



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:43 AM UTC

PDB ID : 3L1A / pdb_00003l1a
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 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

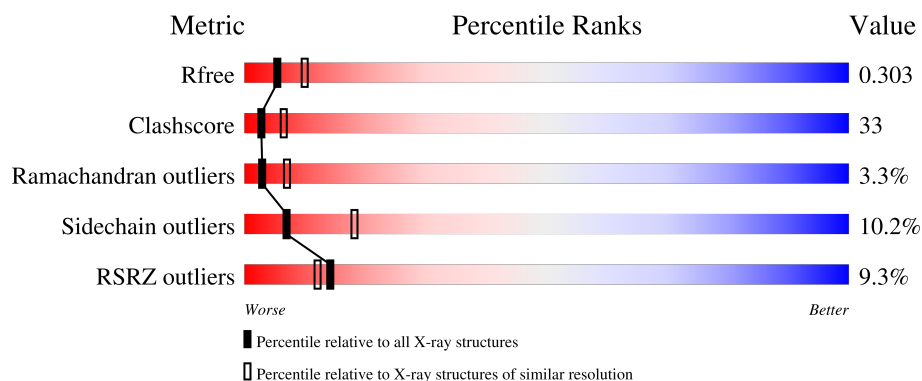
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	266	11% 55% 36% 8%
1	B	266	7% 55% 26% 5% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3610 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 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		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.93Å 63.80Å 103.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.99 – 2.69 23.99 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (23.99-2.69) 99.0 (23.99-2.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.233 , 0.313 (Not available) , 0.303	Depositor DCC
R_{free} test set	1403 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3610	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.55	0/1957	0.89	1/2675 (0.0%)
1	B	0.59	0/1673	1.00	3/2290 (0.1%)
All	All	0.57	0/3630	0.94	4/4965 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ARG	NE-CZ-NH2	8.26	126.64	119.20
1	B	238	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	A	179	ALA	N-CA-C	5.82	118.84	111.69
1	B	238	ARG	CD-NE-CZ	5.43	132.00	124.40

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	1928	0	1931	169	1
1	B	1651	0	1682	75	1
2	A	19	0	0	2	0
2	B	12	0	0	2	0
All	All	3610	0	3613	237	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 33.

All (237) 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: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:O	1:B:20:LEU:HD22	1.41	1.21
1:A:63:GLN:NE2	1:A:66:GLY:HA2	1.58	1.18
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:HB	1:A:167:ASP:HB2	1.21	1.08
1:A:166:VAL:CB	1:A:167:ASP:CB	2.30	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:166:VAL:H	1:A:167:ASP:C	1.67	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:63:GLN:CD	1:A:66:GLY:HA2	1.89	0.98
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: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:HH11	1:B:189:ARG:CG	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:CA	2.42	0.93
1:A:167:ASP:N	1:A:168:PRO:CD	2.30	0.91
1:A:166:VAL:C	1:A:168:PRO:HD3	1.97	0.89
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:20:LEU:HD22	1:B:20:LEU:C	2.05	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:37:GLY:HA2	1:A:64:THR:HG23	1.65	0.77
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:161:GLN:C	1:A:163:PRO:HD3	2.09	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: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:B:189:ARG:HH11	1:B:189:ARG:HB2	1.50	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:166:VAL:N	1:A:167:ASP:C	2.49	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:165:GLU:C	1:A:167:ASP:HB3	2.15	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
1:A:163:PRO:HB2	1:A:164:GLU:HG2	0.67	0.67
1:A:10:PRO:HG3	1:A:79:ARG:NH1	2.10	0.66
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:167:ASP:N	1:A:168:PRO:HD3	2.04	0.66
1:B:20:LEU:O	1:B:20:LEU:CD2	2.32	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:NH1	1:B:189:ARG:HB2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:CG	1:B:189:ARG:NH1	2.47	0.66
1:A:79:ARG:HB3	1:A:183:ARG:NH1	2.11	0.66
1:A:165:GLU:O	1:A:166:VAL:CG2	2.42	0.66
1:B:189:ARG:NH1	1:B:189:ARG:HG2	2.09	0.65
1:B:189:ARG:HH11	1:B:189:ARG:HG2	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: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:239:ASP:O	1:A:247:CYS:HB2	1.97	0.64
1:B:20:LEU:C	1:B:20:LEU:HD13	2.22	0.64
1:A:79:ARG:HB3	1:A:183:ARG:HH12	1.63	0.63
1:A:123:GLU:O	1:A:123:GLU:HG2	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:7:LEU:O	1:A:8:ARG:CB	2.48	0.62
1:A:8:ARG:NE	1:A:160:THR:HG21	2.09	0.62
1:A:81:GLN:HB2	1:A:157:LEU:O	2.00	0.62
1:A:239:ASP:CG	1:A:240:ILE:N	2.58	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:43:LEU:HD12	1:A:85:SER:HB3	1.83	0.60
1:A:253:ARG:CZ	1:B:260:GLY:HA3	2.31	0.60
1:A:164:GLU:C	1:A:167:ASP:O	2.45	0.60
1:B:179:ALA:C	1:B:181:PRO:HD3	2.27	0.60
1:A:19:GLN:O	1:A:19:GLN:HG2	2.01	0.60
1:A:112:SER:HA	1:A:189:ARG:HG2	1.84	0.59
1:B:39:THR:HG22	1:B:58:LEU:HD23	1.83	0.59
1:B:168:PRO:O	1:B:169:ASP:HB2	2.02	0.59
1:A:44:LEU:HD13	1:A:69:ARG:HB2	1.82	0.59
1:B:25:SER:O	1:B:195:GLU:CD	2.43	0.59
1:B:40:ASN:OD1	1:B:152:VAL:HG12	2.03	0.58
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:84:LEU:C	1:B:84:LEU:HD12	2.30	0.57
1:A:79:ARG:CG	1:A:183:ARG:HH12	2.16	0.57
1:B:161:GLN:HG3	1:B:163:PRO:HD2	1.86	0.57
1:A:161:GLN:HA	1:A:172:SER:HB3	1.87	0.56
1:B:160:THR:HG22	1:B:161:GLN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:128:TRP:CH2	1:B:259:ALA:HA	2.41	0.55
1:B:178:VAL:HB	1:B:181:PRO:HG3	1.89	0.55
1:B:163:PRO:HB3	2:B:2031:HOH:O	2.05	0.55
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:127:LYS:CE	1:A:262:VAL:O	2.53	0.54
1:B:119:VAL:HB	1:B:123:GLU:OE2	2.08	0.54
1:A:112:SER:OG	1:A:190:LEU:HA	2.09	0.53
1:A:145:GLU:O	1:A:151:VAL:HG13	2.09	0.53
1:B:43:LEU:HD13	1:B:58:LEU:HD22	1.91	0.53
1:A:167:ASP:H	1:A:168:PRO:HD2	1.72	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:A:84:LEU:C	1:A:84:LEU:HD12	2.35	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
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:4:ARG:O	1:A:5:ASP:CG	2.54	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:231:GLN:O	1:A:232:ASP:OD1	2.30	0.50
1:A:253:ARG:NH1	1:B:260:GLY:HA3	2.27	0.50
1:A:28:ARG:NE	1:A:54:ASP:O	2.44	0.50
1:A:63:GLN:CD	1:A:66:GLY:N	2.71	0.49
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:B:147:ALA:O	1:B:148:GLN:C	2.56	0.49
1:A:11:LEU:N	1:A:183:ARG:HH21	2.11	0.48
1:A:119:VAL:HG13	1:A:119:VAL:O	2.13	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:A:255:VAL:HG13	1:B:255:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLY:O	1:B:27:TRP:O	2.31	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:239:ASP:O	1:A:247:CYS:CB	2.62	0.48
1:B:20:LEU:O	1:B:21:ILE:C	2.55	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:240:ILE:HG23	1:A:245:ARG:C	2.39	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:239:ASP:CG	1:A:240:ILE:H	2.21	0.47
1:B:241:ASP:C	1:B:243:GLN:H	2.23	0.47
1:A:121:PRO:HB2	1:A:135:ARG:CG	2.45	0.47
1:A:16:LEU:O	1:A:20:LEU:HB2	2.14	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: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:B:43:LEU:HD11	1:B:58:LEU:HD13	1.97	0.46
1:B:258:SER:O	1:B:259:ALA:C	2.59	0.46
1:A:159:VAL:HG22	1:A:173:LEU:HD11	1.98	0.46
1:A:58:LEU:HD12	1:A:59:ILE:N	2.31	0.45
1:A:163:PRO:HB3	1:A:164:GLU:CD	2.41	0.45
1:B:58:LEU:O	1:B:84:LEU:HB2	2.16	0.45
1:A:101:LEU:HA	1:A:101:LEU:HD23	1.67	0.45
1:A:227:LEU:O	1:A:228:PRO:C	2.58	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:B:26:GLY:C	1:B:27:TRP:O	2.59	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:HD12	1:B:110:LEU:O	2.17	0.44
1:A:79:ARG:HG2	1:A:183:ARG:HH12	1.80	0.44
1:A:9:PRO:O	1:A:183:ARG:CZ	2.66	0.44
1:A:38:SER:CB	1:A:67:ARG:H	2.21	0.44
1:B:180:ALA:N	1:B:181:PRO:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:B:101:LEU:HA	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:228:PRO:HG2	1:B:250:VAL:O	2.18	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:90:VAL:HG11	1:A:151:VAL:HG23	2.00	0.43
1:B:225:VAL:HG11	1:B:248:LEU:CD2	2.49	0.43
1:B:266:ARG:NH1	2:B:2024:HOH:O	2.51	0.42
1:A:21:ILE:HD13	1:A:21:ILE:HA	1.85	0.42
1:A:227:LEU:HD21	1:A:257:VAL:HG21	2.00	0.42
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:O	1:A:123:GLU:HG3	2.19	0.41
1:B:148:GLN:HA	1:B:149:PRO:HA	1.87	0.41
1:A:74:TRP:CG	1:A:166:VAL:HG13	2.55	0.41
1:A:163:PRO:HA	1:A:164:GLU:HA	1.80	0.41
1:B:40:ASN:ND2	1:B:145:GLU:OE1	2.48	0.41
1:B:178:VAL:O	1:B:181:PRO:HG3	2.21	0.41
1:A:132:VAL:HB	1:A:140:ALA:HB3	2.03	0.41
1:A:221:SER:HB2	1:A:266:ARG:HG2	2.01	0.41
1:A:138:LYS:N	1:A:170:ALA:HA	2.36	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:O	1:B:35:GLN:O[2_444]	2.17	0.03

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	262/266 (98%)	224 (86%)	29 (11%)	9 (3%)	3	7
1	B	224/266 (84%)	200 (89%)	17 (8%)	7 (3%)	3	8
All	All	486/532 (91%)	424 (87%)	46 (10%)	16 (3%)	3	7

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 [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	186/202 (92%)	164 (88%)	22 (12%)	5	13
1	B	168/202 (83%)	154 (92%)	14 (8%)	10	26
All	All	354/404 (88%)	318 (90%)	36 (10%)	7	18

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	69	ARG
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	203	ASN
1	A	231	GLN
1	A	233	VAL
1	A	238	ARG
1	A	240	ILE
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	148	GLN
1	B	174	LEU
1	B	175	ASP
1	B	178	VAL
1	B	189	ARG
1	B	190	LEU
1	B	194	LEU
1	B	225	VAL
1	B	233	VAL

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Mol	Chain	Res	Type
1	B	248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	63	GLN
1	A	81	GLN
1	B	81	GLN
1	B	130	ASN
1	B	161	GLN
1	B	231	GLN

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	264/266 (99%)	0.61	28 (10%) 11 9	25, 37, 68, 121	12 (4%)
1	B	228/266 (85%)	0.52	18 (7%) 18 16	20, 40, 80, 107	7 (3%)
All	All	492/532 (92%)	0.57	46 (9%) 14 12	20, 39, 75, 121	19 (3%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	VAL	6.6
1	A	75	ALA	6.4
1	A	162	ALA	5.0
1	B	162	ALA	5.0
1	A	76	ALA	5.0
1	A	67	ARG	4.6
1	A	65	ALA	4.4
1	A	70	HIS	4.2
1	A	163	PRO	3.9
1	B	23	ALA	3.9
1	A	66	GLY	3.8
1	B	168	PRO	3.8
1	B	21	ILE	3.8
1	A	74	TRP	3.8
1	B	163	PRO	3.8
1	A	160	THR	3.7
1	A	71	GLY	3.4
1	A	63	GLN	3.3
1	A	64	THR	3.1
1	B	179	ALA	3.1
1	A	73	GLY	3.1
1	B	22	GLY	2.9
1	B	24	GLY	2.8
1	A	72	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	5	ASP	2.7
1	B	180	ALA	2.6
1	A	239	ASP	2.6
1	A	161	GLN	2.6
1	B	20	LEU	2.6
1	A	166	VAL	2.6
1	A	168	PRO	2.6
1	A	229	GLY	2.5
1	A	230	GLY	2.5
1	A	92	ASP	2.5
1	B	181	PRO	2.5
1	B	189	ARG	2.4
1	A	204	ALA	2.4
1	B	25	SER	2.3
1	B	167	ASP	2.3
1	A	164	GLU	2.3
1	B	34	ALA	2.2
1	A	68	GLY	2.2
1	B	165	GLU	2.1
1	A	206	PRO	2.1
1	A	69	ARG	2.0
1	B	203	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 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.