



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:45 AM UTC

PDB ID : 4XLX / pdb_00004xlx
Title : Crystal structure of BJKS from Bradyrhizobium japonicum
Authors : Hu, Y.; Zheng, Y.; Ko, T.P.; Liu, W.; Guo, R.T.
Deposited on : 2015-01-14
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

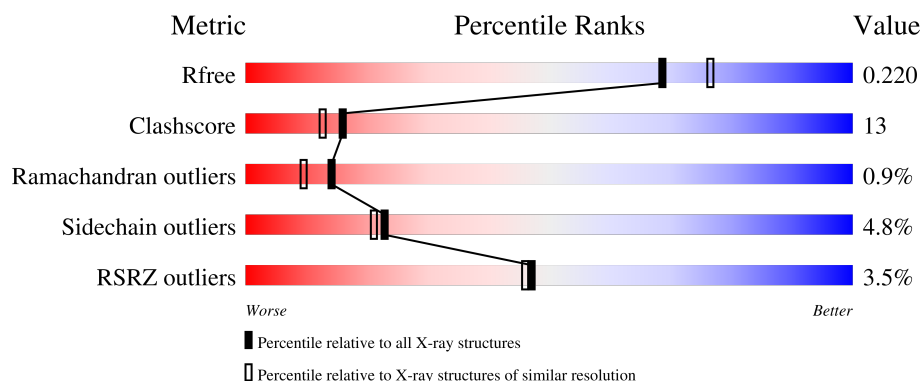
1 Overall quality at a glance

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	300	4% 74% 18% • •
1	B	300	4% 67% 23% • 7%
1	C	300	3% 72% 18% • • 6%
1	D	300	3% 65% 18% 5% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9417 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 Uncharacterized protein blr2150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2263	1421	413	417	12			
1	B	279	Total	C	N	O	S	0	0	0
			2189	1379	398	400	12			
1	C	281	Total	C	N	O	S	0	0	0
			2211	1394	402	403	12			
1	D	267	Total	C	N	O	S	0	0	0
			2103	1334	379	379	11			

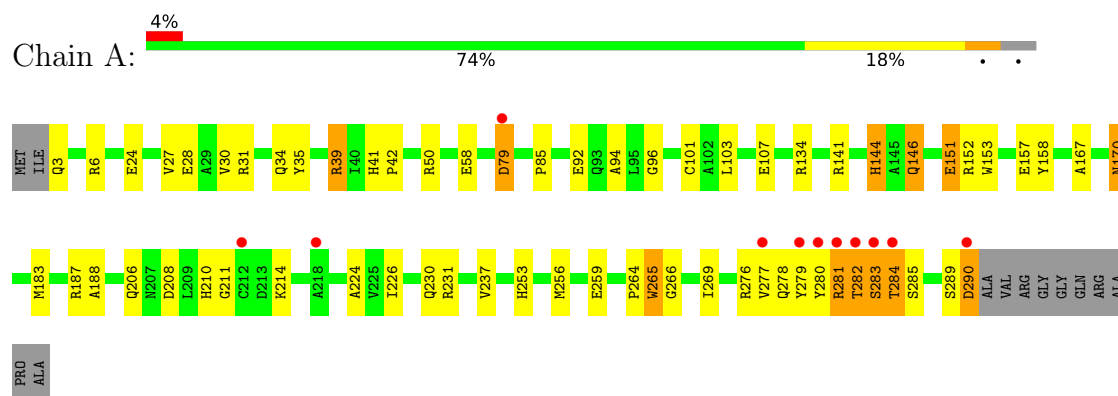
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	188	Total	O	0	0
			188	188		
2	B	137	Total	O	0	0
			137	137		
2	C	183	Total	O	0	0
			183	183		
2	D	143	Total	O	0	0
			143	143		

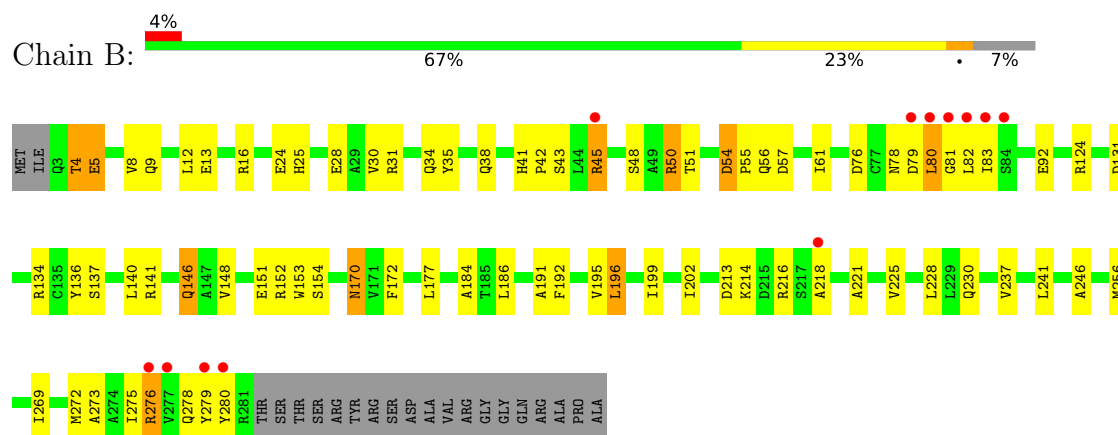
3 Residue-property plots [i](#)

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.

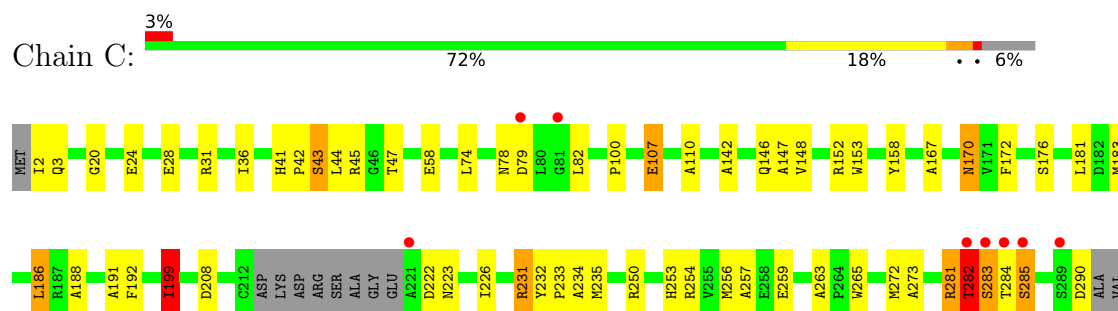
• Molecule 1: Uncharacterized protein blr2150



• Molecule 1: Uncharacterized protein blr2150

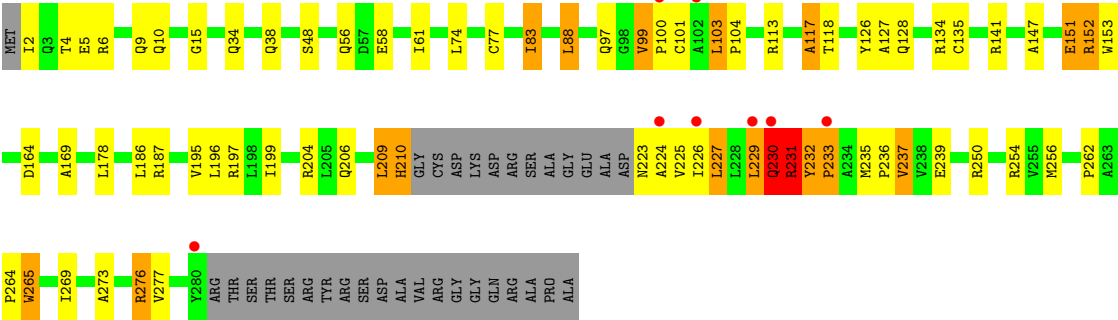


• Molecule 1: Uncharacterized protein blr2150



ARG
GLY
GLN
ARG
ALA
PRO
ALA

● Molecule 1: Uncharacterized protein blr2150



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.03Å 130.07Å 66.39Å 90.00° 95.62° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (25.00-2.00) 95.3 (25.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.02 (at 1.99Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.176 , 0.220 0.176 , 0.220	Depositor DCC
R_{free} test set	3582 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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	1.15	1/2310 (0.0%)	1.16	9/3138 (0.3%)
1	B	1.06	2/2235 (0.1%)	1.13	11/3037 (0.4%)
1	C	1.15	5/2257 (0.2%)	1.17	11/3067 (0.4%)
1	D	1.08	3/2148 (0.1%)	1.15	12/2921 (0.4%)
All	All	1.11	11/8950 (0.1%)	1.15	43/12163 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	256	MET	SD-CE	8.40	2.00	1.79
1	D	256	MET	CG-SD	-6.59	1.64	1.80
1	C	142	ALA	CA-CB	5.99	1.62	1.53
1	B	148	VAL	CA-CB	5.99	1.60	1.54
1	B	246	ALA	CA-CB	5.96	1.62	1.53
1	C	183	MET	CA-C	5.54	1.60	1.52
1	C	199	ILE	CA-CB	5.53	1.61	1.54
1	C	263	ALA	CA-CB	5.40	1.61	1.53
1	D	169	ALA	CA-CB	5.36	1.61	1.53
1	A	183	MET	SD-CE	5.27	1.92	1.79
1	D	127	ALA	CA-CB	5.25	1.61	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	THR	N-CA-C	9.46	130.95	110.80
1	A	259	GLU	N-CA-C	8.88	122.12	111.82
1	B	4	THR	N-CA-C	8.84	121.81	111.02
1	D	224	ALA	N-CA-C	-8.81	101.12	112.23
1	C	281	ARG	N-CA-C	7.48	120.18	110.53
1	A	167	ALA	N-CA-C	7.47	121.97	112.86
1	A	265	TRP	N-CA-C	7.36	119.31	111.28
1	A	103	LEU	CA-C-N	-7.04	113.56	120.52
1	A	103	LEU	C-N-CA	-7.04	113.56	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	VAL	N-CA-C	6.52	116.68	110.42
1	D	83	ILE	N-CA-C	-6.42	99.12	108.11
1	B	83	ILE	N-CA-C	6.38	117.90	108.65
1	D	151	GLU	N-CA-C	6.25	120.62	113.19
1	B	51	THR	N-CA-C	6.22	121.05	112.90
1	C	283	SER	N-CA-C	-6.17	104.18	111.03
1	D	4	THR	N-CA-C	6.01	118.36	111.02
1	D	232	TYR	CA-C-N	5.87	127.18	119.84
1	D	232	TYR	C-N-CA	5.87	127.18	119.84
1	C	78	ASN	N-CA-C	-5.85	101.98	111.04
1	B	54	ASP	CA-C-N	5.83	125.52	119.05
1	B	54	ASP	C-N-CA	5.83	125.52	119.05
1	C	167	ALA	N-CA-C	5.73	119.85	112.86
1	C	234	ALA	N-CA-C	5.72	119.53	112.54
1	D	117	ALA	N-CA-C	-5.65	105.20	111.36
1	D	103	LEU	N-CA-C	5.60	117.56	109.04
1	C	188	ALA	N-CA-C	-5.58	106.43	113.18
1	A	237	VAL	N-CA-C	5.57	116.20	110.36
1	C	281	ARG	CA-C-N	5.56	132.15	121.54
1	C	281	ARG	C-N-CA	5.56	132.15	121.54
1	D	209	LEU	N-CA-C	-5.55	104.86	111.69
1	B	276	ARG	N-CA-C	-5.39	102.48	110.46
1	D	265	TRP	N-CA-C	5.34	117.10	111.28
1	B	154	SER	N-CA-C	-5.31	103.68	110.53
1	A	188	ALA	N-CA-C	-5.28	106.79	113.18
1	A	79	ASP	N-CA-C	5.25	119.78	112.90
1	C	79	ASP	N-CA-C	5.24	120.01	111.37
1	D	178	LEU	N-CA-C	5.23	118.13	111.69
1	D	15	GLY	N-CA-C	5.12	119.95	113.24
1	A	224	ALA	N-CA-C	5.11	116.85	111.28
1	B	202	ILE	N-CA-C	-5.08	105.54	110.42
1	C	265	TRP	N-CA-C	5.07	116.80	111.28
1	B	54	ASP	N-CA-C	5.03	116.22	109.83
1	B	25	HIS	N-CA-C	-5.01	105.70	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2263	0	2220	48	0
1	B	2189	0	2152	67	0
1	C	2211	0	2177	55	0
1	D	2103	0	2079	67	0
2	A	188	0	0	6	0
2	B	137	0	0	8	0
2	C	183	0	0	3	0
2	D	143	0	0	3	0
All	All	9417	0	8628	230	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 13.

All (230) 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:199:ILE:HD11	1:B:273:ALA:HA	1.29	1.12
1:C:235:MET:HE2	1:D:235:MET:HG3	1.25	1.10
1:D:135:CYS:HB2	2:D:513:HOH:O	1.57	1.05
1:C:281:ARG:HG3	1:C:282:THR:HG23	1.45	0.95
1:B:199:ILE:HD11	1:B:273:ALA:CA	1.99	0.92
1:C:28:GLU:OE2	1:C:281:ARG:HD3	1.70	0.92
1:D:152:ARG:HH11	1:D:231:ARG:HD2	1.31	0.91
1:D:34:GLN:O	1:D:38:GLN:HG2	1.74	0.86
1:D:226:ILE:O	1:D:230:GLN:HB2	1.74	0.86
1:B:131:ASP:OD1	1:B:134:ARG:NH2	2.11	0.84
1:B:199:ILE:CD1	1:B:273:ALA:HA	2.07	0.82
1:C:235:MET:CE	1:D:235:MET:HG3	2.09	0.82
1:B:81:GLY:O	2:B:506:HOH:O	1.96	0.81
1:C:281:ARG:HG3	1:C:282:THR:N	1.96	0.80
1:B:31:ARG:HD2	1:B:280:TYR:HA	1.62	0.79
1:B:131:ASP:HB3	2:B:529:HOH:O	1.82	0.79
1:D:152:ARG:NH1	1:D:231:ARG:HD2	1.97	0.79
1:A:24:GLU:O	1:A:28:GLU:HG3	1.82	0.78
1:C:31:ARG:NH2	1:C:283:SER:OG	2.17	0.77
1:C:281:ARG:CG	1:C:282:THR:HG23	2.16	0.76
1:C:281:ARG:HG3	1:C:282:THR:H	1.51	0.76
1:A:3:GLN:HG2	1:A:6:ARG:H	1.50	0.75
1:B:24:GLU:O	1:B:28:GLU:HG3	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:HD22	1:A:170:ASN:H	1.34	0.74
1:B:13:GLU:OE2	1:B:16:ARG:HD2	1.88	0.74
1:A:31:ARG:NH1	1:A:283:SER:HB2	2.03	0.73
1:C:172:PHE:CE1	1:C:272:MET:HG3	2.23	0.72
1:D:210:HIS:ND1	1:D:210:HIS:C	2.48	0.71
1:D:152:ARG:HD2	1:D:231:ARG:NE	2.06	0.69
1:D:250:ARG:O	1:D:254:ARG:HG3	1.92	0.69
1:C:152:ARG:HG3	1:C:231:ARG:HD2	1.74	0.69
1:D:204:ARG:O	1:D:204:ARG:HD3	1.92	0.68
1:D:229:LEU:CA	1:D:237:VAL:HG21	2.23	0.68
1:A:30:VAL:O	1:A:34:GLN:HG3	1.93	0.68
1:B:131:ASP:CB	2:B:529:HOH:O	2.38	0.68
1:D:206:GLN:NE2	1:D:276:ARG:HH22	1.93	0.67
1:D:153:TRP:O	1:D:231:ARG:NH2	2.28	0.66
1:D:229:LEU:HA	1:D:237:VAL:HG21	1.78	0.66
1:B:79:ASP:C	1:B:81:GLY:N	2.52	0.64
1:A:24:GLU:HG3	1:A:284:THR:HB	1.78	0.64
1:A:146:GLN:HG2	1:A:153:TRP:CE2	2.33	0.63
1:C:24:GLU:HG3	1:C:284:THR:CG2	2.27	0.63
1:C:172:PHE:HE1	1:C:272:MET:HG3	1.63	0.63
1:B:50:ARG:HG3	1:B:50:ARG:HH11	1.62	0.63
1:B:79:ASP:O	1:B:81:GLY:N	2.32	0.63
1:C:148:VAL:HG12	1:C:148:VAL:O	1.98	0.63
1:A:31:ARG:HG2	1:A:280:TYR:HA	1.80	0.62
1:A:152:ARG:HD2	1:A:231:ARG:HG2	1.82	0.62
1:C:31:ARG:HH22	1:C:283:SER:HG	1.45	0.62
1:D:227:LEU:O	1:D:231:ARG:HB2	1.98	0.62
1:A:289:SER:O	1:A:290:ASP:HB2	2.00	0.62
1:A:277:VAL:HG22	1:A:281:ARG:HB3	1.81	0.61
1:A:28:GLU:OE2	1:A:281:ARG:HD3	1.99	0.61
1:C:232:TYR:HB2	1:C:235:MET:HG2	1.82	0.61
1:C:2:ILE:HD12	1:C:58:GLU:HG3	1.81	0.60
1:C:3:GLN:OE1	2:C:579:HOH:O	2.16	0.60
1:C:43:SER:HB2	2:C:455:HOH:O	2.00	0.60
1:A:35:TYR:O	1:A:39:ARG:HG2	2.00	0.60
1:D:225:VAL:O	1:D:229:LEU:HB3	2.02	0.60
1:B:81:GLY:HA3	2:B:506:HOH:O	2.01	0.59
1:C:24:GLU:HG3	1:C:284:THR:HG22	1.84	0.59
1:C:232:TYR:CG	1:C:235:MET:HE3	2.37	0.59
1:A:107:GLU:CD	1:A:107:GLU:H	2.11	0.58
1:B:79:ASP:C	1:B:81:GLY:H	2.11	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ARG:HD2	1:D:231:ARG:CD	2.34	0.58
1:B:79:ASP:O	1:B:80:LEU:C	2.47	0.57
1:B:276:ARG:HB2	1:B:279:TYR:CE1	2.39	0.57
1:B:177:LEU:HD23	1:B:177:LEU:C	2.28	0.57
1:B:230:GLN:HG2	2:C:563:HOH:O	2.04	0.57
1:B:41:HIS:HB3	1:B:42:PRO:HD3	1.87	0.57
1:A:6:ARG:NH1	1:A:58:GLU:OE1	2.37	0.57
1:C:235:MET:HE2	1:D:235:MET:CG	2.18	0.57
1:D:152:ARG:HD2	1:D:231:ARG:HE	1.68	0.57
1:A:226:ILE:O	1:A:230:GLN:HG3	2.05	0.56
1:A:96:GLY:O	1:A:134:ARG:NH1	2.38	0.56
1:D:88:LEU:HD23	1:D:141:ARG:HG3	1.87	0.56
1:C:41:HIS:HB3	1:C:42:PRO:HD3	1.87	0.56
1:A:276:ARG:HB3	1:A:278:GLN:HG2	1.88	0.55
1:C:146:GLN:HG3	1:C:153:TRP:CE2	2.41	0.55
1:B:199:ILE:CD1	1:B:273:ALA:CA	2.77	0.55
1:B:50:ARG:HH11	1:B:50:ARG:CG	2.19	0.55
1:D:101:CYS:O	1:D:103:LEU:N	2.37	0.55
1:B:16:ARG:CZ	2:B:402:HOH:O	2.55	0.55
1:D:77:CYS:HB2	1:D:83:ILE:HD12	1.90	0.54
1:D:204:ARG:HD3	1:D:204:ARG:C	2.33	0.54
1:C:199:ILE:HD11	1:C:273:ALA:N	2.23	0.54
1:D:227:LEU:C	1:D:227:LEU:HD12	2.33	0.54
1:B:170:ASN:H	1:B:170:ASN:HD22	1.55	0.53
1:D:134:ARG:NH2	2:D:513:HOH:O	2.41	0.53
1:C:235:MET:SD	1:D:235:MET:HE2	2.48	0.53
1:A:277:VAL:HG22	1:A:281:ARG:CB	2.38	0.53
1:B:192:PHE:O	1:B:195:VAL:HG22	2.09	0.53
1:A:277:VAL:HA	1:A:280:TYR:CE2	2.44	0.53
2:B:477:HOH:O	1:C:253:HIS:HD2	1.92	0.52
1:A:92:GLU:OE2	2:A:546:HOH:O	2.19	0.52
1:B:54:ASP:OD1	1:B:56:GLN:N	2.38	0.52
1:B:172:PHE:CE1	1:B:272:MET:HG3	2.45	0.51
1:B:196:LEU:HD12	1:B:196:LEU:O	2.10	0.51
1:D:2:ILE:HD11	1:D:6:ARG:HG2	1.91	0.51
1:D:101:CYS:C	1:D:103:LEU:H	2.19	0.51
1:D:229:LEU:N	1:D:237:VAL:HG21	2.26	0.51
1:C:186:LEU:HD13	1:C:192:PHE:CE1	2.46	0.51
1:D:227:LEU:O	1:D:231:ARG:HD3	2.11	0.51
1:B:221:ALA:HB2	1:B:230:GLN:HE22	1.76	0.51
1:D:97:GLN:O	1:D:99:VAL:HG12	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:NH1	1:D:58:GLU:OE1	2.43	0.51
1:C:146:GLN:HG3	1:C:153:TRP:CD2	2.45	0.50
1:D:195:VAL:HG11	1:D:269:ILE:HD13	1.92	0.50
1:D:2:ILE:HD12	1:D:58:GLU:CD	2.36	0.50
1:B:214:LYS:H	1:B:214:LYS:HD2	1.76	0.50
1:A:79:ASP:OD1	1:A:144:HIS:CE1	2.64	0.50
1:D:276:ARG:NE	1:D:276:ARG:HA	2.27	0.50
1:B:199:ILE:HD11	1:B:273:ALA:N	2.26	0.49
1:A:170:ASN:HD22	1:A:170:ASN:N	2.07	0.49
1:B:172:PHE:HE1	1:B:272:MET:HG3	1.78	0.49
1:D:230:GLN:O	1:D:231:ARG:C	2.56	0.49
1:C:152:ARG:HG3	1:C:231:ARG:HH21	1.77	0.49
1:C:232:TYR:CB	1:C:235:MET:HE3	2.43	0.49
1:A:206:GLN:NE2	2:A:527:HOH:O	2.44	0.49
1:A:253:HIS:HD2	2:A:559:HOH:O	1.95	0.49
1:D:206:GLN:CD	1:D:276:ARG:HH22	2.21	0.49
1:B:92:GLU:OE2	1:B:141:ARG:HD3	2.13	0.48
1:C:42:PRO:O	1:C:45:ARG:HB2	2.12	0.48
1:D:199:ILE:HD11	1:D:273:ALA:CA	2.43	0.48
1:A:211:GLY:HA2	1:A:214:LYS:HD2	1.94	0.48
1:B:276:ARG:HB2	1:B:279:TYR:CD1	2.49	0.48
1:D:56:GLN:HA	1:D:61:ILE:HD11	1.94	0.48
1:C:223:ASN:HB3	1:C:226:ILE:HD12	1.96	0.48
1:B:131:ASP:CG	2:B:529:HOH:O	2.55	0.48
1:D:100:PRO:HA	1:D:113:ARG:NH1	2.29	0.48
1:D:229:LEU:O	1:D:230:GLN:O	2.31	0.48
1:A:170:ASN:H	1:A:170:ASN:ND2	2.05	0.48
1:A:170:ASN:N	1:A:170:ASN:ND2	2.62	0.48
1:B:225:VAL:HG22	1:B:241:LEU:HD12	1.96	0.48
1:B:76:ASP:HB3	1:B:82:LEU:HD11	1.96	0.47
1:B:213:ASP:CG	1:B:216:ARG:HH21	2.22	0.47
1:D:236:PRO:HB2	1:D:239:GLU:HB3	1.95	0.47
1:B:57:ASP:OD1	1:B:57:ASP:C	2.58	0.47
1:D:223:ASN:CB	1:D:226:ILE:HG12	2.45	0.47
1:B:146:GLN:HG2	1:B:153:TRP:CE3	2.49	0.47
1:A:31:ARG:HG2	1:A:279:TYR:O	2.15	0.47
1:A:276:ARG:C	1:A:278:GLN:N	2.70	0.47
1:B:41:HIS:HE1	1:B:45:ARG:NE	2.13	0.47
1:D:232:TYR:HA	1:D:233:PRO:HD2	1.64	0.47
1:A:210:HIS:CE1	1:A:278:GLN:HE22	2.33	0.47
1:B:256:MET:HE2	1:B:269:ILE:CG2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:GLN:CD	1:D:276:ARG:NH2	2.73	0.47
1:C:147:ALA:HB2	1:C:222:ASP:HB2	1.97	0.47
1:C:36:ILE:HD11	1:C:272:MET:SD	2.55	0.47
1:D:197:ARG:NH1	2:D:540:HOH:O	2.47	0.47
1:B:136:TYR:CZ	1:B:140:LEU:HD11	2.51	0.46
1:C:158:TYR:OH	1:C:208:ASP:OD2	2.31	0.46
1:A:141:ARG:HH11	1:A:141:ARG:HB3	1.81	0.46
1:D:134:ARG:HG2	1:D:134:ARG:HH11	1.81	0.46
1:B:56:GLN:HA	1:B:61:ILE:HD11	1.98	0.46
1:B:9:GLN:OE1	1:B:13:GLU:HG2	2.16	0.46
1:B:50:ARG:CG	1:B:50:ARG:NH1	2.78	0.46
1:D:74:LEU:HD23	1:D:83:ILE:HD13	1.98	0.46
1:C:41:HIS:O	1:C:42:PRO:C	2.57	0.45
1:A:151:GLU:CD	2:A:572:HOH:O	2.59	0.45
1:A:282:THR:HG23	1:A:283:SER:N	2.31	0.45
1:A:27:VAL:HB	1:A:284:THR:HG21	1.99	0.45
1:A:107:GLU:CD	1:A:107:GLU:N	2.74	0.45
1:B:230:GLN:CD	1:C:257:ALA:O	2.59	0.45
1:D:186:LEU:HD11	1:D:265:TRP:CD1	2.52	0.45
1:B:48:SER:OG	1:B:55:PRO:HD3	2.15	0.45
1:C:284:THR:O	1:C:285:SER:HB2	2.16	0.45
1:B:256:MET:HE2	1:B:269:ILE:HG21	1.99	0.45
1:C:36:ILE:CD1	1:C:272:MET:SD	3.05	0.45
1:D:135:CYS:SG	1:D:164:ASP:CG	3.00	0.45
1:C:170:ASN:HD22	1:C:170:ASN:H	1.65	0.45
1:B:9:GLN:NE2	1:B:9:GLN:HA	2.33	0.44
1:A:187:ARG:NH2	2:A:493:HOH:O	2.23	0.44
1:C:191:ALA:HB1	1:C:259:GLU:HG3	2.00	0.44
1:B:199:ILE:HD13	1:B:273:ALA:HB2	1.99	0.44
1:B:34:GLN:O	1:B:38:GLN:HG3	2.17	0.44
1:C:107:GLU:O	1:C:107:GLU:HG3	2.17	0.44
1:D:147:ALA:O	1:D:151:GLU:HG3	2.18	0.44
1:D:5:GLU:OE2	1:D:9:GLN:NE2	2.35	0.44
1:D:117:ALA:HB2	1:D:126:TYR:CE1	2.53	0.44
1:B:218:ALA:O	1:C:253:HIS:HB2	2.18	0.43
1:C:176:SER:HA	1:C:181:LEU:HB2	1.99	0.43
1:D:101:CYS:O	1:D:101:CYS:SG	2.76	0.43
1:D:231:ARG:CB	1:D:231:ARG:HH11	2.31	0.43
1:C:100:PRO:HA	1:C:110:ALA:HB2	2.00	0.43
1:C:172:PHE:HE1	1:C:272:MET:CG	2.31	0.43
1:D:223:ASN:N	1:D:226:ILE:HD11	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:HA	1:A:284:THR:HG21	2.00	0.43
1:C:44:LEU:O	1:C:47:THR:N	2.47	0.43
1:C:250:ARG:O	1:C:254:ARG:HG3	2.18	0.43
1:A:94:ALA:HB2	1:A:101:CYS:HA	1.99	0.43
1:B:124:ARG:NH2	1:B:184:ALA:HB3	2.34	0.43
1:D:186:LEU:HD21	1:D:262:PRO:CD	2.49	0.43
1:B:35:TYR:CE2	1:B:275:ILE:HG13	2.54	0.43
1:B:230:GLN:NE2	1:C:257:ALA:HB1	2.34	0.42
1:C:186:LEU:HD13	1:C:192:PHE:CD1	2.54	0.42
1:A:158:TYR:OH	1:A:208:ASP:OD2	2.26	0.42
1:D:101:CYS:C	1:D:103:LEU:N	2.74	0.42
1:B:152:ARG:NE	1:B:230:GLN:OE1	2.41	0.42
1:A:153:TRP:HB2	1:A:157:GLU:HB2	2.02	0.42
1:A:289:SER:O	1:A:290:ASP:CB	2.67	0.42
1:B:279:TYR:CD1	1:B:279:TYR:N	2.87	0.42
1:C:232:TYR:O	1:C:233:PRO:C	2.62	0.42
1:D:2:ILE:CD1	1:D:10:GLN:NE2	2.83	0.42
1:B:9:GLN:HA	1:B:9:GLN:HE21	1.85	0.41
1:A:141:ARG:NH1	1:A:141:ARG:CB	2.83	0.41
1:A:277:VAL:HA	1:A:280:TYR:CZ	2.55	0.41
1:C:20:GLY:O	1:C:82:LEU:HD13	2.20	0.41
1:B:4:THR:O	1:B:8:VAL:HG23	2.20	0.41
1:A:6:ARG:CZ	2:A:530:HOH:O	2.69	0.41
1:A:265:TRP:O	1:A:269:ILE:HG12	2.21	0.41
1:D:103:LEU:HA	1:D:104:PRO:HD3	1.97	0.41
1:B:12:LEU:O	1:B:16:ARG:HG3	2.20	0.41
1:B:30:VAL:O	1:B:34:GLN:HB2	2.21	0.41
1:D:209:LEU:HD23	1:D:209:LEU:HA	1.82	0.41
1:A:41:HIS:HB3	1:A:42:PRO:HD3	2.02	0.41
1:B:5:GLU:OE2	1:B:5:GLU:O	2.39	0.41
1:B:191:ALA:O	1:B:195:VAL:HG13	2.21	0.41
1:D:100:PRO:HA	1:D:113:ARG:HH12	1.86	0.41
1:B:78:ASN:HD21	1:B:141:ARG:HG3	1.85	0.41
1:C:147:ALA:CB	1:C:222:ASP:HB2	2.50	0.41
1:C:148:VAL:O	1:C:148:VAL:CG1	2.67	0.41
1:D:199:ILE:HD11	1:D:273:ALA:HA	2.03	0.41
1:B:137:SER:HB2	2:B:520:HOH:O	2.21	0.40
1:B:228:LEU:HA	1:B:228:LEU:HD23	1.84	0.40
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.89	0.40
1:C:199:ILE:HD11	1:C:273:ALA:CA	2.51	0.40
1:D:128:GLN:HG2	1:D:187:ARG:NH2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:HE2	1:A:266:GLY:HA2	2.03	0.40
1:D:135:CYS:SG	1:D:164:ASP:OD2	2.79	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	286/300 (95%)	281 (98%)	2 (1%)	3 (1%)	12	8
1	B	277/300 (92%)	272 (98%)	4 (1%)	1 (0%)	30	27
1	C	277/300 (92%)	269 (97%)	6 (2%)	2 (1%)	18	14
1	D	263/300 (88%)	252 (96%)	7 (3%)	4 (2%)	8	4
All	All	1103/1200 (92%)	1074 (97%)	19 (2%)	10 (1%)	14	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	THR
1	C	282	THR
1	D	230	GLN
1	D	233	PRO
1	C	285	SER
1	A	285	SER
1	B	80	LEU
1	A	281	ARG
1	D	231	ARG
1	D	237	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/237 (97%)	219 (95%)	11 (5%)	23	21
1	B	221/237 (93%)	211 (96%)	10 (4%)	24	23
1	C	225/237 (95%)	217 (96%)	8 (4%)	31	31
1	D	213/237 (90%)	199 (93%)	14 (7%)	15	12
All	All	889/948 (94%)	846 (95%)	43 (5%)	23	21

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	50	ARG
1	A	85	PRO
1	A	144	HIS
1	A	146	GLN
1	A	151	GLU
1	A	170	ASN
1	A	264	PRO
1	A	283	SER
1	A	284	THR
1	A	290	ASP
1	B	5	GLU
1	B	43	SER
1	B	45	ARG
1	B	50	ARG
1	B	146	GLN
1	B	151	GLU
1	B	170	ASN
1	B	186	LEU
1	B	196	LEU
1	B	278	GLN
1	C	43	SER
1	C	74	LEU
1	C	107	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	170	ASN
1	C	186	LEU
1	C	199	ILE
1	C	231	ARG
1	C	290	ASP
1	D	48	SER
1	D	88	LEU
1	D	99	VAL
1	D	118	THR
1	D	152	ARG
1	D	196	LEU
1	D	210	HIS
1	D	227	LEU
1	D	229	LEU
1	D	230	GLN
1	D	231	ARG
1	D	264	PRO
1	D	276	ARG
1	D	277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	160	HIS
1	A	170	ASN
1	A	194	GLN
1	A	206	GLN
1	B	34	GLN
1	B	41	HIS
1	B	56	GLN
1	B	78	ASN
1	B	93	GLN
1	B	170	ASN
1	B	278	GLN
1	C	38	GLN
1	C	78	ASN
1	C	144	HIS
1	C	146	GLN
1	C	170	ASN
1	C	210	HIS
1	C	253	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	34	GLN
1	D	41	HIS
1	D	97	GLN
1	D	170	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/300 (96%)	-0.33	11 (3%) 44 43	10, 20, 62, 83	0
1	B	279/300 (93%)	-0.03	12 (4%) 40 39	12, 26, 54, 79	0
1	C	281/300 (93%)	-0.26	8 (2%) 55 54	11, 21, 48, 74	0
1	D	267/300 (89%)	-0.18	8 (2%) 52 51	11, 24, 51, 62	0
All	All	1115/1200 (92%)	-0.20	39 (3%) 47 46	10, 23, 54, 83	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	284	THR	6.4
1	B	81	GLY	4.3
1	B	80	LEU	4.2
1	D	229	LEU	3.9
1	C	285	SER	3.7
1	B	218	ALA	3.6
1	B	83	ILE	3.4
1	A	282	THR	3.3
1	A	212	CYS	3.1
1	A	277	VAL	3.1
1	B	277	VAL	3.0
1	B	82	LEU	2.9
1	A	284	THR	2.9
1	C	282	THR	2.8
1	D	280	TYR	2.8
1	A	283	SER	2.7
1	C	79	ASP	2.7
1	D	233	PRO	2.6
1	D	226	ILE	2.6
1	A	218	ALA	2.6
1	B	84	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	221	ALA	2.5
1	A	281	ARG	2.5
1	B	79	ASP	2.4
1	B	276	ARG	2.4
1	B	279	TYR	2.3
1	A	290	ASP	2.3
1	A	279	TYR	2.3
1	A	280	TYR	2.3
1	C	283	SER	2.2
1	B	280	TYR	2.1
1	C	81	GLY	2.1
1	D	102	ALA	2.1
1	A	79	ASP	2.1
1	D	230	GLN	2.1
1	B	45	ARG	2.1
1	C	289	SER	2.1
1	D	224	ALA	2.0
1	D	100	PRO	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.