



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:12 AM GMT

PDB ID : 3L1A  
Title : Structural ordering of disordered ligand binding loops of biotin protein ligase into active conformations as a consequence of dehydration  
Authors : Gupta, V.  
Deposited on : 2009-12-11  
Resolution : 2.69 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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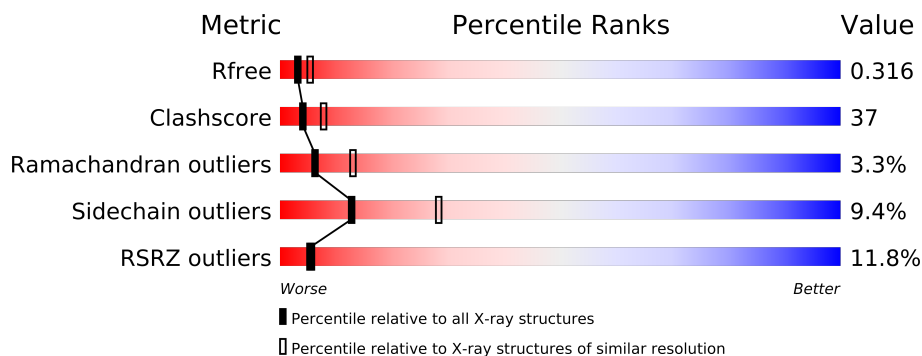
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.69 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	266	
1	B	266	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3610 atoms, of which 0 are hydrogen and 0 are deuterium.

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 BirA bifunctional protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			1928	1200	363	364	1			
1	B	228	Total	C	N	O	S	0	0	0
			1651	1039	298	313	1			

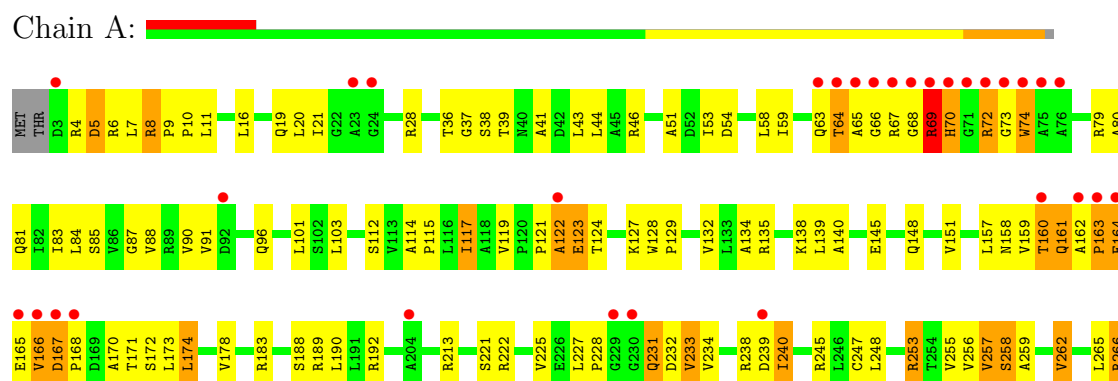
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	12	Total	O	0	0
			12	12		

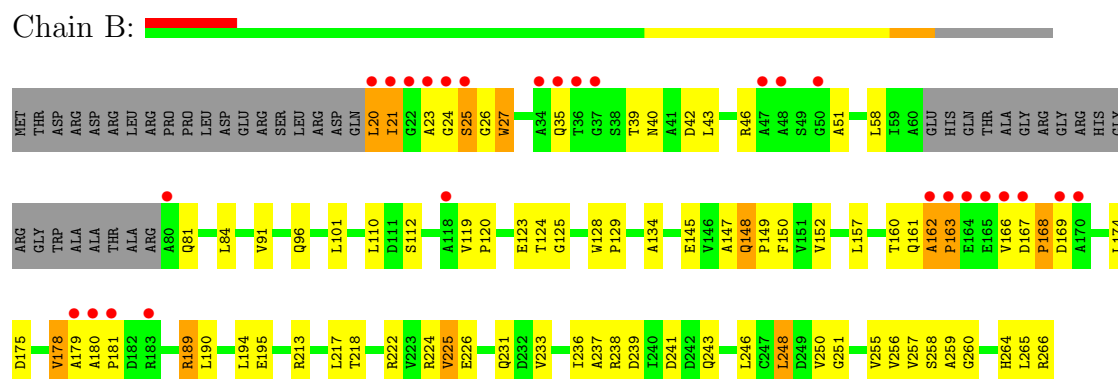
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: BirA bifunctional protein



- Molecule 1: BirA bifunctional protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.93Å 63.80Å 103.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.99 – 2.69 24.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (23.99-2.69) 98.9 (24.74-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.233 , 0.313 0.252 , 0.316	Depositor DCC
$R_{free}$ test set	1148 reflections (11.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 14096 reflections (0.014%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.41	1/1957 (0.1%)	0.60	0/2675
1	B	0.43	0/1673	0.76	3/2290 (0.1%)
All	All	0.42	1/3630 (0.0%)	0.68	3/4965 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	GLU	CD-OE2	6.89	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ARG	NE-CZ-NH1	-13.14	113.73	120.30
1	B	238	ARG	NE-CZ-NH2	12.67	126.64	120.30
1	B	238	ARG	CD-NE-CZ	6.00	132.00	123.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1928	0	1931	187	1
1	B	1651	0	1682	86	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	0	2	0
2	B	12	0	0	2	0
All	All	3610	0	3613	266	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

All (266) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:PRO:CB	1:A:164:GLU:HG2	1.18	1.52
1:A:163:PRO:HB2	1:A:164:GLU:CG	1.46	1.40
1:A:166:VAL:HB	1:A:167:ASP:CB	1.56	1.34
1:A:166:VAL:N	1:A:167:ASP:HB3	1.52	1.24
1:B:20:LEU:HD22	1:B:20:LEU:O	1.41	1.21
1:A:63:GLN:NE2	1:A:66:GLY:HA2	1.58	1.18
1:A:69:ARG:CB	1:A:69:ARG:HH11	1.63	1.11
1:A:166:VAL:HB	1:A:167:ASP:HB3	1.32	1.10
1:B:25:SER:O	1:B:195:GLU:OE1	1.65	1.10
1:A:166:VAL:CB	1:A:167:ASP:HB3	1.82	1.10
1:B:189:ARG:CB	1:B:189:ARG:HH11	1.65	1.09
1:A:166:VAL:CB	1:A:167:ASP:CB	2.30	1.08
1:A:166:VAL:HB	1:A:167:ASP:HB2	1.21	1.08
1:A:166:VAL:CA	1:A:167:ASP:HB3	1.83	1.08
1:A:163:PRO:HB3	1:A:164:GLU:HG2	1.31	1.06
1:A:163:PRO:CB	1:A:164:GLU:CG	2.15	1.05
1:A:121:PRO:HG2	1:A:124:THR:HG21	1.08	1.05
1:A:165:GLU:O	1:A:166:VAL:HG23	1.60	1.02
1:A:69:ARG:HH11	1:A:69:ARG:HB3	1.23	1.01
1:A:121:PRO:HG2	1:A:124:THR:CG2	1.89	1.01
1:A:121:PRO:CG	1:A:124:THR:HG21	1.93	0.99
1:A:70:HIS:HA	2:A:2016:HOH:O	1.64	0.97
1:A:124:THR:HG22	1:A:135:ARG:H	1.29	0.97
1:A:166:VAL:H	1:A:167:ASP:C	1.67	0.96
1:A:8:ARG:HE	1:A:160:THR:HG21	1.26	0.96
1:A:64:THR:O	1:A:74:TRP:O	1.85	0.95
1:B:189:ARG:CG	1:B:189:ARG:HH11	1.78	0.95
1:A:227:LEU:HB3	1:A:228:PRO:HD2	1.50	0.94
1:A:166:VAL:N	1:A:167:ASP:CB	2.30	0.93
1:A:63:GLN:CD	1:A:66:GLY:HA2	1.89	0.93
1:A:167:ASP:N	1:A:168:PRO:CD	2.30	0.91
1:B:166:VAL:HG12	1:B:168:PRO:HG3	1.54	0.89
1:A:65:ALA:HB1	1:A:73:GLY:HA3	1.54	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:GLN:CD	1:A:66:GLY:CA	2.42	0.88
1:B:26:GLY:HA3	1:B:195:GLU:OE2	1.73	0.87
1:A:74:TRP:HB2	1:A:166:VAL:HG22	1.57	0.87
1:A:166:VAL:CA	1:A:167:ASP:CB	2.48	0.86
1:A:166:VAL:CB	1:A:167:ASP:HB2	1.98	0.86
1:A:74:TRP:CB	1:A:166:VAL:HG22	2.06	0.86
1:A:166:VAL:C	1:A:168:PRO:HD3	1.97	0.84
1:A:38:SER:HB2	1:A:67:ARG:H	1.40	0.83
1:A:80:ALA:CB	1:A:162:ALA:HB2	2.09	0.83
1:A:127:LYS:HE2	1:A:262:VAL:O	1.79	0.82
1:A:213:ARG:HD3	1:A:239:ASP:OD1	1.79	0.81
1:A:225:VAL:HB	1:A:233:VAL:HG23	1.64	0.79
1:A:128:TRP:CZ2	1:A:258:SER:O	2.36	0.79
1:A:124:THR:HG22	1:A:135:ARG:N	1.98	0.78
1:A:162:ALA:N	1:A:163:PRO:HD3	1.98	0.78
1:A:74:TRP:HB2	1:A:166:VAL:CG2	2.13	0.77
1:A:69:ARG:NH1	1:A:69:ARG:HB3	1.99	0.77
1:A:37:GLY:HA2	1:A:64:THR:HG23	1.65	0.77
1:B:20:LEU:HD22	1:B:20:LEU:C	2.05	0.76
1:A:162:ALA:N	1:A:163:PRO:CD	2.48	0.76
1:A:227:LEU:HB3	1:A:228:PRO:CD	2.16	0.76
1:A:128:TRP:HZ2	1:A:258:SER:O	1.68	0.75
1:A:222:ARG:HB3	1:A:266:ARG:HB3	1.67	0.74
1:A:38:SER:HA	1:A:63:GLN:HE21	1.51	0.74
1:B:166:VAL:HG12	1:B:168:PRO:CG	2.17	0.74
1:B:189:ARG:CB	1:B:189:ARG:NH1	2.47	0.74
1:A:63:GLN:NE2	1:A:66:GLY:CA	2.45	0.73
1:A:188:SER:O	1:A:192:ARG:HG3	1.89	0.72
1:A:161:GLN:C	1:A:163:PRO:HD3	2.09	0.72
1:B:189:ARG:HB2	1:B:189:ARG:HH11	1.50	0.71
1:A:167:ASP:N	1:A:168:PRO:HD3	2.04	0.71
1:A:63:GLN:OE1	1:A:66:GLY:CA	2.37	0.70
1:A:167:ASP:N	1:A:168:PRO:HD2	2.06	0.70
1:A:256:VAL:HB	1:B:256:VAL:HB	1.74	0.70
1:A:7:LEU:O	1:A:8:ARG:HB2	1.91	0.70
1:A:123:GLU:CG	1:A:123:GLU:O	2.39	0.69
1:A:166:VAL:N	1:A:167:ASP:CA	2.57	0.68
1:A:240:ILE:HG23	1:A:245:ARG:O	1.94	0.68
1:A:245:ARG:HG2	1:A:258:SER:HA	1.74	0.68
1:A:166:VAL:H	1:A:167:ASP:CA	2.06	0.67
1:B:120:PRO:HD2	1:B:123:GLU:OE2	1.95	0.67
1:A:158:ASN:O	1:A:172:SER:HA	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:PRO:HB2	1:A:164:GLU:HG2	0.67	0.67
1:B:20:LEU:HD13	1:B:21:ILE:N	2.10	0.66
1:B:237:ALA:HA	1:B:248:LEU:HD12	1.76	0.66
1:A:10:PRO:HG3	1:A:79:ARG:NH1	2.10	0.66
1:B:20:LEU:CD2	1:B:20:LEU:O	2.32	0.66
1:B:189:ARG:HB2	1:B:189:ARG:NH1	2.09	0.66
1:B:23:ALA:N	1:B:24:GLY:HA3	2.10	0.66
1:B:174:LEU:HA	1:B:178:VAL:O	1.95	0.66
1:B:189:ARG:CG	1:B:189:ARG:NH1	2.47	0.66
1:A:165:GLU:O	1:A:166:VAL:CG2	2.42	0.66
1:A:79:ARG:HB3	1:A:183:ARG:NH1	2.11	0.66
1:B:189:ARG:NH1	1:B:189:ARG:HG2	2.09	0.65
1:B:189:ARG:HG2	1:B:189:ARG:HH11	1.56	0.65
1:A:240:ILE:CG2	1:A:245:ARG:O	2.45	0.65
1:A:163:PRO:HB3	1:A:164:GLU:CG	2.09	0.65
1:A:69:ARG:CG	1:A:69:ARG:HH11	2.10	0.64
1:A:63:GLN:OE1	1:A:66:GLY:HA3	1.96	0.64
1:A:165:GLU:N	1:A:167:ASP:O	2.30	0.64
1:A:165:GLU:C	1:A:167:ASP:HB3	2.15	0.64
1:A:239:ASP:O	1:A:247:CYS:HB2	1.97	0.64
1:A:69:ARG:CB	1:A:69:ARG:NH1	2.49	0.64
1:A:65:ALA:HB1	1:A:73:GLY:CA	2.28	0.64
1:A:79:ARG:HB3	1:A:183:ARG:HH12	1.63	0.63
1:B:166:VAL:CG1	1:B:168:PRO:HG3	2.27	0.63
1:A:123:GLU:HG2	1:A:123:GLU:O	1.97	0.63
1:B:81:GLN:HB2	1:B:157:LEU:O	1.99	0.62
1:A:80:ALA:HB3	1:A:162:ALA:HB2	1.78	0.62
1:A:8:ARG:NE	1:A:160:THR:HG21	2.09	0.62
1:A:7:LEU:O	1:A:8:ARG:CB	2.48	0.62
1:A:81:GLN:HB2	1:A:157:LEU:O	2.00	0.62
1:A:221:SER:HA	1:A:266:ARG:HD3	1.81	0.61
1:A:79:ARG:CB	1:A:183:ARG:HH12	2.14	0.60
1:A:253:ARG:CZ	1:B:260:GLY:HA3	2.31	0.60
1:A:43:LEU:HD12	1:A:85:SER:HB3	1.83	0.60
1:A:19:GLN:HG2	1:A:19:GLN:O	2.01	0.60
1:A:112:SER:HA	1:A:189:ARG:HG2	1.84	0.59
1:B:168:PRO:O	1:B:169:ASP:HB2	2.02	0.59
1:B:39:THR:HG22	1:B:58:LEU:HD23	1.83	0.59
1:B:20:LEU:C	1:B:20:LEU:HD13	2.22	0.59
1:A:44:LEU:HD13	1:A:69:ARG:HB2	1.82	0.59
1:B:40:ASN:OD1	1:B:152:VAL:HG12	2.03	0.58
1:B:162:ALA:H	1:B:163:PRO:CD	2.17	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:VAL:H	1:B:231:GLN:HE22	1.52	0.58
1:A:80:ALA:HB1	1:A:162:ALA:HB2	1.84	0.58
1:A:159:VAL:HG22	1:A:173:LEU:CD1	2.34	0.58
1:B:125:GLY:HA3	1:B:217:LEU:HG	1.87	0.57
1:B:161:GLN:HG3	1:B:163:PRO:HD2	1.86	0.57
1:A:239:ASP:CG	1:A:240:ILE:N	2.58	0.57
1:A:79:ARG:CG	1:A:183:ARG:HH12	2.16	0.57
1:B:166:VAL:HG12	1:B:168:PRO:HD3	1.87	0.56
1:A:161:GLN:HA	1:A:172:SER:HB3	1.87	0.56
1:A:68:GLY:O	1:A:69:ARG:C	2.43	0.56
1:B:162:ALA:N	1:B:163:PRO:CD	2.68	0.56
1:A:166:VAL:N	1:A:167:ASP:C	2.49	0.56
1:B:160:THR:HG22	1:B:161:GLN:O	2.06	0.56
1:B:179:ALA:C	1:B:181:PRO:HD3	2.27	0.55
1:B:166:VAL:HG12	1:B:168:PRO:CD	2.37	0.55
1:A:114:ALA:HB3	1:A:115:PRO:HD3	1.89	0.55
1:B:225:VAL:HG11	1:B:248:LEU:HD21	1.88	0.55
1:B:178:VAL:HB	1:B:181:PRO:HG3	1.89	0.55
1:B:128:TRP:CH2	1:B:259:ALA:HA	2.41	0.55
1:B:163:PRO:HB3	2:B:2031:HOH:O	2.05	0.55
1:A:69:ARG:O	1:A:70:HIS:ND1	2.41	0.54
1:A:70:HIS:CA	2:A:2016:HOH:O	2.36	0.54
1:A:124:THR:HG22	1:A:134:ALA:HA	1.89	0.54
1:A:164:GLU:C	1:A:167:ASP:O	2.45	0.54
1:A:127:LYS:CE	1:A:262:VAL:O	2.53	0.54
1:B:25:SER:O	1:B:195:GLU:CD	2.43	0.54
1:B:119:VAL:HB	1:B:123:GLU:OE2	2.08	0.54
1:A:69:ARG:CG	1:A:69:ARG:NH1	2.70	0.53
1:A:112:SER:OG	1:A:190:LEU:HA	2.09	0.53
1:B:43:LEU:HD13	1:B:58:LEU:HD22	1.91	0.53
1:A:145:GLU:O	1:A:151:VAL:HG13	2.09	0.53
1:A:167:ASP:H	1:A:168:PRO:HD2	1.72	0.53
1:B:84:LEU:C	1:B:84:LEU:HD12	2.30	0.53
1:A:159:VAL:HG13	1:A:173:LEU:HD12	1.91	0.52
1:B:224:ARG:HB2	1:B:265:LEU:HD21	1.90	0.52
1:A:128:TRP:CH2	1:A:259:ALA:HA	2.44	0.52
1:A:37:GLY:O	1:A:63:GLN:HG3	2.09	0.52
1:A:41:ALA:HB2	1:A:68:GLY:HA2	1.91	0.52
1:B:162:ALA:H	1:B:163:PRO:HD3	1.74	0.52
1:A:74:TRP:CD2	1:A:74:TRP:N	2.78	0.52
1:B:161:GLN:CG	1:B:163:PRO:HD2	2.40	0.52
1:A:59:ILE:HG23	1:A:83:ILE:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:PRO:HB2	1:A:164:GLU:CB	2.30	0.51
1:B:218:THR:HA	1:B:264:HIS:NE2	2.25	0.51
1:A:10:PRO:HG3	1:A:79:ARG:CZ	2.40	0.51
1:A:138:LYS:O	1:A:170:ALA:HB1	2.10	0.50
1:A:53:ILE:O	1:A:87:GLY:HA3	2.12	0.50
1:A:174:LEU:HD12	1:A:178:VAL:O	2.12	0.50
1:A:253:ARG:NH1	1:B:260:GLY:HA3	2.27	0.50
1:A:231:GLN:O	1:A:232:ASP:OD1	2.30	0.50
1:A:28:ARG:NE	1:A:54:ASP:O	2.44	0.50
1:A:80:ALA:HA	1:A:160:THR:OG1	2.13	0.49
1:A:4:ARG:O	1:A:5:ASP:OD1	2.30	0.49
1:A:63:GLN:HE22	1:A:66:GLY:HA2	1.62	0.49
1:A:11:LEU:N	1:A:183:ARG:HH21	2.11	0.48
1:A:119:VAL:O	1:A:119:VAL:HG13	2.13	0.48
1:B:163:PRO:HG3	1:B:166:VAL:HB	1.95	0.48
1:A:227:LEU:HD21	1:A:257:VAL:CG2	2.43	0.48
1:A:228:PRO:HB2	1:B:251:GLY:HA3	1.95	0.48
1:B:26:GLY:O	1:B:27:TRP:O	2.31	0.48
1:A:255:VAL:HG13	1:B:255:VAL:HG13	1.95	0.48
1:B:42:ASP:O	1:B:46:ARG:HG3	2.13	0.48
1:B:222:ARG:HG3	1:B:265:LEU:HD12	1.96	0.48
1:A:69:ARG:O	1:A:70:HIS:CB	2.59	0.48
1:A:239:ASP:O	1:A:247:CYS:CB	2.62	0.48
1:B:163:PRO:HB2	1:B:166:VAL:HG23	1.95	0.48
1:A:79:ARG:CB	1:A:183:ARG:NH1	2.76	0.48
1:A:59:ILE:HG12	1:A:84:LEU:HB2	1.96	0.47
1:A:74:TRP:HB2	1:A:166:VAL:HG21	1.96	0.47
1:A:139:LEU:HD12	1:A:171:THR:O	2.15	0.47
1:A:90:VAL:HG11	1:A:151:VAL:CG2	2.45	0.47
1:A:121:PRO:HB2	1:A:135:ARG:CG	2.45	0.47
1:A:84:LEU:HD12	1:A:84:LEU:C	2.35	0.47
1:A:128:TRP:CD1	1:A:240:ILE:HD12	2.50	0.47
1:B:124:THR:HG22	1:B:134:ALA:CB	2.45	0.47
1:A:16:LEU:O	1:A:20:LEU:HB2	2.14	0.47
1:A:159:VAL:HG22	1:A:173:LEU:HD12	1.96	0.46
1:A:157:LEU:HD23	1:A:159:VAL:HG23	1.98	0.46
1:A:74:TRP:HB3	1:A:166:VAL:HG22	1.93	0.46
1:B:225:VAL:CG1	1:B:248:LEU:HD21	2.45	0.46
1:A:4:ARG:O	1:A:5:ASP:CG	2.54	0.46
1:B:43:LEU:HD11	1:B:58:LEU:HD13	1.97	0.46
1:A:74:TRP:N	1:A:74:TRP:CE3	2.84	0.46
1:A:159:VAL:HG22	1:A:173:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:58:LEU:O	1:B:84:LEU:HB2	2.16	0.45
1:A:58:LEU:HD12	1:A:59:ILE:N	2.31	0.45
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.67	0.45
1:A:68:GLY:O	1:A:70:HIS:N	2.50	0.45
1:B:112:SER:OG	1:B:190:LEU:HA	2.17	0.45
1:B:124:THR:HG22	1:B:134:ALA:HB2	1.97	0.45
1:B:149:PRO:HD2	1:B:150:PHE:CD1	2.52	0.45
1:B:46:ARG:HB3	1:B:51:ALA:HB3	1.98	0.45
1:A:63:GLN:CD	1:A:66:GLY:N	2.71	0.45
1:B:112:SER:HA	1:B:189:ARG:CG	2.47	0.45
1:A:121:PRO:O	1:A:122:ALA:O	2.35	0.44
1:B:110:LEU:O	1:B:110:LEU:HD12	2.17	0.44
1:A:69:ARG:HB2	1:A:69:ARG:HH11	1.71	0.44
1:A:68:GLY:O	1:A:70:HIS:O	2.35	0.44
1:A:79:ARG:HG2	1:A:183:ARG:HH12	1.80	0.44
1:A:38:SER:CB	1:A:67:ARG:H	2.21	0.44
1:A:9:PRO:O	1:A:183:ARG:CZ	2.66	0.44
1:B:180:ALA:N	1:B:181:PRO:HD3	2.32	0.44
1:B:147:ALA:O	1:B:148:GLN:C	2.56	0.44
1:B:213:ARG:HD3	1:B:239:ASP:OD1	2.17	0.44
1:A:46:ARG:HB3	1:A:51:ALA:HB3	2.00	0.44
1:A:39:THR:HB	1:A:85:SER:HB2	1.99	0.44
1:B:246:LEU:HB3	1:B:257:VAL:CG2	2.47	0.44
1:B:128:TRP:HA	1:B:129:PRO:HA	1.78	0.44
1:B:101:LEU:HA	1:B:101:LEU:HD23	1.69	0.43
1:B:124:THR:HA	1:B:134:ALA:HA	1.99	0.43
1:B:236:ILE:N	1:B:236:ILE:HD12	2.34	0.43
1:A:221:SER:CA	1:A:266:ARG:HD3	2.47	0.43
1:A:72:ARG:HA	1:A:72:ARG:HD2	1.49	0.43
1:A:228:PRO:HG2	1:B:250:VAL:O	2.18	0.43
1:B:20:LEU:O	1:B:21:ILE:C	2.55	0.43
1:A:124:THR:CB	1:A:134:ALA:HA	2.48	0.43
1:A:88:VAL:O	1:A:90:VAL:HG13	2.19	0.43
1:A:240:ILE:HG23	1:A:245:ARG:C	2.39	0.43
1:B:225:VAL:HG11	1:B:248:LEU:CD2	2.49	0.43
1:A:90:VAL:HG11	1:A:151:VAL:HG23	2.00	0.43
1:A:69:ARG:O	1:A:70:HIS:HB3	2.19	0.42
1:B:266:ARG:NH1	2:B:2024:HOH:O	2.51	0.42
1:B:241:ASP:C	1:B:243:GLN:H	2.23	0.42
1:A:227:LEU:HD21	1:A:257:VAL:HG21	2.00	0.42
1:A:239:ASP:CG	1:A:240:ILE:H	2.21	0.42
1:A:21:ILE:HD13	1:A:21:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:ARG:H	1:A:266:ARG:HG2	1.84	0.42
1:A:248:LEU:HB3	1:A:255:VAL:O	2.18	0.42
1:A:128:TRP:HA	1:A:129:PRO:HA	1.73	0.42
1:A:124:THR:CG2	1:A:134:ALA:HA	2.50	0.42
1:A:117:ILE:H	1:A:117:ILE:HG12	1.46	0.42
1:A:36:THR:O	1:A:63:GLN:HA	2.19	0.41
1:A:121:PRO:HB2	1:A:135:ARG:HG3	2.01	0.41
1:A:240:ILE:HG22	1:A:245:ARG:O	2.20	0.41
1:A:123:GLU:HG3	1:A:123:GLU:O	2.19	0.41
1:B:148:GLN:HA	1:B:149:PRO:HA	1.87	0.41
1:A:163:PRO:HA	1:A:164:GLU:HA	1.80	0.41
1:A:74:TRP:CG	1:A:166:VAL:HG13	2.55	0.41
1:B:166:VAL:C	1:B:168:PRO:HD3	2.41	0.41
1:B:40:ASN:ND2	1:B:145:GLU:OE1	2.48	0.41
1:B:258:SER:O	1:B:259:ALA:C	2.59	0.41
1:A:227:LEU:O	1:A:228:PRO:C	2.58	0.41
1:B:178:VAL:O	1:B:181:PRO:HG3	2.21	0.41
1:A:221:SER:HB2	1:A:266:ARG:HG2	2.01	0.41
1:A:132:VAL:HB	1:A:140:ALA:HB3	2.03	0.41
1:B:26:GLY:C	1:B:27:TRP:O	2.59	0.40
1:A:138:LYS:N	1:A:170:ALA:HA	2.36	0.40
1:A:69:ARG:O	1:A:70:HIS:CG	2.74	0.40
1:A:10:PRO:HA	1:A:183:ARG:NH2	2.36	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	Distance(Å)	Clash(Å)
1:A:265:LEU:O	1:B:35:GLN:O[2_444]	2.17	0.03

## 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	262/266 (98%)	224 (86%)	29 (11%)	9 (3%)	6 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	224/266 (84%)	200 (89%)	17 (8%)	7 (3%)	7	14
All	All	486/532 (91%)	424 (87%)	46 (10%)	16 (3%)	6	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA
1	A	161	GLN
1	A	166	VAL
1	A	167	ASP
1	A	6	ARG
1	A	69	ARG
1	B	27	TRP
1	A	5	ASP
1	B	167	ASP
1	A	8	ARG
1	B	148	GLN
1	B	163	PRO
1	A	163	PRO
1	B	168	PRO
1	B	21	ILE
1	B	162	ALA

### 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	192/202 (95%)	170 (88%)	22 (12%)	8	19
1	B	168/202 (83%)	156 (93%)	12 (7%)	21	46
All	All	360/404 (89%)	326 (91%)	34 (9%)	13	28

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	69	ARG

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Mol	Chain	Res	Type
1	A	70	HIS
1	A	72	ARG
1	A	74	TRP
1	A	91	VAL
1	A	96	GLN
1	A	103	LEU
1	A	117	ILE
1	A	123	GLU
1	A	148	GLN
1	A	160	THR
1	A	174	LEU
1	A	231	GLN
1	A	233	VAL
1	A	238	ARG
1	A	240	ILE
1	A	253	ARG
1	A	257	VAL
1	A	258	SER
1	A	262	VAL
1	A	266	ARG
1	B	20	LEU
1	B	25	SER
1	B	91	VAL
1	B	96	GLN
1	B	175	ASP
1	B	178	VAL
1	B	189	ARG
1	B	194	LEU
1	B	225	VAL
1	B	226	GLU
1	B	233	VAL
1	B	248	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	158	ASN
1	B	161	GLN
1	B	231	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/266 (99%)	0.55	31 (11%) 5 6	25, 39, 70, 121	12 (4%)
1	B	228/266 (85%)	0.40	27 (11%) 5 5	20, 41, 81, 107	7 (3%)
All	All	492/532 (92%)	0.48	58 (11%) 5 5	20, 39, 79, 121	19 (3%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	PRO	13.1
1	A	162	ALA	10.6
1	A	73	GLY	9.8
1	A	66	GLY	8.7
1	A	75	ALA	8.7
1	A	74	TRP	8.2
1	A	72	ARG	7.2
1	B	164	GLU	6.6
1	A	69	ARG	6.5
1	A	71	GLY	6.4
1	B	162	ALA	6.2
1	B	21	ILE	6.1
1	B	163	PRO	6.1
1	B	165	GLU	5.7
1	B	34	ALA	5.7
1	B	167	ASP	5.6
1	A	65	ALA	5.5
1	B	24	GLY	4.6
1	B	20	LEU	4.5
1	B	23	ALA	4.2
1	A	164	GLU	4.0
1	B	179	ALA	4.0
1	A	68	GLY	3.7
1	B	22	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	166	VAL	3.6
1	A	3	ASP	3.6
1	A	67	ARG	3.5
1	B	37	GLY	3.5
1	B	166	VAL	3.2
1	A	160	THR	3.1
1	B	48	ALA	3.0
1	B	170	ALA	3.0
1	B	169	ASP	3.0
1	A	70	HIS	3.0
1	B	47	ALA	2.9
1	A	92	ASP	2.9
1	A	122	ALA	2.8
1	B	118	ALA	2.8
1	A	230	GLY	2.7
1	A	76	ALA	2.7
1	A	204	ALA	2.7
1	A	167	ASP	2.7
1	A	64	THR	2.6
1	B	183	ARG	2.6
1	A	24	GLY	2.5
1	B	35	GLN	2.5
1	B	80	ALA	2.5
1	A	168	PRO	2.4
1	A	239	ASP	2.4
1	A	23	ALA	2.4
1	B	180	ALA	2.4
1	B	50	GLY	2.3
1	A	229	GLY	2.3
1	A	165	GLU	2.2
1	B	25	SER	2.1
1	B	181	PRO	2.1
1	A	63	GLN	2.0
1	B	36	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.