



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:02 PM UTC

PDB ID : 1B9N / pdb_00001b9n
Title : REGULATOR FROM ESCHERICHIA COLI
Authors : Hall, D.R.; Gourley, D.G.; Hunter, W.N.
Deposited on : 1999-02-12
Resolution : 2.09 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

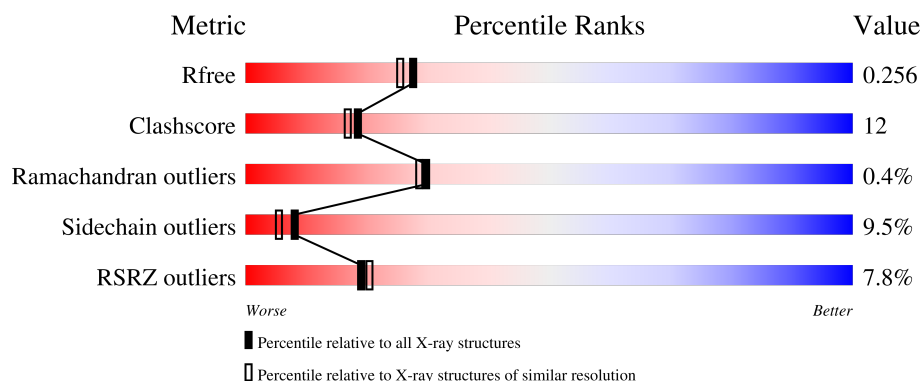
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	265	10% 60% 26% 8% • •
1	B	265	5% 56% 28% 7% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4132 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 PROTEIN (MODE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	3	0
			1957	1232	344	375	6			
1	B	245	Total	C	N	O	S	0	4	0
			1865	1174	321	363	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	SEE REMARK 999	UNP P0A9G8
A	-2	SER	-	SEE REMARK 999	UNP P0A9G8
A	-1	HIS	-	SEE REMARK 999	UNP P0A9G8
B	-3	GLY	-	SEE REMARK 999	UNP P0A9G8
B	-2	SER	-	SEE REMARK 999	UNP P0A9G8
B	-1	HIS	-	SEE REMARK 999	UNP P0A9G8

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

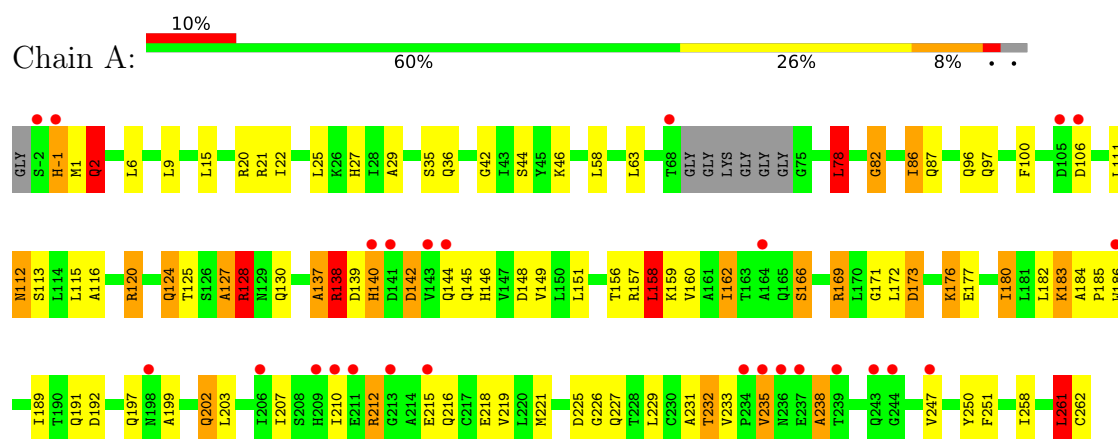
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	138	Total	O	0	0
			138	138		

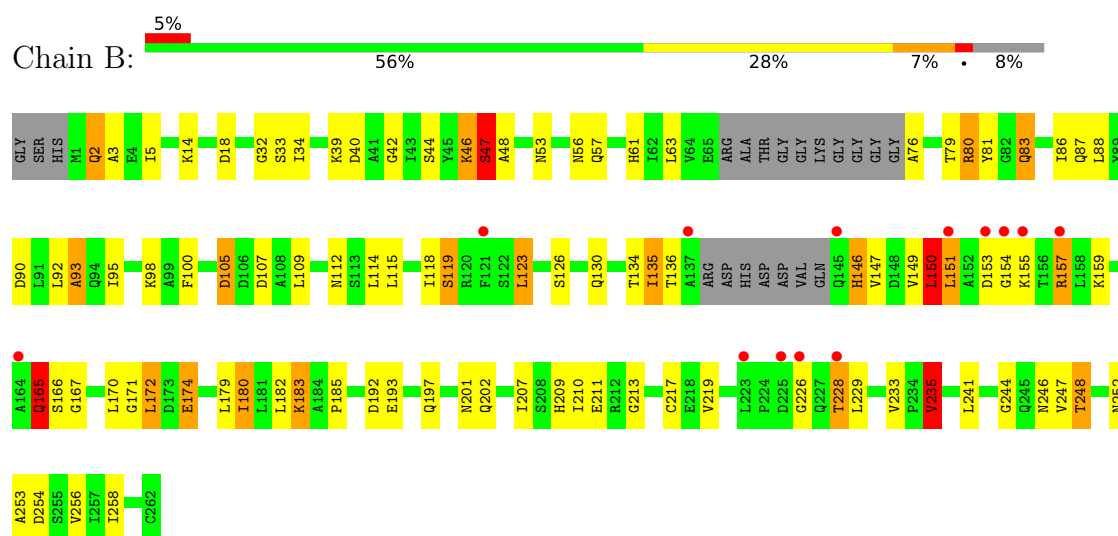
3 Residue-property plots [i](#)

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: PROTEIN (MODE)



• Molecule 1: PROTEIN (MODE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	81.11Å 127.36Å 62.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.63 – 2.09 28.63 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.63-2.09) 98.7 (28.63-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.286 0.199 , 0.256	Depositor DCC
R_{free} test set	1934 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4132	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NI

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	1.11	0/1999	2.10	77/2715 (2.8%)
1	B	1.02	1/1909 (0.1%)	1.98	55/2590 (2.1%)
All	All	1.07	1/3908 (0.0%)	2.04	132/5305 (2.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	7
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	GLY	N-CA	5.94	1.49	1.44

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ARG	CD-NE-CZ	10.94	139.72	124.40
1	B	233	VAL	N-CA-CB	-10.43	96.61	111.21
1	A	148	ASP	CA-CB-CG	-10.17	102.43	112.60
1	B	235	VAL	CB-CA-C	-9.72	99.02	112.14
1	A	-1	HIS	CA-C-N	8.64	138.04	121.54
1	A	-1	HIS	C-N-CA	8.64	138.04	121.54
1	A	250	TYR	CA-C-O	-8.35	111.64	120.99
1	B	112	ASN	OD1-CG-ND2	-8.16	114.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	A	20	ARG	NE-CZ-NH2	8.04	126.44	119.20
1	A	87	GLN	CA-C-O	8.00	129.22	120.82
1	B	248	THR	CA-CB-OG1	7.75	121.23	109.60
1	A	137	ALA	CA-C-O	-7.74	112.68	121.19
1	B	149	VAL	O-C-N	7.71	131.34	123.10
1	B	235	VAL	N-CA-CB	7.64	120.93	110.54
1	A	25	LEU	CA-C-O	-7.62	111.48	120.10
1	B	18	ASP	N-CA-C	-7.61	101.28	108.13
1	A	78	LEU	CA-C-O	-7.52	112.74	121.16
1	A	140	HIS	CA-CB-CG	-7.44	106.36	113.80
1	A	-1	HIS	N-CA-C	7.43	126.63	110.80
1	B	244	GLY	CA-C-O	7.43	126.77	119.27
1	A	2	GLN	CB-CG-CD	7.37	125.12	112.60
1	A	2	GLN	OE1-CD-NE2	-7.18	115.42	122.60
1	A	227	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	B	154	GLY	N-CA-C	7.09	124.76	115.40
1	A	96	GLN	CB-CA-C	-7.07	98.83	110.85
1	B	165	GLN	CB-CG-CD	7.04	124.58	112.60
1	B	248	THR	N-CA-CB	6.88	121.58	110.77
1	B	92	LEU	O-C-N	-6.84	114.97	122.09
1	B	146	HIS	CA-CB-CG	-6.84	106.96	113.80
1	A	158	LEU	CA-C-O	-6.82	113.46	121.44
1	A	-1	HIS	CA-C-O	6.70	130.09	120.51
1	A	250	TYR	O-C-N	6.69	130.88	123.33
1	B	149	VAL	CA-C-O	-6.65	113.22	120.67
1	A	262	CYS	CA-C-O	-6.52	109.72	120.80
1	A	22	ILE	O-C-N	-6.51	115.55	121.87
1	B	201	ASN	OD1-CG-ND2	6.49	129.09	122.60
1	B	107	ASP	CA-CB-CG	-6.48	106.12	112.60
1	A	127	ALA	O-C-N	-6.41	113.84	122.43
1	A	120	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	B	192	ASP	CA-CB-CG	6.33	118.92	112.60
1	B	202	GLN	CA-C-O	-6.29	113.57	120.24
1	A	173	ASP	CA-CB-CG	-6.28	106.32	112.60
1	B	81	TYR	CA-C-N	6.26	126.89	119.94
1	B	81	TYR	C-N-CA	6.26	126.89	119.94
1	B	166	SER	N-CA-C	-6.24	104.02	111.69
1	A	36	GLN	CG-CD-NE2	6.22	125.73	116.40
1	A	138	ARG	N-CA-CB	6.22	119.87	109.92
1	A	261	LEU	CA-C-O	-6.21	113.77	120.92
1	A	216	GLN	N-CA-C	6.18	119.48	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LYS	CA-CB-CG	6.15	126.40	114.10
1	B	228	THR	N-CA-CB	6.08	120.12	110.57
1	A	46	LYS	CA-C-O	-6.05	114.01	120.42
1	A	212	ARG	CA-C-N	6.05	129.77	122.03
1	A	212	ARG	C-N-CA	6.05	129.77	122.03
1	B	93	ALA	CA-C-O	-6.03	112.19	119.49
1	B	126	SER	N-CA-C	-6.03	105.92	113.28
1	A	172	LEU	O-C-N	-6.00	114.61	122.59
1	A	192	ASP	CA-C-N	5.99	128.58	120.38
1	A	192	ASP	C-N-CA	5.99	128.58	120.38
1	A	87	GLN	O-C-N	-5.97	115.92	122.07
1	A	82	GLY	N-CA-C	-5.90	105.65	112.50
1	A	183	LYS	CA-CB-CG	5.89	125.89	114.10
1	B	246	ASN	CA-C-O	-5.89	113.84	120.43
1	B	211	GLU	CA-C-O	-5.81	114.06	120.33
1	B	80	ARG	CD-NE-CZ	-5.76	116.34	124.40
1	A	21	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	B	147	VAL	CA-C-O	-5.72	115.67	121.67
1	B	87	GLN	O-C-N	5.71	128.17	122.12
1	B	95	ILE	O-C-N	5.64	127.61	122.14
1	A	120	ARG	CD-NE-CZ	5.64	132.29	124.40
1	B	80	ARG	N-CA-C	-5.61	105.08	111.14
1	A	202	GLN	CA-C-O	-5.61	114.09	120.32
1	B	48	ALA	CA-C-O	-5.58	114.63	120.55
1	A	251	PHE	CA-C-O	-5.57	115.27	121.23
1	A	-1	HIS	O-C-N	-5.54	115.22	122.59
1	A	27	HIS	CG-CD2-NE2	-5.53	101.67	107.20
1	A	124	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	B	219	VAL	O-C-N	-5.50	117.40	123.18
1	A	35	SER	CA-C-N	-5.49	112.49	120.29
1	A	35	SER	C-N-CA	-5.49	112.49	120.29
1	A	169	ARG	N-CA-CB	-5.49	101.82	110.06
1	B	53	ASN	N-CA-CB	5.48	118.17	110.12
1	A	58	LEU	N-CA-C	5.47	117.24	111.28
1	B	90	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	9	LEU	N-CA-CB	5.44	119.04	110.23
1	A	9	LEU	CA-C-O	-5.43	114.67	120.92
1	B	235	VAL	CA-CB-CG2	5.41	119.59	110.40
1	B	183	LYS	CA-C-N	5.41	127.72	120.58
1	B	183	LYS	C-N-CA	5.41	127.72	120.58
1	B	171	GLY	CA-C-O	5.39	126.18	119.88
1	A	86	ILE	CB-CG1-CD1	-5.38	102.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	GLY	N-CA-C	5.38	125.92	113.18
1	B	18	ASP	N-CA-CB	5.37	116.32	111.27
1	B	42	GLY	CA-C-O	-5.37	112.64	119.19
1	A	100	PHE	CA-CB-CG	-5.34	108.46	113.80
1	A	177	GLU	O-C-N	-5.32	116.81	123.04
1	A	232	THR	CB-CA-C	5.32	118.99	110.16
1	A	44	SER	CA-C-N	5.32	127.35	120.44
1	A	44	SER	C-N-CA	5.32	127.35	120.44
1	B	150	LEU	CA-C-O	-5.31	114.64	120.43
1	A	238	ALA	CA-C-N	5.29	128.10	120.38
1	A	238	ALA	C-N-CA	5.29	128.10	120.38
1	A	226	GLY	CA-C-O	5.26	124.74	119.27
1	A	22	ILE	CA-C-O	5.25	126.41	120.95
1	A	231	ALA	CA-C-N	-5.23	115.62	123.00
1	A	231	ALA	C-N-CA	-5.23	115.62	123.00
1	A	191	GLN	N-CA-C	-5.23	106.58	113.17
1	B	56	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	169	ARG	CD-NE-CZ	-5.21	117.10	124.40
1	A	97	GLN	CB-CG-CD	-5.17	103.82	112.60
1	B	14	LYS	CA-C-N	5.17	128.68	121.24
1	B	14	LYS	C-N-CA	5.17	128.68	121.24
1	B	248	THR	CA-CB-CG2	5.16	119.28	110.50
1	B	171	GLY	O-C-N	-5.15	116.31	122.34
1	A	189	ILE	CA-C-N	-5.15	113.79	122.29
1	A	189	ILE	C-N-CA	-5.15	113.79	122.29
1	A	128	ARG	N-CA-CB	5.15	119.19	110.49
1	A	191	GLN	OE1-CD-NE2	5.14	127.74	122.60
1	A	180	ILE	CB-CG1-CD1	-5.12	103.05	113.80
1	A	111	LEU	O-C-N	-5.11	115.16	122.41
1	A	145	GLN	CB-CA-C	5.09	119.76	112.12
1	B	209	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	160	VAL	CA-C-O	-5.07	114.98	120.36
1	B	241	LEU	N-CA-C	5.07	117.78	110.28
1	B	105	ASP	CA-CB-CG	-5.06	107.54	112.60
1	B	201	ASN	CA-CB-CG	-5.04	107.56	112.60
1	B	123	LEU	CA-C-O	-5.04	114.74	120.58
1	A	173	ASP	CA-C-O	-5.03	115.51	121.89
1	B	47	SER	N-CA-CB	-5.02	102.74	110.16
1	A	159	LYS	CB-CA-C	-5.01	99.80	109.37
1	A	156	THR	CA-C-O	-5.01	114.82	120.43

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	SER	Mainchain
1	A	127	ALA	Mainchain
1	A	128	ARG	Mainchain
1	A	130	GLN	Mainchain
1	A	158	LEU	Mainchain
1	A	162	ILE	Mainchain
1	A	2	GLN	Mainchain
1	A	219	VAL	Mainchain
1	A	42	GLY	Mainchain
1	B	135	ILE	Mainchain
1	B	172	LEU	Mainchain
1	B	182	LEU	Mainchain
1	B	34	ILE	Mainchain
1	B	5	ILE	Mainchain
1	B	83	GLN	Mainchain
1	B	93	ALA	Mainchain

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	1957	0	1955	47	0
1	B	1865	0	1877	47	0
2	A	1	0	0	0	0
3	A	171	0	0	3	0
3	B	138	0	0	2	0
All	All	4132	0	3832	92	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 12.

All (92) 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:167:GLY:HA2	1:B:172:LEU:HD12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASN:HD22	1:A:112:ASN:H	1.25	0.85
1:B:180:ILE:HD12	1:B:256:VAL:HG13	1.59	0.82
1:A:158:LEU:HD12	1:A:180:ILE:HD13	1.71	0.73
1:A:183:LYS:HE2	3:A:347:HOH:O	1.87	0.72
1:A:183:LYS:HB2	1:A:186[B]:TRP:CE3	2.24	0.72
1:B:44:SER:OG	1:B:47:SER:HB2	1.89	0.71
1:B:183:LYS:HB3	1:B:185:PRO:HD2	1.72	0.70
1:A:151:LEU:HD21	1:A:158:LEU:HD11	1.72	0.70
1:B:114:LEU:O	1:B:118:ILE:HG12	1.92	0.68
1:B:180:ILE:HD12	1:B:256:VAL:CG1	2.24	0.68
3:A:277:HOH:O	1:B:61:HIS:HE1	1.75	0.67
1:B:135:ILE:HD11	1:B:172:LEU:HD22	1.77	0.67
1:A:29:ALA:HB2	1:A:78:LEU:HD22	1.77	0.66
1:A:149:VAL:HG11	1:A:180:ILE:HD11	1.79	0.65
1:B:146:HIS:CG	1:B:159:LYS:HE2	2.32	0.65
1:A:199:ALA:O	1:A:202:GLN:NE2	2.31	0.63
1:B:136:THR:CG2	1:B:150:LEU:HB2	2.28	0.62
1:A:139:ASP:HB3	1:A:157:ARG:CZ	2.30	0.61
1:A:184:ALA:CB	1:A:232:THR:HG23	2.31	0.61
1:A:215:GLU:O	1:A:235:VAL:HG22	2.02	0.60
1:A:233:VAL:HG23	1:A:238:ALA:HB2	1.84	0.60
1:A:184:ALA:HB1	1:A:232:THR:HG23	1.83	0.59
1:A:139:ASP:HB3	1:A:157:ARG:NH1	2.18	0.59
1:A:142:ASP:CG	1:A:144:GLN:HE21	2.11	0.58
1:A:158:LEU:HD22	1:A:203:LEU:HD21	1.88	0.55
1:A:171:GLY:O	1:A:176:LYS:HG3	2.07	0.55
1:B:32:GLY:O	1:B:76:ALA:N	2.41	0.55
1:B:88:LEU:HD23	1:B:88:LEU:C	2.32	0.54
1:B:115:LEU:O	1:B:119:SER:HB3	2.07	0.54
1:A:158:LEU:CD2	1:A:203:LEU:HD21	2.38	0.53
1:B:167:GLY:CA	1:B:172:LEU:HD12	2.35	0.53
1:A:138:ARG:HD2	1:A:140:HIS:CE1	2.45	0.52
1:A:183:LYS:HB3	1:A:185:PRO:HD2	1.91	0.51
1:B:2:GLN:H	1:B:2:GLN:CD	2.18	0.51
1:A:115:LEU:HB2	1:A:261:LEU:HD22	1.91	0.51
1:A:221:MET:HE2	1:A:229:LEU:HD13	1.92	0.51
1:A:151:LEU:HB3	1:A:225:ASP:OD2	2.11	0.50
1:A:157:ARG:O	1:A:158:LEU:HD23	2.11	0.50
1:A:112:ASN:HD22	1:A:112:ASN:N	1.96	0.50
1:B:151:LEU:N	1:B:151:LEU:HD23	2.27	0.50
1:B:235:VAL:HG12	3:B:343:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD13	1:A:82:GLY:HA2	1.95	0.48
1:A:158:LEU:HD12	1:A:180:ILE:CD1	2.42	0.48
1:A:203:LEU:O	1:A:221:MET:HE1	2.13	0.48
1:B:109:LEU:HD22	1:B:109:LEU:N	2.28	0.48
1:A:212:ARG:NH2	1:A:238:ALA:O	2.47	0.48
1:B:109:LEU:N	1:B:109:LEU:CD2	2.76	0.48
1:B:155:LYS:O	1:B:157:ARG:NH2	2.47	0.47
1:B:210:ILE:HG23	1:B:217:CYS:SG	2.54	0.47
1:A:158:LEU:CD1	1:A:180:ILE:HD13	2.44	0.47
1:A:207:ILE:HG21	1:A:210:ILE:HG13	1.97	0.47
1:A:162:ILE:HG13	1:A:166:SER:OG	2.15	0.46
1:A:140:HIS:NE2	1:A:146:HIS:CE1	2.83	0.46
1:B:130:GLN:HG2	1:B:179:LEU:HD11	1.96	0.46
1:B:167:GLY:HA2	1:B:172:LEU:CD1	2.37	0.45
1:A:233:VAL:CG2	1:A:238:ALA:HB2	2.46	0.45
1:B:98:LYS:HB3	1:B:118:ILE:CG2	2.46	0.45
1:A:139:ASP:CB	3:A:378:HOH:O	2.64	0.45
1:A:142:ASP:OD1	1:A:144:GLN:NE2	2.49	0.45
1:A:124:GLN:HB3	1:B:170:LEU:HD22	1.98	0.45
1:A:112:ASN:H	1:A:112:ASN:ND2	2.03	0.45
1:A:106:ASP:OD2	1:B:80:ARG:NH1	2.42	0.44
1:B:229:LEU:C	1:B:229:LEU:HD23	2.42	0.44
1:B:79:THR:O	1:B:83:GLN:HG3	2.17	0.44
1:B:118:ILE:HD13	1:B:118:ILE:HG21	1.79	0.44
1:B:258:ILE:HD13	1:B:258:ILE:HG21	1.72	0.44
1:A:137:ALA:O	1:A:138:ARG:C	2.57	0.44
1:A:157:ARG:C	1:A:158:LEU:HD23	2.43	0.44
1:A:128:ARG:NH2	1:A:218:GLU:OE1	2.45	0.43
1:B:136:THR:HG21	1:B:150:LEU:HB2	2.01	0.43
1:B:98:LYS:HB3	1:B:118:ILE:HG22	2.01	0.43
1:B:207:ILE:HD11	1:B:247:VAL:HG11	2.01	0.42
1:B:3:ALA:HB1	1:B:100:PHE:CE2	2.55	0.42
1:B:151:LEU:N	1:B:151:LEU:CD2	2.82	0.42
1:A:86:ILE:HG21	1:A:86:ILE:HD13	1.82	0.42
1:A:215:GLU:C	1:A:235:VAL:HG22	2.44	0.42
1:A:183:LYS:HB2	1:A:186[B]:TRP:CZ3	2.54	0.41
1:B:136:THR:HG23	1:B:150:LEU:HB2	2.01	0.41
1:A:116:ALA:O	1:A:120:ARG:HG3	2.21	0.41
1:B:109:LEU:CD2	1:B:109:LEU:H	2.33	0.41
1:B:105:ASP:OD1	1:B:105:ASP:C	2.63	0.41
1:B:165:GLN:H	1:B:165:GLN:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:HIS:CD2	1:B:159:LYS:HG3	2.56	0.40
1:B:159:LYS:HD3	1:B:253:ALA:HB2	2.03	0.40
1:B:183:LYS:NZ	3:B:325:HOH:O	2.41	0.40
1:B:86:ILE:HG21	1:B:86:ILE:HD13	1.78	0.40
1:B:39:LYS:O	1:B:40:ASP:C	2.63	0.40
1:B:46:LYS:HG3	1:B:47:SER:N	2.37	0.40
1:B:252:ASN:HB3	1:B:254:ASP:OD1	2.21	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	257/265 (97%)	243 (95%)	12 (5%)	2 (1%)	16	12
1	B	243/265 (92%)	233 (96%)	10 (4%)	0	100	100
All	All	500/530 (94%)	476 (95%)	22 (4%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	1	MET

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	205/213 (96%)	188 (92%)	17 (8%)	10	8
1	B	201/213 (94%)	180 (90%)	21 (10%)	7	4
All	All	406/426 (95%)	368 (91%)	38 (9%)	8	6

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	6	LEU
1	A	15	LEU
1	A	78	LEU
1	A	112	ASN
1	A	125	THR
1	A	138	ARG
1	A	142	ASP
1	A	166	SER
1	A	169	ARG
1	A	176	LYS
1	A	182	LEU
1	A	197	GLN
1	A	235	VAL
1	A	247	VAL
1	A	258	ILE
1	A	261	LEU
1	B	2	GLN
1	B	33	SER
1	B	46	LYS
1	B	47	SER
1	B	57	GLN
1	B	63	LEU
1	B	119	SER
1	B	123	LEU
1	B	134	THR
1	B	150	LEU
1	B	151	LEU
1	B	153	ASP
1	B	157	ARG
1	B	165	GLN
1	B	174	GLU
1	B	180	ILE
1	B	193	GLU
1	B	197	GLN

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Mol	Chain	Res	Type
1	B	228	THR
1	B	235	VAL
1	B	248	THR

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

Mol	Chain	Res	Type
1	A	97	GLN
1	A	112	ASN
1	A	144	GLN
1	B	236	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	258/265 (97%)	0.26	26 (10%) 12 13	19, 33, 70, 83	3 (1%)
1	B	245/265 (92%)	0.30	13 (5%) 32 34	19, 36, 63, 90	4 (1%)
All	All	503/530 (94%)	0.28	39 (7%) 19 20	19, 35, 66, 90	7 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	THR	5.4
1	B	154	GLY	3.9
1	A	239	THR	3.8
1	B	137	ALA	3.6
1	B	225	ASP	3.4
1	B	226	GLY	3.3
1	A	198	ASN	3.2
1	B	121	PHE	3.2
1	B	157	ARG	3.2
1	A	141	ASP	3.0
1	B	164	ALA	3.0
1	B	228	THR	3.0
1	A	143	VAL	3.0
1	A	186[A]	TRP	2.9
1	A	140	HIS	2.8
1	A	144	GLN	2.8
1	A	213	GLY	2.7
1	A	243	GLN	2.7
1	A	-2	SER	2.7
1	A	235	VAL	2.6
1	A	244	GLY	2.5
1	B	223	LEU	2.5
1	A	-1	HIS	2.5
1	A	211	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLU	2.5
1	A	215	GLU	2.4
1	A	209	HIS	2.4
1	A	106	ASP	2.3
1	A	236	ASN	2.3
1	B	145	GLN	2.2
1	A	234	PRO	2.1
1	A	210	ILE	2.1
1	B	155	LYS	2.1
1	B	153	ASP	2.1
1	A	247	VAL	2.1
1	B	151	LEU	2.1
1	A	206	ILE	2.1
1	A	164	ALA	2.0
1	A	105	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NI	A	263	1/1	0.95	0.22	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.