:343:ILE:HG23	1:A:346:ALA:HB3	1.91	0.52
1:A:1419:LEU:O	1:A:1420:ALA:HB3	2.11	0.51
1:A:1370:SER:OG	1:A:1374:THR:OG1	2.21	0.51
1:A:613:ASP:OD1	1:A:653:ARG:NH2	2.45	0.50
1:A:529:ASN:HD21	1:A:577:ARG:HH22	1.60	0.50
1:A:766:ILE:HD12	1:A:766:ILE:N	2.27	0.50
1:A:1062:PRO:O	2:J:2388:ARG:NH2	2.44	0.50
1:A:755:THR:HG22	1:A:796:LEU:HD21	1.93	0.50
1:A:614:ILE:HG23	3:A:2301:HOH:O	2.12	0.49
1:A:1426:ASN:HD21	1:A:1428:LEU:CD2	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1544:LEU:HD21	1:A:1720:VAL:HG23	1.94	0.49
1:A:557:ILE:CD1	1:A:604:VAL:HG22	2.42	0.49
2:J:2330:GLU:HB3	2:J:2332:THR:HG22	1.93	0.49
1:A:1123:HIS:HB3	1:A:1124:PRO:HD3	1.95	0.49
1:A:1226:TRP:O	1:A:1264:VAL:HG11	2.13	0.49
1:A:1351:ILE:HG23	1:A:1535:PHE:CE2	2.48	0.48
1:A:1236:LEU:HD11	1:A:1258:PHE:HB3	1.96	0.48
1:A:360:ILE:HD11	1:A:365:SER:OG	2.14	0.48
1:A:1758:ILE:HG22	1:A:1846:THR:HG23	1.95	0.48
1:A:1359:LEU:HD21	1:A:1379:MET:HB3	1.94	0.48
1:A:1962:VAL:HG22	1:A:1976:ALA:HB3	1.96	0.48
1:A:610:GLU:OE2	1:A:643:ARG:HD2	2.14	0.47
1:A:750:THR:HG21	1:A:803:THR:HG23	1.95	0.47
1:A:828:LEU:HG	1:A:830:CYS:SG	2.53	0.47
1:A:1204:VAL:HG13	1:A:1222:ILE:HG12	1.96	0.47
1:A:1015:MET:HE1	1:A:1111:ALA:HB1	1.96	0.47
1:A:169:ILE:HG23	1:A:716:LEU:HD13	1.96	0.47
1:A:556:LYS:NZ	1:A:602:THR:O	2.45	0.47
1:A:421:PRO:O	1:A:422:ALA:HB3	2.14	0.47
1:A:1476:ALA:HB1	1:A:1521:PHE:CZ	2.50	0.47
1:A:1194:ASP:O	1:A:1198:ARG:HG2	2.15	0.47
1:A:963:ASP:O	1:A:965:GLN:N	2.48	0.47
1:A:1370:SER:O	1:A:1513:ASN:HA	2.14	0.47
1:A:1429:GLY:O	1:A:1431:ASP:N	2.47	0.47
1:A:285:ILE:HD11	1:A:355:THR:HG22	1.97	0.47
1:A:774:ASP:HA	1:A:778:LYS:HB2	1.97	0.46
1:A:1608:ASP:O	1:A:1609:MET:HG2	2.16	0.46
1:A:1631:ALA:HB3	1:A:1632:PRO:HD3	1.97	0.46
1:A:1674:ALA:HB1	1:A:1709:LEU:HD13	1.97	0.46
1:A:283:VAL:HG11	1:A:355:THR:CB	2.45	0.46
1:A:285:ILE:HD12	1:A:285:ILE:N	2.31	0.46
1:A:1782:ILE:HG21	1:A:1803:LEU:HD21	1.97	0.46
1:A:1200:PRO:HG2	1:A:1297:TRP:CD1	2.51	0.46
1:A:1241:LEU:HD11	1:A:1290:LEU:HD11	1.98	0.45
1:A:1582:SER:HA	1:A:1664:LEU:O	2.17	0.45
1:A:2111:LEU:HD21	1:A:2114:ILE:HB	1.98	0.45
1:A:1419:LEU:O	1:A:1420:ALA:CB	2.65	0.45
2:J:2152:TRP:CE2	2:J:2391:HIS:CE1	3.05	0.45
1:A:283:VAL:HG22	1:A:352:ASN:ND2	2.31	0.45
1:A:270:ILE:HD11	1:A:1733:LYS:HG3	1.99	0.44
1:A:1062:PRO:HD3	2:J:2395:PHE:CG	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1853:ALA:HB2	1:A:1863:ILE:HD12	1.99	0.44
1:A:497:THR:O	1:A:498:SER:CB	2.65	0.44
1:A:1349:ASN:HB2	3:A:2213:HOH:O	2.16	0.44
1:A:1759:ALA:HB2	1:A:1846:THR:HG21	1.98	0.44
2:J:2205:ALA:HB2	2:J:2226:LEU:HD23	2.00	0.44
1:A:449:PRO:HG2	1:A:465:ILE:HG23	2.00	0.44
1:A:653:ARG:NH1	1:A:923:GLU:OE2	2.51	0.44
1:A:1459:TRP:CG	1:A:1498:ILE:HD11	2.52	0.44
1:A:280:ILE:HG22	1:A:280:ILE:O	2.18	0.44
1:A:1015:MET:CE	1:A:1111:ALA:HB1	2.48	0.44
1:A:2055:TYR:CG	1:A:2055:TYR:O	2.71	0.44
1:A:1426:ASN:OD1	1:A:1426:ASN:O	2.36	0.44
1:A:345:LEU:HD13	1:A:345:LEU:O	2.18	0.43
2:J:2226:LEU:O	2:J:2352:PRO:HD3	2.19	0.43
1:A:1476:ALA:HB1	1:A:1521:PHE:HZ	1.82	0.43
1:A:151:LEU:C	1:A:151:LEU:HD12	2.39	0.43
1:A:370:ILE:N	1:A:371:PRO:HD2	2.34	0.43
1:A:1899:ARG:O	1:A:1903:VAL:HG23	2.19	0.43
1:A:1085:SER:HB3	2:J:2396:SER:HA	2.01	0.43
1:A:1477:HIS:CG	1:A:1513:ASN:OD1	2.71	0.43
2:J:2388:ARG:N	2:J:2389:PRO:HD3	2.33	0.43
1:A:1264:VAL:HG12	1:A:1265:GLY:N	2.34	0.42
1:A:1425:ILE:HG22	1:A:1426:ASN:O	2.19	0.42
1:A:1631:ALA:HB3	1:A:1632:PRO:CD	2.50	0.42
2:J:2189:LEU:HD13	2:J:2224:VAL:HG23	2.01	0.42
1:A:2075:LEU:HD21	1:A:2144:CYS:SG	2.59	0.42
1:A:420:ASN:N	1:A:421:PRO:HD2	2.34	0.42
1:A:1370:SER:HG	1:A:1374:THR:HG1	1.45	0.42
1:A:1605:ILE:HG22	1:A:1606:GLU:N	2.34	0.42
1:A:331:GLU:O	1:A:335:VAL:HG23	2.19	0.42
1:A:1403:GLU:HG2	1:A:1673:PHE:HZ	1.84	0.42
1:A:176:ASN:HD22	1:A:176:ASN:N	2.18	0.42
2:J:2388:ARG:O	2:J:2389:PRO:C	2.57	0.42
1:A:1424:ILE:O	1:A:1425:ILE:HD13	2.19	0.42
1:A:1935:SER:HB2	1:A:1937:LEU:HD13	2.01	0.42
1:A:1429:GLY:HA3	1:A:1451:GLN:HG2	2.01	0.41
1:A:1003:ASN:HD22	1:A:1003:ASN:C	2.23	0.41
1:A:895:VAL:O	1:A:899:LEU:HB2	2.21	0.41
1:A:1004:ILE:HG22	1:A:1015:MET:HE1	2.02	0.41
2:J:2204:ALA:CB	2:J:2238:ILE:HD11	2.50	0.41
2:J:2238:ILE:HG22	2:J:2239:SER:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:HG22	1:A:557:ILE:HD12	2.02	0.41
1:A:819:LEU:HD23	1:A:824:LEU:HD12	2.03	0.41
1:A:1201:LYS:HA	1:A:1302:PHE:CZ	2.55	0.41
1:A:1117:LEU:HD11	1:A:1254:TYR:CG	2.56	0.41
1:A:1427:LYS:NZ	1:A:1445:LEU:HD13	2.36	0.40
1:A:1430:ASN:ND2	1:A:1952:GLU:O	2.55	0.40
1:A:1167:TRP:CZ3	1:A:1171:LEU:HD21	2.57	0.40
1:A:1339:PHE:CE1	1:A:1419:LEU:HD23	2.57	0.40
1:A:726:CYS:O	1:A:730:VAL:HG23	2.22	0.40
1:A:770:LEU:HD21	1:A:801:ILE:HG13	2.02	0.40
1:A:785:ALA:O	1:A:788:VAL:HG22	2.22	0.40
1:A:2091:TYR:HA	1:A:2092:PRO:HD3	1.83	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	1937/1948 (99%)	1823 (94%)	97 (5%)	17 (1%)	17 46
2	J	247/251 (98%)	231 (94%)	16 (6%)	0	100 100
All	All	2184/2199 (99%)	2054 (94%)	113 (5%)	17 (1%)	19 49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
1	A	498	SER
1	A	767	THR
1	A	172	GLU
1	A	321	GLU
1	A	422	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	443	VAL
1	A	1430	ASN
1	A	339	LYS
1	A	964	GLY
1	A	1644	MET
1	A	283	VAL
1	A	1972	ASN
1	A	1609	MET
1	A	1611	ASN
1	A	265	ILE
1	A	1676	LYS

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	1762/1762 (100%)	1714 (97%)	48 (3%)	44	78
2	J	223/223 (100%)	220 (99%)	3 (1%)	69	91
All	All	1985/1985 (100%)	1934 (97%)	51 (3%)	46	79

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LEU
1	A	176	ASN
1	A	311	ASP
1	A	350	LEU
1	A	532	LEU
1	A	585	VAL
1	A	594	LEU
1	A	607	SER
1	A	659	LYS
1	A	715	SER
1	A	748	LYS
1	A	752	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	763	GLU
1	A	766	ILE
1	A	767	THR
1	A	770	LEU
1	A	771	THR
1	A	803	THR
1	A	845	VAL
1	A	963	ASP
1	A	1003	ASN
1	A	1136	THR
1	A	1204	VAL
1	A	1323	LEU
1	A	1326	ASN
1	A	1428	LEU
1	A	1433	SER
1	A	1435	ASN
1	A	1460	ARG
1	A	1461	GLN
1	A	1466	GLN
1	A	1488	TYR
1	A	1544	LEU
1	A	1553	ASP
1	A	1562	SER
1	A	1608	ASP
1	A	1624	LEU
1	A	1809	THR
1	A	1818	SER
1	A	1824	ASP
1	A	1842	GLU
1	A	1938	GLU
1	A	1954	VAL
1	A	2024	ASP
1	A	2057	LEU
1	A	2124	GLN
1	A	2132	THR
1	A	2145	VAL
2	J	2155	SER
2	J	2235	SER
2	J	2310	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	176	ASN
1	A	264	ASN
1	A	503	GLN
1	A	529	ASN
1	A	621	ASN
1	A	676	ASN
1	A	739	GLN
1	A	984	GLN
1	A	1003	ASN
1	A	1086	GLN
1	A	1191	GLN
1	A	1426	ASN
1	A	1864	GLN
1	A	2161	ASN
2	J	2240	ASN

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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
2	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	192:ILE	C	258:ASN	N	48.54
1	A	393:GLU	C	420:ASN	N	23.97
1	A	1828:GLU	C	1841:THR	N	9.71
1	A	1556:HIS	C	1557:ILE	N	2.56
1	A	1555:GLU	C	1556:HIS	N	2.41
1	J	2387:HIS	C	2388:ARG	N	2.05

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	1948/1948 (100%)	0.10	87 (4%)	33	23	57, 90, 184, 237	0
2	J	251/251 (100%)	-0.23	2 (0%)	86	81	59, 88, 151, 194	0
All	All	2199/2199 (100%)	0.06	89 (4%)	38	28	57, 89, 182, 237	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	ASN	13.4
1	A	440	LEU	12.8
1	A	342	ASN	12.3
1	A	441	MET	12.1
1	A	173	LEU	9.2
1	A	385	LEU	9.1
1	A	278	SER	8.8
1	A	164	GLU	8.6
1	A	435	ASP	8.3
1	A	281	GLU	8.3
1	A	386	VAL	8.1
1	A	389	TYR	8.0
1	A	277	THR	7.4
1	A	437	SER	7.2
1	A	182	PHE	6.9
1	A	325	HIS	6.5
1	A	378	VAL	6.4
1	A	163	GLU	6.3
1	A	442	THR	6.3
1	A	275	SER	6.2
1	A	172	GLU	6.1
1	A	162	ILE	5.7
1	A	434	PHE	5.5
1	A	273	SER	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	276	LYS	5.4
1	A	438	SER	5.2
1	A	169	ILE	5.1
1	A	341	GLU	5.0
2	J	2148	SER	4.9
1	A	1716	MET	4.6
1	A	174	GLY	4.6
1	A	167	GLU	4.6
1	A	1172	GLN	4.5
1	A	443	VAL	4.4
1	A	1164	THR	4.4
1	A	363	ALA	4.4
1	A	158	GLU	4.3
1	A	1827	ALA	4.2
1	A	436	GLU	4.1
1	A	154	ASN	4.1
1	A	184	GLU	4.1
1	A	1173	LEU	4.1
1	A	382	LEU	4.0
1	A	1715	SER	3.9
1	A	274	ASP	3.9
1	A	287	SER	3.8
1	A	280	ILE	3.7
1	A	367	GLU	3.6
1	A	272	LEU	3.6
1	A	156	GLU	3.6
2	J	2398	LEU	3.6
1	A	165	ARG	3.5
1	A	343	ILE	3.5
1	A	181	LYS	3.4
1	A	328	VAL	3.4
1	A	2065	SER	3.3
1	A	439	LYS	3.2
1	A	2064	ILE	3.2
1	A	662	GLN	3.2
1	A	1712	GLY	3.1
1	A	372	ASN	3.1
1	A	282	SER	3.0
1	A	161	ASN	2.9
1	A	183	ASN	2.9
1	A	545	PRO	2.9
1	A	433	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	370	ILE	2.8
1	A	114	PRO	2.8
1	A	159	ASP	2.8
1	A	2066	GLY	2.7
1	A	292	PHE	2.7
1	A	117	VAL	2.7
1	A	592	SER	2.5
1	A	258	ASN	2.5
1	A	390	LYS	2.4
1	A	496	THR	2.4
1	A	1428	LEU	2.4
1	A	1174	GLU	2.3
1	A	1170	TYR	2.3
1	A	1167	TRP	2.3
1	A	1714	ASP	2.3
1	A	178	ASP	2.2
1	A	1169	ASP	2.2
1	A	591	ASP	2.1
1	A	1146	LEU	2.1
1	A	185	LEU	2.1
1	A	775	ALA	2.1
1	A	377	MET	2.0
1	A	493	SER	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.