



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:15 PM UTC

PDB ID : 2G6V / pdb_00002g6v
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

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
Mogul : 2022.3.0, CSD as543be (2022)
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

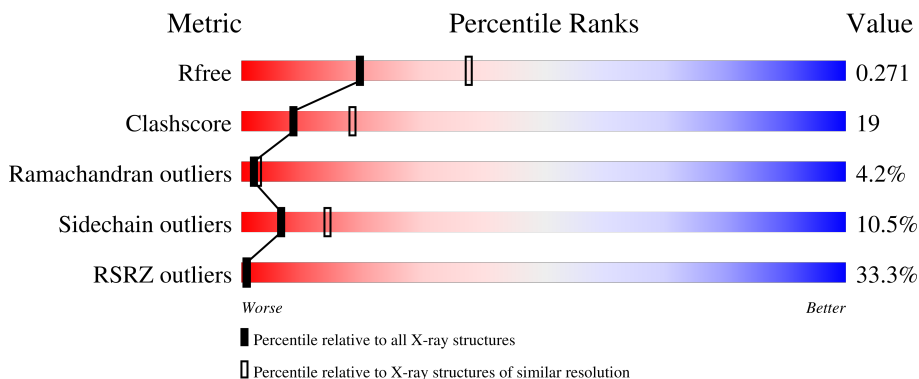
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	71.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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	0.61	0/2753	0.93	4/3723 (0.1%)
1	B	0.55	0/2800	0.90	3/3790 (0.1%)
All	All	0.58	0/5553	0.91	7/7513 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	LEU	N-CA-C	-8.59	99.54	110.19
1	A	173	SER	N-CA-C	8.20	115.60	108.22
1	A	168	SER	N-CA-C	-7.14	105.75	114.75
1	B	173	SER	N-CA-C	6.99	114.51	108.22
1	A	67	THR	N-CA-C	6.69	125.04	110.80
1	B	66	ALA	N-CA-C	6.08	115.87	107.73
1	B	213	GLU	N-CA-C	5.22	121.92	110.80

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	112	0
1	B	2756	0	2735	100	0
2	A	42	0	0	6	0
2	B	23	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5530	0	5433	206	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 (206) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:104:ASN:O	1:B:105:PRO:C	2.43	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:A:108:ALA:C	1:A:110:ARG:H	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:144:THR:C	1:A:146:PHE:H	2.13	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:212:ASP:CG	1:B:214:GLN:OE1	2.49	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
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:332:GLY:C	1:B:334:CYS:N	2.66	0.53
1:B:149:ILE:HD11	1:B:285:MSE:SE	2.59	0.53
1:A:212:ASP:C	1:A:212:ASP:OD2	2.52	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: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: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: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:B:366:GLY:O	1:B:367:ALA:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:HB	1:A:242:HIS:ND1	2.27	0.50
1:B:345:ALA:O	1:B:346:PRO:C	2.55	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:332:GLY:C	1:B:334:CYS:H	2.18	0.49
1:B:166:GLY:C	1:B:168:SER:H	2.21	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:B:101:GLN:O	1:B:102:ASP:HB3	2.11	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
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:216:GLN:C	1:B:217:ALA:O	2.54	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: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:B:334:CYS:O	1:B:335:THR:C	2.59	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:217:ALA:O	1:B:218:LEU:C	2.57	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:B:217:ALA:C	1:B:218:LEU:O	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:302:PRO:HA	1:A:333:LEU:O	2.17	0.43
1:B:110:ARG:C	1:B:112:LEU:N	2.73	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:165:SER:O	1:B:166:GLY:C	2.63	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:275:HIS:O	1:A:276:LYS:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLN:CG	1:A:109:GLY:HA2	2.50	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:A:167:GLU:HB3	1:A:170:TRP:HE1	1.86	0.41
1:B:105:PRO:C	1:B:107:VAL:N	2.79	0.40
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	3
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

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Mol	Chain	Res	Type
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
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%)	249 (89%)	32 (11%)	5	11
1	B	282/321 (88%)	255 (90%)	27 (10%)	8	17
All	All	563/642 (88%)	504 (90%)	59 (10%)	6	14

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	LEU
1	A	15	GLN

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Mol	Chain	Res	Type
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	117	GLN
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	215	THR
1	A	218	LEU
1	A	219	TYR
1	A	222	GLN
1	A	224	LEU
1	A	226	GLN
1	A	241	VAL
1	A	251	THR
1	A	256	THR
1	A	269	THR
1	A	304	LEU
1	A	329	ASP
1	A	333	LEU
1	A	334	CYS
1	A	336	LEU
1	A	347	GLN
1	A	365	VAL
1	B	21	THR
1	B	36	GLU
1	B	48	GLU
1	B	56	LEU
1	B	67	THR
1	B	71	THR
1	B	96	VAL
1	B	101	GLN
1	B	110	ARG
1	B	117	GLN
1	B	126	LEU
1	B	142	MSE

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Mol	Chain	Res	Type
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	286	MSE
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	44	GLN
1	A	116	GLN
1	A	188	HIS
1	A	223	ASN
1	A	226	GLN
1	A	247	GLN
1	A	291	GLN
1	A	294	ASN
1	B	2	GLN
1	B	15	GLN
1	B	101	GLN
1	B	117	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	347	GLN
1	B	363	HIS

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	346/402 (86%)	1.41	84 (24%) 2 1	74, 86, 100, 111	0
1	B	354/402 (88%)	1.87	149 (42%) 0 0	75, 87, 99, 106	0
All	All	700/804 (87%)	1.64	233 (33%) 1 1	74, 86, 100, 111	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ASP	6.2
1	B	164	ALA	6.2
1	A	218	LEU	5.5
1	B	334	CYS	5.3
1	B	233	ASP	5.2
1	B	162	ALA	5.1
1	B	335	THR	5.0
1	B	327	GLY	4.8
1	A	335	THR	4.8
1	B	218	LEU	4.7
1	B	219	TYR	4.6
1	A	83	PRO	4.5
1	A	346	PRO	4.4
1	B	-4	THR	4.4
1	A	217	ALA	4.4
1	A	75	CYS	4.2
1	B	337	PRO	4.1
1	A	338	GLY	4.1
1	B	342	LEU	4.0
1	A	334	CYS	4.0
1	A	19	PHE	3.9
1	B	96	VAL	3.9
1	A	-4	THR	3.8
1	A	84	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	233	ASP	3.8
1	B	328	SER	3.8
1	B	108	ALA	3.8
1	A	331	ARG	3.7
1	A	170	TRP	3.6
1	A	367	ALA	3.6
1	A	67	THR	3.6
1	B	217	ALA	3.6
1	B	357	GLY	3.5
1	A	94	ALA	3.5
1	B	367	ALA	3.5
1	A	336	LEU	3.5
1	B	104	ASN	3.5
1	B	166	GLY	3.5
1	B	171	ILE	3.5
1	B	338	GLY	3.5
1	A	167	GLU	3.5
1	B	107	VAL	3.4
1	A	162	ALA	3.4
1	B	45	ARG	3.3
1	B	325	LEU	3.3
1	B	323	PRO	3.3
1	A	-2	TYR	3.2
1	B	312	GLY	3.2
1	B	333	LEU	3.2
1	B	21	THR	3.2
1	B	222	GLN	3.2
1	A	332	GLY	3.2
1	B	131	ALA	3.2
1	B	176	ALA	3.2
1	A	107	VAL	3.2
1	B	19	PHE	3.2
1	B	160	ARG	3.1
1	B	208	TRP	3.1
1	B	165	SER	3.1
1	A	219	TYR	3.1
1	B	44	GLN	3.1
1	B	345	ALA	3.1
1	A	105	PRO	3.1
1	A	337	PRO	3.0
1	B	175	GLN	3.0
1	A	18	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	66	ALA	3.0
1	A	71	THR	3.0
1	B	155	ALA	3.0
1	A	15	GLN	3.0
1	A	110	ARG	3.0
1	B	145	GLY	3.0
1	A	91	ALA	3.0
1	A	330	ALA	3.0
1	B	360	VAL	3.0
1	B	-1	ILE	3.0
1	A	174	PRO	2.9
1	B	353	ILE	2.9
1	A	269	THR	2.9
1	B	72	LEU	2.9
1	B	134	LEU	2.9
1	B	262	GLU	2.9
1	B	168	SER	2.9
1	A	45	ARG	2.9
1	B	214	GLN	2.9
1	B	178	ARG	2.9
1	A	329	ASP	2.9
1	A	109	GLY	2.9
1	B	6	TYR	2.9
1	B	109	GLY	2.8
1	B	136	LYS	2.8
1	A	134	LEU	2.8
1	B	182	LEU	2.8
1	B	362	LEU	2.8
1	A	101	GLN	2.8
1	B	216	GLN	2.8
1	A	171	ILE	2.8
1	B	41	GLY	2.8
1	B	159	GLY	2.8
1	B	256	THR	2.8
1	A	103	PRO	2.8
1	B	105	PRO	2.8
1	A	135	ASN	2.8
1	A	145	GLY	2.8
1	A	198	LEU	2.8
1	A	326	LEU	2.8
1	B	66	ALA	2.8
1	B	15	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	325	LEU	2.8
1	B	22	HIS	2.8
1	A	161	THR	2.8
1	B	343	ALA	2.8
1	B	42	TYR	2.8
1	A	46	ALA	2.7
1	B	241	VAL	2.7
1	B	140	LYS	2.7
1	B	172	THR	2.7
1	A	44	GLN	2.7
1	A	104	ASN	2.7
1	A	168	SER	2.7
1	B	65	GLY	2.7
1	B	26	ASN	2.7
1	A	131	ALA	2.7
1	A	12	LYS	2.7
1	B	64	LYS	2.7
1	B	355	HIS	2.7
1	B	18	ARG	2.7
1	B	137	GLY	2.7
1	A	90	ALA	2.7
1	B	330	ALA	2.7
1	B	2	GLN	2.6
1	A	157	LEU	2.6
1	B	110	ARG	2.6
1	B	14	ALA	2.6
1	B	91	ALA	2.6
1	A	-3	LEU	2.6
1	A	16	ARG	2.6
1	A	289	GLY	2.6
1	B	27	VAL	2.6
1	B	53	VAL	2.6
1	B	170	TRP	2.6
1	B	321	ILE	2.6
1	B	320	TYR	2.6
1	B	339	LEU	2.6
1	A	327	GLY	2.6
1	B	99	SER	2.6
1	A	112	LEU	2.6
1	B	71	THR	2.5
1	B	310	GLN	2.6
1	A	132	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	137	GLY	2.5
1	B	356	VAL	2.5
1	A	347	GLN	2.5
1	B	215	THR	2.5
1	A	63	ALA	2.5
1	A	214	GLN	2.5
1	B	101	GLN	2.5
1	B	173	SER	2.5
1	B	211	LEU	2.5
1	B	97	VAL	2.5
1	B	8	ALA	2.5
1	B	336	LEU	2.5
1	B	1	GLY	2.5
1	A	20	THR	2.4
1	B	187	SER	2.4
1	B	359	ASP	2.4
1	B	40	GLU	2.4
1	B	125	GLY	2.4
1	B	274	GLU	2.4
1	A	133	GLN	2.4
1	B	255	ARG	2.4
1	A	228	ILE	2.4
1	A	333	LEU	2.4
1	A	129	SER	2.4
1	A	213	GLU	2.4
1	B	273	PRO	2.4
1	B	207	ARG	2.4
1	B	48	GLU	2.4
1	B	212	ASP	2.4
1	B	117	GLN	2.4
1	B	322	ALA	2.4
1	A	159	GLY	2.3
1	B	177	ARG	2.3
1	B	30	VAL	2.3
1	B	12	LYS	2.3
1	B	68	ALA	2.3
1	B	213	GLU	2.3
1	B	76	SER	2.3
1	B	220	PRO	2.3
1	B	346	PRO	2.3
1	B	221	GLN	2.3
1	B	89	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	135	ASN	2.3
1	B	0	GLN	2.3
1	B	90	ALA	2.2
1	B	16	ARG	2.2
1	A	17	GLY	2.2
1	B	326	LEU	2.2
1	B	311	ALA	2.2
1	B	363	HIS	2.2
1	A	34	ASP	2.2
1	B	332	GLY	2.2
1	A	54	HIS	2.2
1	A	115	LEU	2.2
1	A	126	LEU	2.2
1	A	172	THR	2.2
1	B	223	ASN	2.2
1	A	290	LYS	2.2
1	B	236	ASN	2.1
1	B	290	LYS	2.1
1	B	43	HIS	2.1
1	B	358	PRO	2.1
1	B	133	GLN	2.1
1	B	86	ASP	2.1
1	A	57	ARG	2.1
1	B	248	PRO	2.1
1	A	42	TYR	2.1
1	B	269	THR	2.1
1	B	246	GLN	2.1
1	B	13	LEU	2.1
1	B	139	LEU	2.1
1	B	224	LEU	2.1
1	B	271	LEU	2.1
1	A	293	ILE	2.1
1	B	102	ASP	2.0
1	A	108	ALA	2.0
1	B	94	ALA	2.0
1	B	156	SER	2.0
1	B	239	THR	2.0
1	B	257	GLN	2.0
1	B	258	GLU	2.0
1	B	47	GLY	2.0
1	B	365	VAL	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.