



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 08:40 PM EST

PDB ID : 2G6V  
Title : The crystal structure of ribD from Escherichia coli  
Authors : Stenmark, P.; Moche, M.; Gurmu, D.; Nordlund, P.; Structural Proteomics in Europe (SPINE)  
Deposited on : 2006-02-25  
Resolution : 2.60 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](mailto: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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

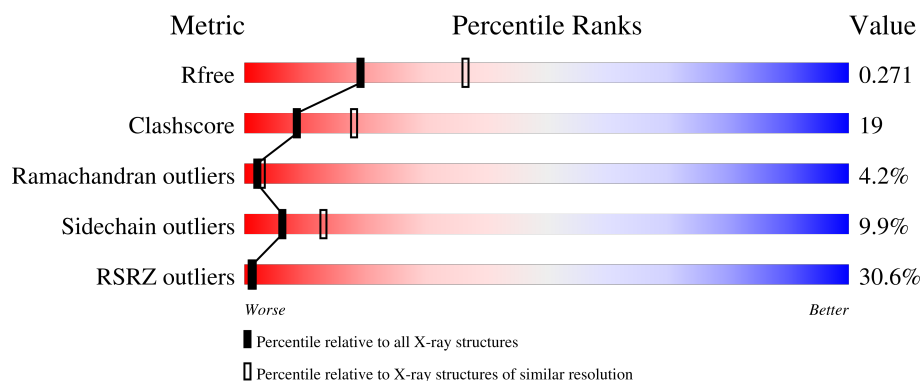
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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	402	
1	B	402	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5530 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 Riboflavin biosynthesis protein ribD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	Se	0	0	0
			2709	1708	488	498	6	9			
1	B	363	Total	C	N	O	S	Se	0	0	0
			2756	1730	503	511	3	9			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP P25539
A	-25	ASP	-	expression tag	UNP P25539
A	-24	TYR	-	expression tag	UNP P25539
A	-23	LYS	-	expression tag	UNP P25539
A	-22	ASP	-	expression tag	UNP P25539
A	-21	ASP	-	expression tag	UNP P25539
A	-20	ASP	-	expression tag	UNP P25539
A	-19	ASP	-	expression tag	UNP P25539
A	-18	LYS	-	expression tag	UNP P25539
A	-17	GLY	-	expression tag	UNP P25539
A	-16	SER	-	expression tag	UNP P25539
A	-15	SER	-	expression tag	UNP P25539
A	-14	THR	-	expression tag	UNP P25539
A	-13	SER	-	expression tag	UNP P25539
A	-12	LEU	-	expression tag	UNP P25539
A	-11	TYR	-	expression tag	UNP P25539
A	-10	LYS	-	expression tag	UNP P25539
A	-9	LYS	-	expression tag	UNP P25539
A	-8	ALA	-	expression tag	UNP P25539
A	-7	GLY	-	expression tag	UNP P25539
A	-6	SER	-	expression tag	UNP P25539
A	-5	GLU	-	expression tag	UNP P25539
A	-4	THR	-	expression tag	UNP P25539
A	-3	LEU	-	expression tag	UNP P25539
A	-2	TYR	-	expression tag	UNP P25539

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ILE	-	expression tag	UNP P25539
A	0	GLN	-	expression tag	UNP P25539
A	1	GLY	-	expression tag	UNP P25539
A	7	MSE	MET	modified residue	UNP P25539
A	58	MSE	MET	modified residue	UNP P25539
A	100	MSE	MET	modified residue	UNP P25539
A	127	MSE	MET	modified residue	UNP P25539
A	128	MSE	MET	modified residue	UNP P25539
A	142	MSE	MET	modified residue	UNP P25539
A	163	MSE	MET	modified residue	UNP P25539
A	285	MSE	MET	modified residue	UNP P25539
A	286	MSE	MET	modified residue	UNP P25539
A	368	SER	-	expression tag	UNP P25539
A	369	THR	-	expression tag	UNP P25539
A	370	HIS	-	expression tag	UNP P25539
A	371	HIS	-	expression tag	UNP P25539
A	372	HIS	-	expression tag	UNP P25539
A	373	HIS	-	expression tag	UNP P25539
A	374	HIS	-	expression tag	UNP P25539
A	375	HIS	-	expression tag	UNP P25539
B	-26	MET	-	expression tag	UNP P25539
B	-25	ASP	-	expression tag	UNP P25539
B	-24	TYR	-	expression tag	UNP P25539
B	-23	LYS	-	expression tag	UNP P25539
B	-22	ASP	-	expression tag	UNP P25539
B	-21	ASP	-	expression tag	UNP P25539
B	-20	ASP	-	expression tag	UNP P25539
B	-19	ASP	-	expression tag	UNP P25539
B	-18	LYS	-	expression tag	UNP P25539
B	-17	GLY	-	expression tag	UNP P25539
B	-16	SER	-	expression tag	UNP P25539
B	-15	SER	-	expression tag	UNP P25539
B	-14	THR	-	expression tag	UNP P25539
B	-13	SER	-	expression tag	UNP P25539
B	-12	LEU	-	expression tag	UNP P25539
B	-11	TYR	-	expression tag	UNP P25539
B	-10	LYS	-	expression tag	UNP P25539
B	-9	LYS	-	expression tag	UNP P25539
B	-8	ALA	-	expression tag	UNP P25539
B	-7	GLY	-	expression tag	UNP P25539
B	-6	SER	-	expression tag	UNP P25539
B	-5	GLU	-	expression tag	UNP P25539

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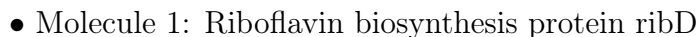
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	THR	-	expression tag	UNP P25539
B	-3	LEU	-	expression tag	UNP P25539
B	-2	TYR	-	expression tag	UNP P25539
B	-1	ILE	-	expression tag	UNP P25539
B	0	GLN	-	expression tag	UNP P25539
B	1	GLY	-	expression tag	UNP P25539
B	7	MSE	MET	modified residue	UNP P25539
B	58	MSE	MET	modified residue	UNP P25539
B	100	MSE	MET	modified residue	UNP P25539
B	127	MSE	MET	modified residue	UNP P25539
B	128	MSE	MET	modified residue	UNP P25539
B	142	MSE	MET	modified residue	UNP P25539
B	163	MSE	MET	modified residue	UNP P25539
B	285	MSE	MET	modified residue	UNP P25539
B	286	MSE	MET	modified residue	UNP P25539
B	368	SER	-	expression tag	UNP P25539
B	369	THR	-	expression tag	UNP P25539
B	370	HIS	-	expression tag	UNP P25539
B	371	HIS	-	expression tag	UNP P25539
B	372	HIS	-	expression tag	UNP P25539
B	373	HIS	-	expression tag	UNP P25539
B	374	HIS	-	expression tag	UNP P25539
B	375	HIS	-	expression tag	UNP P25539

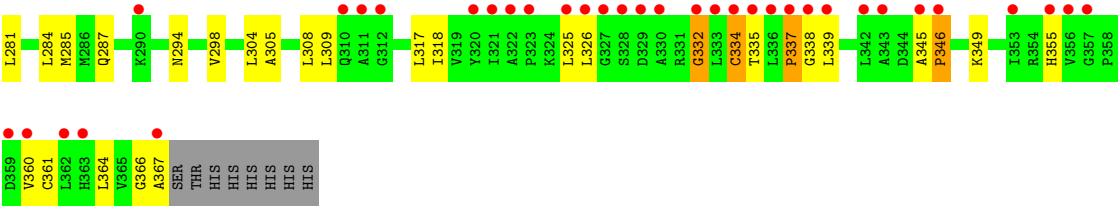
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	42	Total O 42 42	0	0
2	B	23	Total O 23 23	0	0



- Molecule 1: Riboflavin biosynthesis protein ribD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.60Å 172.60Å 76.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.25 – 2.60 28.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.25-2.60) 99.9 (28.25-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.244 , 0.285 0.237 , 0.271	Depositor DCC
$R_{free}$ test set	2010 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 81.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.47	0/2753	0.66	2/3723 (0.1%)
1	B	0.41	0/2800	0.62	0/3790
All	All	0.44	0/5553	0.64	2/7513 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	67	THR	N-CA-C	5.20	125.04	111.00

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	2709	0	2698	111	0
1	B	2756	0	2735	97	0
2	A	42	0	0	6	0
2	B	23	0	0	6	0
All	All	5530	0	5433	202	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 19.

All (202) 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:213:GLU:HA	2:B:395:HOH:O	1.32	1.25
1:B:194:SER:HB3	1:B:233:ASP:HB3	1.14	1.11
1:B:206:VAL:H	1:B:226:GLN:HE22	1.04	1.00
1:B:194:SER:CB	1:B:233:ASP:HB3	1.99	0.91
1:B:141:ARG:HH11	1:B:294:ASN:HD21	1.20	0.87
1:B:160:ARG:HA	1:B:332:GLY:HA3	1.59	0.85
1:A:194:SER:HB3	1:A:233:ASP:HB3	1.58	0.84
1:A:152:LYS:HE3	1:A:163:MSE:SE	2.28	0.83
1:A:141:ARG:HH11	1:A:294:ASN:HD21	1.26	0.82
1:A:206:VAL:H	1:A:226:GLN:NE2	1.77	0.81
1:A:229:ARG:NH2	1:A:248:PRO:O	2.15	0.78
1:A:39:GLY:HA2	1:A:58:MSE:HE2	1.63	0.78
1:A:33:LYS:HE3	1:A:65:GLY:HA3	1.65	0.78
1:A:218:LEU:HG	1:A:219:TYR:N	1.98	0.77
1:A:24:ASN:ND2	1:A:46:ALA:HA	1.98	0.77
1:A:206:VAL:H	1:A:226:GLN:HE22	1.31	0.77
1:B:160:ARG:HA	1:B:332:GLY:CA	2.15	0.77
1:B:142:MSE:HA	1:B:142:MSE:HE2	1.67	0.77
1:A:332:GLY:HA3	1:B:335:THR:HG22	1.65	0.76
1:A:208:TRP:CZ2	1:A:215:THR:HG23	2.20	0.76
1:A:28:GLY:H	1:A:71:THR:CG2	2.00	0.75
1:B:21:THR:HG23	1:B:24:ASN:O	1.88	0.74
1:B:215:THR:OG1	2:B:387:HOH:O	2.05	0.74
1:B:33:LYS:HD3	1:B:65:GLY:HA3	1.68	0.73
1:B:137:GLY:HA2	1:B:148:TYR:HB2	1.72	0.71
1:A:21:THR:HG23	1:A:24:ASN:O	1.90	0.71
1:B:168:SER:HB2	1:B:200:ASP:OD2	1.90	0.71
1:A:208:TRP:CH2	1:A:215:THR:HG23	2.25	0.70
1:A:269:THR:HG21	2:A:408:HOH:O	1.91	0.70
1:A:218:LEU:HB3	2:A:415:HOH:O	1.92	0.70
1:B:212:ASP:OD2	1:B:214:GLN:OE1	2.09	0.69
1:A:19:PHE:O	1:A:225:ARG:NH1	2.23	0.69
1:B:206:VAL:N	1:B:226:GLN:HE22	1.85	0.69
1:B:194:SER:HB3	1:B:233:ASP:CB	2.08	0.69
1:A:144:THR:O	1:A:146:PHE:N	2.24	0.69
1:A:45:ARG:NH1	1:A:223:ASN:O	2.27	0.67
1:B:141:ARG:HH11	1:B:294:ASN:ND2	1.92	0.67
1:A:239:THR:HG22	1:A:241:VAL:H	1.58	0.67
1:A:194:SER:CB	1:A:233:ASP:HB3	2.25	0.67
1:B:206:VAL:H	1:B:226:GLN:NE2	1.85	0.67
1:A:347:GLN:HA	1:A:347:GLN:OE1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:OE1	1:B:214:GLN:N	2.24	0.65
1:A:28:GLY:H	1:A:71:THR:HG22	1.62	0.64
1:A:99:SER:O	1:A:128:MSE:HB2	1.97	0.64
1:A:162:ALA:HB1	1:A:171:ILE:HD12	1.78	0.64
1:B:24:ASN:ND2	1:B:46:ALA:HA	2.13	0.64
1:B:105:PRO:O	1:B:107:VAL:N	2.28	0.62
1:B:161:THR:O	1:B:163:MSE:N	2.31	0.62
1:A:239:THR:HG23	1:A:240:PRO:HD2	1.82	0.61
1:A:39:GLY:CA	1:A:58:MSE:HE2	2.29	0.61
1:A:108:ALA:O	1:A:110:ARG:N	2.32	0.61
1:A:128:MSE:SE	1:A:128:MSE:O	2.68	0.60
1:A:17:GLY:O	1:A:21:THR:HB	2.00	0.60
1:A:28:GLY:H	1:A:71:THR:HG21	1.66	0.60
1:A:132:GLU:OE2	1:A:143:ARG:NH2	2.35	0.60
1:B:208:TRP:CH2	1:B:215:THR:HG23	2.37	0.59
1:A:71:THR:HG23	2:A:402:HOH:O	2.01	0.59
1:A:219:TYR:N	1:A:220:PRO:HD2	2.18	0.59
1:B:64:LYS:HA	1:B:92:GLY:O	2.02	0.59
1:A:178:ARG:HH11	1:A:178:ARG:HB3	1.67	0.59
1:B:245:VAL:HA	1:B:251:THR:HG21	1.85	0.58
1:B:141:ARG:NH1	1:B:294:ASN:HD21	1.97	0.58
1:A:302:PRO:HG3	1:A:332:GLY:O	2.04	0.58
1:A:141:ARG:HE	1:A:294:ASN:HD22	1.51	0.58
1:A:21:THR:CG2	2:A:376:HOH:O	2.52	0.58
1:A:229:ARG:NH1	1:A:251:THR:HG22	2.19	0.58
1:A:95:ARG:HA	1:A:121:ASP:O	2.04	0.57
1:B:229:ARG:NH2	1:B:248:PRO:O	2.37	0.57
1:A:332:GLY:CA	1:B:335:THR:HG22	2.34	0.57
1:B:110:ARG:O	1:B:110:ARG:HG2	2.04	0.57
1:A:33:LYS:CE	1:A:65:GLY:HA3	2.35	0.57
1:B:142:MSE:HA	1:B:142:MSE:CE	2.35	0.57
1:B:217:ALA:O	1:B:218:LEU:O	2.23	0.56
1:B:96:VAL:HG22	1:B:122:VAL:HG12	1.87	0.56
1:B:104:ASN:O	1:B:105:PRO:C	2.43	0.56
1:A:137:GLY:HA2	1:A:148:TYR:HB2	1.88	0.56
1:B:98:ALA:O	1:B:124:HIS:HA	2.06	0.56
1:B:116:GLN:OE1	1:B:122:VAL:HG22	2.06	0.55
1:A:154:GLY:HA3	1:A:163:MSE:HB3	1.88	0.55
1:B:42:TYR:CE1	1:B:44:GLN:HG2	2.42	0.55
1:B:141:ARG:HE	1:B:294:ASN:HD22	1.53	0.54
1:A:66:ALA:HA	1:A:94:ALA:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:O	1:A:62:LYS:HE3	2.08	0.54
1:A:187:SER:OG	1:A:297:TRP:HB2	2.08	0.53
1:B:17:GLY:O	1:B:21:THR:HB	2.08	0.53
1:B:52:GLU:O	1:B:56:LEU:HB2	2.07	0.53
1:A:98:ALA:O	1:A:124:HIS:HA	2.08	0.53
1:A:45:ARG:HH22	1:A:223:ASN:HD22	1.57	0.53
1:B:149:ILE:HD11	1:B:285:MSE:SE	2.59	0.53
1:B:258:GLU:OE1	1:B:269:THR:HG21	2.09	0.53
1:A:141:ARG:HH11	1:A:294:ASN:ND2	2.03	0.52
1:B:139:LEU:O	1:B:143:ARG:HG3	2.08	0.52
1:B:222:GLN:NE2	1:B:222:GLN:H	2.08	0.52
1:A:149:ILE:HD11	1:A:285:MSE:SE	2.59	0.52
1:B:198:LEU:HD11	1:B:237:ARG:HB3	1.92	0.52
1:A:188:HIS:HD2	1:A:294:ASN:H	1.57	0.52
1:A:64:LYS:O	1:A:92:GLY:O	2.27	0.52
1:A:108:ALA:C	1:A:110:ARG:H	2.11	0.52
1:A:309:LEU:HD13	1:B:325:LEU:HD13	1.90	0.52
1:A:67:THR:HG23	1:A:95:ARG:HG2	1.92	0.51
1:B:188:HIS:HA	1:B:225:ARG:NH2	2.25	0.51
1:A:245:VAL:HA	1:A:251:THR:HG21	1.92	0.51
1:A:144:THR:C	1:A:146:PHE:H	2.13	0.51
1:A:150:GLN:HG2	1:A:316:GLU:HG2	1.92	0.51
1:A:188:HIS:CD2	1:A:294:ASN:H	2.28	0.51
1:B:100:MSE:HE2	1:B:131:ALA:HB1	1.92	0.51
1:B:212:ASP:CG	1:B:214:GLN:OE1	2.49	0.51
1:A:21:THR:HG21	1:A:26:ASN:OD1	2.11	0.51
1:A:158:ASP:O	1:B:334:CYS:HA	2.11	0.51
1:B:218:LEU:HG	1:B:219:TYR:H	1.75	0.51
1:B:141:ARG:O	1:B:144:THR:O	2.29	0.50
1:A:235:GLN:HB2	1:A:237:ARG:HD2	1.94	0.50
1:A:239:THR:HB	1:A:242:HIS:ND1	2.27	0.50
1:A:139:LEU:O	1:A:143:ARG:HG3	2.12	0.50
1:A:185:ALA:HA	1:A:206:VAL:HG21	1.94	0.50
1:A:126:LEU:HD22	1:A:127:MSE:HG3	1.93	0.50
1:A:141:ARG:HE	1:A:294:ASN:ND2	2.10	0.49
1:B:101:GLN:O	1:B:102:ASP:HB3	2.11	0.49
1:A:160:ARG:HA	1:A:331:ARG:O	2.12	0.49
1:A:310:GLN:OE1	1:A:337:PRO:HD2	2.12	0.48
1:A:255:ARG:HD2	1:A:269:THR:HB	1.95	0.48
1:B:355:HIS:HD2	2:B:377:HOH:O	1.96	0.48
1:A:150:GLN:HG2	1:A:316:GLU:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HE	1:B:294:ASN:ND2	2.10	0.48
1:B:156:SER:OG	1:B:159:GLY:O	2.22	0.48
1:B:332:GLY:C	1:B:334:CYS:N	2.66	0.48
1:B:222:GLN:H	1:B:222:GLN:HE21	1.62	0.48
1:A:206:VAL:N	1:A:226:GLN:HE22	2.05	0.48
1:A:212:ASP:C	1:A:212:ASP:OD2	2.52	0.48
1:B:191:LEU:HB3	1:B:298:VAL:HG22	1.96	0.48
1:A:144:THR:O	1:A:144:THR:OG1	2.32	0.47
1:B:9:ARG:HG3	2:B:392:HOH:O	2.14	0.47
1:B:317:LEU:HB2	1:B:364:LEU:HB2	1.97	0.47
1:B:3:ASP:HB3	1:B:126:LEU:HD11	1.97	0.46
1:A:66:ALA:HB3	2:A:399:HOH:O	2.14	0.46
1:B:160:ARG:NH1	1:B:326:LEU:O	2.49	0.46
1:B:349:LYS:HE2	1:B:367:ALA:CB	2.45	0.46
1:B:67:THR:HA	1:B:95:ARG:O	2.15	0.46
1:B:220:PRO:HB2	1:B:222:GLN:NE2	2.31	0.46
1:A:218:LEU:HG	1:A:219:TYR:H	1.77	0.46
1:B:212:ASP:OD1	1:B:214:GLN:NE2	2.42	0.46
1:B:126:LEU:HD22	1:B:127:MSE:HG3	1.98	0.46
1:B:366:GLY:O	1:B:367:ALA:C	2.55	0.45
1:B:332:GLY:C	1:B:334:CYS:H	2.18	0.45
1:B:345:ALA:O	1:B:346:PRO:C	2.55	0.45
1:B:171:ILE:O	1:B:173:SER:N	2.46	0.45
1:A:219:TYR:N	1:A:220:PRO:CD	2.79	0.45
1:A:137:GLY:HA2	1:A:148:TYR:CB	2.47	0.45
1:B:229:ARG:NH1	1:B:244:ILE:O	2.50	0.45
1:A:316:GLU:HB2	1:A:364:LEU:O	2.17	0.44
1:A:161:THR:HG22	1:A:330:ALA:O	2.18	0.44
1:A:219:TYR:H	1:A:220:PRO:HD2	1.82	0.44
1:B:188:HIS:CD2	1:B:294:ASN:H	2.35	0.44
1:B:166:GLY:C	1:B:168:SER:H	2.21	0.44
1:A:24:ASN:HD22	1:A:46:ALA:HA	1.82	0.44
1:A:96:VAL:HG13	1:A:120:ILE:HG21	2.00	0.44
1:B:48:GLU:HB3	2:B:381:HOH:O	2.18	0.44
1:B:318:ILE:HG23	1:B:361:CYS:SG	2.58	0.44
1:B:19:PHE:HB3	1:B:219:TYR:CZ	2.53	0.43
1:A:45:ARG:HH12	1:A:223:ASN:HB3	1.84	0.43
1:B:216:GLN:C	1:B:217:ALA:O	2.54	0.43
1:B:218:LEU:HG	1:B:219:TYR:N	2.32	0.43
1:B:218:LEU:CG	1:B:219:TYR:H	2.30	0.43
1:B:284:LEU:HG	1:B:285:MSE:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PRO:HA	1:A:333:LEU:O	2.17	0.43
1:B:281:LEU:HD13	1:B:308:LEU:HD23	2.00	0.43
1:A:332:GLY:HA3	1:B:335:THR:CG2	2.43	0.43
1:B:172:THR:N	2:B:397:HOH:O	2.51	0.43
1:A:146:PHE:CZ	1:A:286:MSE:HG3	2.54	0.43
1:B:188:HIS:HD2	1:B:294:ASN:H	1.67	0.43
1:A:34:ASP:HA	2:A:410:HOH:O	2.18	0.42
1:A:174:PRO:O	1:A:178:ARG:HG3	2.20	0.42
1:A:212:ASP:OD2	1:A:213:GLU:N	2.53	0.42
1:A:22:HIS:HB3	1:A:188:HIS:CD2	2.53	0.42
1:A:73:GLU:CB	1:A:101:GLN:OE1	2.67	0.42
1:A:226:GLN:NE2	1:A:226:GLN:HA	2.34	0.42
1:B:151:LEU:HD21	1:B:305:ALA:HB1	2.00	0.42
1:A:103:PRO:O	1:A:105:PRO:HA	2.19	0.42
1:B:194:SER:CB	1:B:233:ASP:CB	2.84	0.42
1:B:219:TYR:HD1	1:B:219:TYR:HA	1.71	0.42
1:B:337:PRO:HB2	1:B:338:GLY:H	1.61	0.42
1:A:184:ARG:NE	1:A:299:GLU:OE1	2.46	0.42
1:B:27:VAL:O	1:B:42:TYR:HA	2.20	0.42
1:A:101:GLN:HG3	1:A:109:GLY:HA2	2.00	0.42
1:A:310:GLN:HE22	1:A:338:GLY:H	1.66	0.42
1:B:219:TYR:N	1:B:220:PRO:CD	2.82	0.42
1:A:218:LEU:CG	1:A:219:TYR:N	2.76	0.42
1:A:220:PRO:HG2	1:A:223:ASN:OD1	2.20	0.42
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.34	0.41
1:A:52:GLU:OE2	1:A:84:CYS:SG	2.70	0.41
1:A:70:VAL:O	1:A:98:ALA:HA	2.19	0.41
1:A:101:GLN:CG	1:A:109:GLY:HA2	2.50	0.41
1:B:110:ARG:C	1:B:112:LEU:N	2.73	0.41
1:B:334:CYS:O	1:B:335:THR:C	2.59	0.41
1:A:33:LYS:CD	1:A:65:GLY:HA3	2.51	0.41
1:A:140:LYS:O	1:A:144:THR:O	2.39	0.41
1:A:91:ALA:O	1:A:93:VAL:N	2.53	0.41
1:B:217:ALA:O	1:B:218:LEU:C	2.57	0.41
1:A:167:GLU:HB3	1:A:170:TRP:HE1	1.86	0.41
1:A:102:ASP:HA	1:A:103:PRO:HD3	1.89	0.40
1:A:325:LEU:HD21	1:B:309:LEU:HD22	2.03	0.40
1:B:159:GLY:HA3	1:B:334:CYS:CB	2.52	0.40

There are no symmetry-related clashes.

## 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	347/402 (86%)	310 (89%)	24 (7%)	13 (4%)	2	4
1	B	359/402 (89%)	319 (89%)	23 (6%)	17 (5%)	2	2
All	All	706/804 (88%)	629 (89%)	47 (7%)	30 (4%)	2	3

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLY
1	A	105	PRO
1	A	172	THR
1	A	213	GLU
1	A	217	ALA
1	A	331	ARG
1	B	103	PRO
1	B	162	ALA
1	B	213	GLU
1	B	217	ALA
1	B	332	GLY
1	B	334	CYS
1	B	337	PRO
1	A	65	GLY
1	A	109	GLY
1	A	129	SER
1	A	145	GLY
1	B	65	GLY
1	B	67	THR
1	B	92	GLY
1	B	95	ARG
1	B	167	GLU
1	B	218	LEU
1	B	221	GLN
1	B	106	GLN

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Mol	Chain	Res	Type
1	A	34	ASP
1	A	329	ASP
1	B	102	ASP
1	B	346	PRO
1	A	219	TYR

### 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	281/321 (88%)	252 (90%)	29 (10%)	6	12
1	B	282/321 (88%)	255 (90%)	27 (10%)	7	14
All	All	563/642 (88%)	507 (90%)	56 (10%)	6	13

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	LEU
1	A	15	GLN
1	A	21	THR
1	A	56	LEU
1	A	64	LYS
1	A	85	CYS
1	A	96	VAL
1	A	114	ARG
1	A	123	SER
1	A	126	LEU
1	A	152	LYS
1	A	153	LEU
1	A	171	ILE
1	A	183	LEU
1	A	219	TYR
1	A	222	GLN
1	A	224	LEU
1	A	226	GLN

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Mol	Chain	Res	Type
1	A	241	VAL
1	A	251	THR
1	A	256	THR
1	A	269	THR
1	A	304	LEU
1	A	324	LYS
1	A	329	ASP
1	A	334	CYS
1	A	336	LEU
1	A	347	GLN
1	A	365	VAL
1	B	2	GLN
1	B	21	THR
1	B	36	GLU
1	B	48	GLU
1	B	56	LEU
1	B	67	THR
1	B	101	GLN
1	B	110	ARG
1	B	114	ARG
1	B	117	GLN
1	B	126	LEU
1	B	142	MSE
1	B	152	LYS
1	B	153	LEU
1	B	167	GLU
1	B	183	LEU
1	B	215	THR
1	B	219	TYR
1	B	222	GLN
1	B	224	LEU
1	B	241	VAL
1	B	251	THR
1	B	269	THR
1	B	287	GLN
1	B	304	LEU
1	B	339	LEU
1	B	360	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	44	GLN
1	A	117	GLN
1	A	188	HIS
1	A	221	GLN
1	A	222	GLN
1	A	223	ASN
1	A	226	GLN
1	A	291	GLN
1	A	294	ASN
1	B	15	GLN
1	B	101	GLN
1	B	133	GLN
1	B	186	GLN
1	B	188	HIS
1	B	222	GLN
1	B	226	GLN
1	B	257	GLN
1	B	294	ASN
1	B	310	GLN
1	B	363	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	346/402 (86%)	1.29	81 (23%) <b>2</b> <b>2</b>	74, 86, 100, 111	0
1	B	354/402 (88%)	1.76	133 (37%) <b>1</b> <b>1</b>	75, 87, 99, 106	0
All	All	700/804 (87%)	1.53	214 (30%) <b>1</b> <b>1</b>	74, 86, 100, 111	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ASP	6.2
1	B	164	ALA	6.0
1	A	218	LEU	5.4
1	B	233	ASP	5.2
1	B	334	CYS	5.2
1	B	162	ALA	5.0
1	B	335	THR	4.9
1	A	335	THR	4.7
1	B	327	GLY	4.7
1	B	218	LEU	4.5
1	B	219	TYR	4.5
1	A	83	PRO	4.4
1	B	-4	THR	4.3
1	A	346	PRO	4.3
1	A	217	ALA	4.2
1	A	75	CYS	4.1
1	B	337	PRO	4.0
1	A	338	GLY	4.0
1	B	342	LEU	3.9
1	A	334	CYS	3.9
1	B	96	VAL	3.8
1	A	19	PHE	3.8
1	A	-4	THR	3.8
1	A	233	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	328	SER	3.7
1	A	331	ARG	3.7
1	A	84	CYS	3.7
1	B	108	ALA	3.6
1	A	67	THR	3.5
1	A	367	ALA	3.5
1	A	170	TRP	3.5
1	B	217	ALA	3.4
1	A	167	GLU	3.4
1	B	104	ASN	3.4
1	B	357	GLY	3.4
1	A	94	ALA	3.4
1	B	367	ALA	3.4
1	A	336	LEU	3.4
1	B	171	ILE	3.4
1	B	166	GLY	3.4
1	B	338	GLY	3.3
1	B	107	VAL	3.3
1	B	45	ARG	3.3
1	A	162	ALA	3.3
1	B	325	LEU	3.2
1	B	323	PRO	3.1
1	B	222	GLN	3.1
1	B	21	THR	3.1
1	B	160	ARG	3.1
1	A	-2	TYR	3.1
1	B	312	GLY	3.1
1	B	333	LEU	3.1
1	B	131	ALA	3.1
1	B	176	ALA	3.1
1	B	165	SER	3.1
1	A	332	GLY	3.1
1	A	107	VAL	3.0
1	B	44	GLN	3.0
1	B	19	PHE	3.0
1	B	208	TRP	3.0
1	A	219	TYR	3.0
1	A	18	ARG	3.0
1	B	345	ALA	3.0
1	B	175	GLN	3.0
1	A	105	PRO	3.0
1	A	110	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	337	PRO	2.9
1	A	71	THR	2.9
1	A	66	ALA	2.9
1	A	15	GLN	2.9
1	B	155	ALA	2.9
1	B	360	VAL	2.9
1	A	91	ALA	2.9
1	A	330	ALA	2.9
1	B	145	GLY	2.9
1	B	-1	ILE	2.8
1	A	45	ARG	2.8
1	B	262	GLU	2.8
1	A	174	PRO	2.8
1	B	178	ARG	2.8
1	B	353	ILE	2.8
1	B	168	SER	2.8
1	A	269	THR	2.8
1	B	214	GLN	2.8
1	A	329	ASP	2.8
1	B	72	LEU	2.8
1	B	134	LEU	2.8
1	B	136	LYS	2.8
1	A	101	GLN	2.7
1	B	216	GLN	2.7
1	A	109	GLY	2.7
1	B	6	TYR	2.7
1	B	256	THR	2.7
1	A	134	LEU	2.7
1	B	182	LEU	2.7
1	B	362	LEU	2.7
1	B	109	GLY	2.7
1	A	171	ILE	2.7
1	A	135	ASN	2.7
1	B	15	GLN	2.7
1	A	103	PRO	2.7
1	B	105	PRO	2.7
1	B	41	GLY	2.7
1	B	159	GLY	2.7
1	A	198	LEU	2.7
1	A	326	LEU	2.7
1	B	66	ALA	2.7
1	A	161	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	2.7
1	B	22	HIS	2.7
1	B	140	LYS	2.6
1	A	325	LEU	2.6
1	B	343	ALA	2.6
1	B	42	TYR	2.6
1	B	241	VAL	2.6
1	A	44	GLN	2.6
1	A	46	ALA	2.6
1	B	18	ARG	2.6
1	B	172	THR	2.6
1	A	168	SER	2.6
1	A	12	LYS	2.6
1	B	64	LYS	2.6
1	A	104	ASN	2.6
1	B	26	ASN	2.6
1	B	110	ARG	2.6
1	B	2	GLN	2.6
1	A	16	ARG	2.6
1	A	131	ALA	2.6
1	B	355	HIS	2.6
1	B	65	GLY	2.6
1	A	90	ALA	2.5
1	B	330	ALA	2.5
1	B	137	GLY	2.5
1	A	157	LEU	2.5
1	B	14	ALA	2.5
1	B	91	ALA	2.5
1	B	99	SER	2.5
1	A	-3	LEU	2.5
1	B	27	VAL	2.5
1	B	53	VAL	2.5
1	B	321	ILE	2.5
1	A	289	GLY	2.5
1	A	132	GLU	2.5
1	B	170	TRP	2.5
1	B	339	LEU	2.5
1	B	310	GLN	2.5
1	B	320	TYR	2.5
1	A	327	GLY	2.5
1	B	71	THR	2.5
1	A	112	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	347	GLN	2.4
1	B	215	THR	2.4
1	B	173	SER	2.4
1	B	356	VAL	2.4
1	A	214	GLN	2.4
1	B	101	GLN	2.4
1	A	137	GLY	2.4
1	A	63	ALA	2.4
1	B	40	GLU	2.4
1	B	211	LEU	2.4
1	B	97	VAL	2.4
1	B	187	SER	2.4
1	B	8	ALA	2.4
1	B	359	ASP	2.4
1	A	20	THR	2.3
1	B	274	GLU	2.3
1	B	336	LEU	2.3
1	B	255	ARG	2.3
1	B	1	GLY	2.3
1	A	213	GLU	2.3
1	B	207	ARG	2.3
1	A	133	GLN	2.3
1	A	129	SER	2.3
1	B	125	GLY	2.3
1	B	48	GLU	2.3
1	A	228	ILE	2.3
1	A	333	LEU	2.3
1	B	177	ARG	2.3
1	B	212	ASP	2.3
1	B	273	PRO	2.3
1	B	117	GLN	2.3
1	B	322	ALA	2.2
1	B	12	LYS	2.2
1	B	213	GLU	2.2
1	B	30	VAL	2.2
1	A	159	GLY	2.2
1	B	76	SER	2.2
1	B	221	GLN	2.2
1	B	68	ALA	2.2
1	B	16	ARG	2.2
1	B	220	PRO	2.2
1	B	346	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	ASN	2.2
1	B	0	GLN	2.2
1	B	89	ILE	2.2
1	B	90	ALA	2.1
1	B	363	HIS	2.1
1	A	34	ASP	2.1
1	B	326	LEU	2.1
1	B	311	ALA	2.1
1	A	17	GLY	2.1
1	A	54	HIS	2.1
1	B	332	GLY	2.1
1	A	290	LYS	2.1
1	A	172	THR	2.1
1	A	115	LEU	2.1
1	A	126	LEU	2.1
1	B	223	ASN	2.1
1	B	290	LYS	2.0
1	A	57	ARG	2.0
1	B	236	ASN	2.0
1	B	43	HIS	2.0
1	B	133	GLN	2.0
1	B	86	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.