



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 07:59 AM UTC

PDB ID : 2YJT / pdb_00002yjt
Title : Crystal structure of E. coli DEAD-box protein SrmB bound to regulator of ribonuclease activity A (RraA)
Authors : Pietras, Z.; Hardwick, S.W.; Luisi, B.F.
Deposited on : 2011-05-23
Resolution : 2.90 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

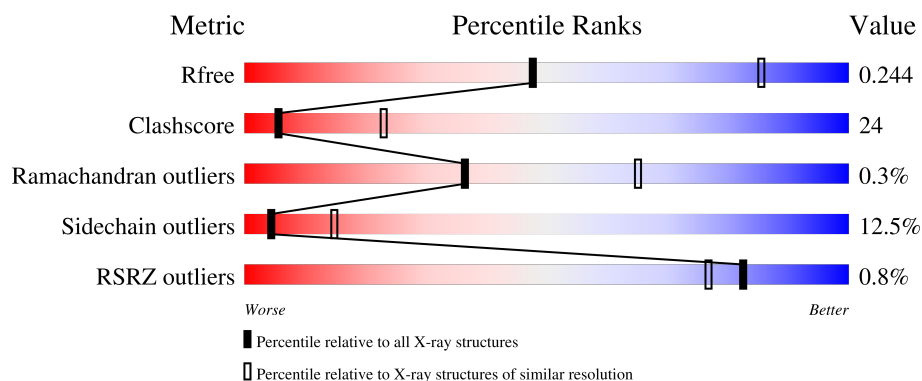
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	161	 70% 19% 9% .
1	B	161	 58% 32% 7% ..
1	C	161	 64% 30% ..
2	D	170	 3% 35% 40% 22% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4993 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 REGULATOR OF RIBONUCLEASE ACTIVITY A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1196	750	200	243	3			
1	B	158	Total	C	N	O	S	0	0	0
			1196	750	200	243	3			
1	C	158	Total	C	N	O	S	0	0	0
			1196	750	200	243	3			

- Molecule 2 is a protein called ATP-DEPENDENT RNA HELICASE SRMB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	170	Total	C	N	O	S	0	0	0
			1376	862	268	243	3			

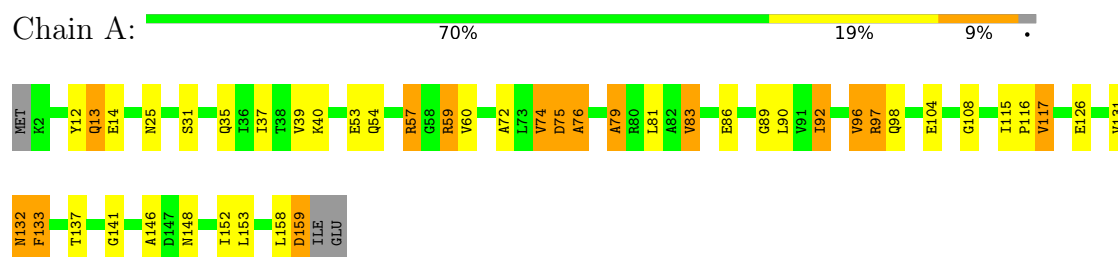
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	10	Total	O	0	0
			10	10		
3	C	6	Total	O	0	0
			6	6		
3	D	3	Total	O	0	0
			3	3		

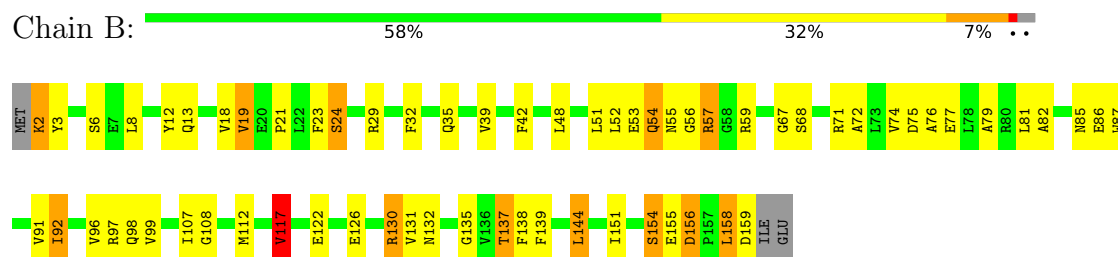
3 Residue-property plots

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.

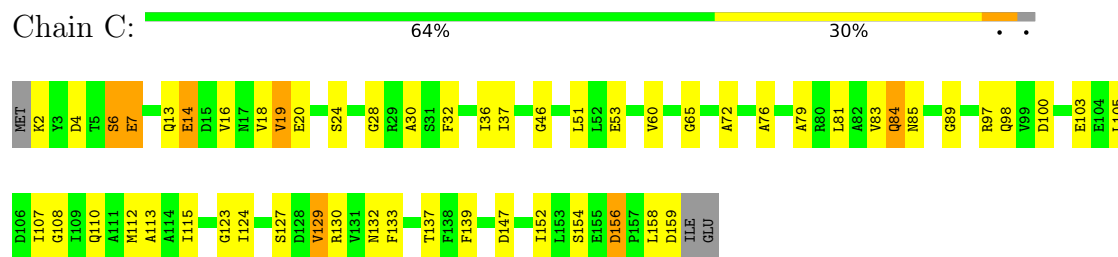
• Molecule 1: REGULATOR OF RIBONUCLEASE ACTIVITY A



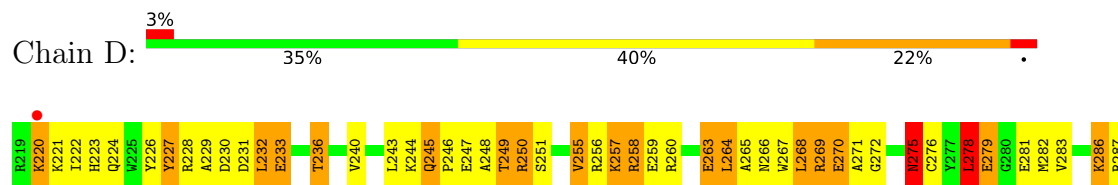
• Molecule 1: REGULATOR OF RIBONUCLEASE ACTIVITY A

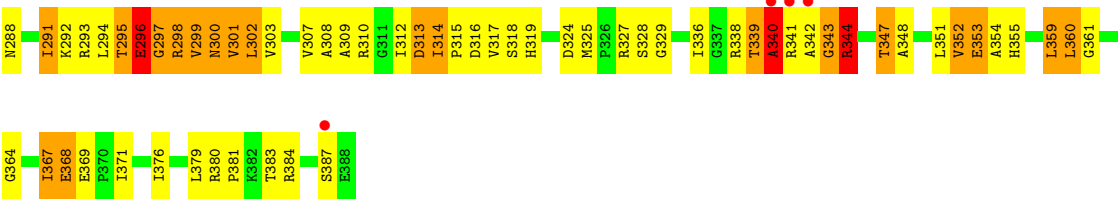


• Molecule 1: REGULATOR OF RIBONUCLEASE ACTIVITY A



• Molecule 2: ATP-DEPENDENT RNA HELICASE SRMB





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.39Å 73.39Å 222.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.30 – 2.90 74.30 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (74.30-2.90) 99.1 (74.30-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.192 , 0.257 0.198 , 0.244	Depositor DCC
R_{free} test set	806 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4993	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

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	1.39	12/1213 (1.0%)	1.12	4/1644 (0.2%)
1	B	1.21	1/1213 (0.1%)	1.12	4/1644 (0.2%)
1	C	1.25	2/1213 (0.2%)	1.18	7/1644 (0.4%)
2	D	1.61	19/1401 (1.4%)	1.44	21/1888 (1.1%)
All	All	1.38	34/5040 (0.7%)	1.23	36/6820 (0.5%)

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
2	D	0	6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	VAL	C-O	-7.38	1.16	1.24
2	D	255	VAL	CA-C	-7.04	1.45	1.52
2	D	278	LEU	C-O	-6.78	1.16	1.24
1	A	76	ALA	CA-CB	-6.48	1.43	1.53
2	D	255	VAL	N-CA	-6.42	1.38	1.46
2	D	229	ALA	CA-CB	-6.33	1.42	1.54
2	D	301	VAL	C-O	-6.31	1.17	1.24
2	D	227	TYR	C-O	-6.20	1.17	1.24
2	D	359	LEU	C-O	-6.14	1.17	1.24
2	D	352	VAL	C-O	-6.12	1.17	1.24
2	D	312	ILE	CA-CB	-6.03	1.47	1.54
2	D	301	VAL	CA-CB	-6.00	1.46	1.54
2	D	303	VAL	CA-CB	-5.83	1.47	1.54
1	C	13	GLN	C-O	-5.82	1.19	1.24
1	A	13	GLN	CA-C	-5.81	1.47	1.52
1	C	129	VAL	C-O	-5.75	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	354	ALA	CA-CB	-5.60	1.43	1.53
1	A	75	ASP	C-O	-5.47	1.17	1.24
1	B	24	SER	C-O	-5.47	1.17	1.23
2	D	244	LYS	CA-C	-5.46	1.46	1.53
1	A	153	LEU	C-O	-5.44	1.17	1.23
2	D	351	LEU	C-O	-5.44	1.17	1.24
1	A	13	GLN	C-O	-5.40	1.19	1.24
1	A	79	ALA	CA-CB	-5.40	1.44	1.53
2	D	348	ALA	CA-CB	-5.35	1.46	1.53
2	D	224	GLN	C-O	-5.30	1.18	1.23
2	D	245	GLN	CA-C	-5.21	1.46	1.52
2	D	248	ALA	CA-CB	-5.20	1.44	1.53
1	A	126	GLU	C-O	-5.16	1.17	1.23
2	D	255	VAL	CA-CB	-5.14	1.47	1.54
1	A	152	ILE	C-O	-5.11	1.18	1.23
1	A	131	VAL	C-O	-5.09	1.18	1.23
1	A	133	PHE	C-O	-5.03	1.18	1.23
1	A	60	VAL	C-O	-5.02	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	297	GLY	N-CA-C	-13.18	98.97	115.31
2	D	298	ARG	N-CA-C	-10.89	99.41	111.28
2	D	368	GLU	N-CA-C	-10.08	100.28	111.07
2	D	312	ILE	N-CA-C	7.88	119.20	108.17
2	D	339	THR	CB-CA-C	-7.86	98.44	111.41
2	D	387	SER	N-CA-C	7.71	120.43	111.02
1	C	115	ILE	CA-C-N	7.49	127.20	119.56
1	C	115	ILE	C-N-CA	7.49	127.20	119.56
2	D	269	ARG	N-CA-C	-7.46	103.08	111.07
2	D	361	GLY	N-CA-C	7.25	121.26	112.49
2	D	270	GLU	N-CA-C	-6.70	103.22	111.33
2	D	340	ALA	CB-CA-C	-6.67	108.90	116.63
2	D	268	LEU	CA-C-N	-6.38	112.15	120.44
2	D	268	LEU	C-N-CA	-6.38	112.15	120.44
2	D	264	LEU	N-CA-C	-6.30	104.46	111.71
1	A	75	ASP	N-CA-C	-6.25	100.06	108.86
1	B	57	ARG	N-CA-C	-6.09	101.26	110.28
2	D	275	ASN	N-CA-C	-6.09	98.47	108.76
2	D	295	THR	N-CA-C	-6.05	105.88	113.20
1	B	3	TYR	N-CA-C	5.97	118.69	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	279	GLU	N-CA-C	5.93	119.08	109.40
1	B	54	GLN	N-CA-C	-5.82	102.98	110.19
2	D	232	LEU	N-CA-C	-5.79	105.10	111.82
2	D	353	GLU	N-CA-C	-5.56	103.05	110.55
1	B	117	VAL	CB-CA-C	-5.51	104.63	111.08
2	D	250	ARG	N-CA-C	-5.43	98.35	108.02
1	C	37	ILE	N-CA-C	-5.37	99.77	107.78
1	C	53	GLU	N-CA-C	-5.32	106.76	113.20
2	D	352	VAL	N-CA-C	5.28	115.45	107.75
1	A	13	GLN	CB-CA-C	-5.25	110.09	117.23
2	D	329	GLY	N-CA-C	-5.24	108.17	114.66
1	A	53	GLU	N-CA-C	-5.24	106.57	113.17
1	C	156	ASP	CA-C-N	5.10	125.00	119.85
1	C	156	ASP	C-N-CA	5.10	125.00	119.85
1	A	92	ILE	N-CA-C	5.07	115.34	107.28
1	C	19	VAL	CB-CA-C	-5.01	104.72	111.63

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	296	GLU	Peptide
2	D	340	ALA	Peptide
2	D	342	ALA	Peptide
2	D	343	GLY	Peptide
2	D	344	ARG	Peptide
2	D	367	ILE	Peptide

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	1196	0	1147	38	0
1	B	1196	0	1147	52	0
1	C	1196	0	1147	38	1
2	D	1376	0	1407	112	3
3	A	10	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	3	0
3	C	6	0	0	3	0
3	D	3	0	0	6	0
All	All	4993	0	4848	231	3

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 24.

All (231) 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)
2:D:340:ALA:O	2:D:341:ARG:CG	1.84	1.25
2:D:233:GLU:HB3	3:D:2001:HOH:O	1.39	1.22
1:B:29:ARG:HD3	3:B:2003:HOH:O	1.42	1.16
1:C:124:ILE:O	3:C:2003:HOH:O	1.59	1.15
1:C:65:GLY:O	3:C:2004:HOH:O	1.59	1.14
2:D:340:ALA:O	2:D:341:ARG:HG2	0.95	1.13
2:D:233:GLU:CB	3:D:2001:HOH:O	1.93	1.11
1:B:57:ARG:NH2	1:B:86:GLU:OE1	1.87	1.08
1:A:79:ALA:O	1:A:83:VAL:HG23	1.52	1.06
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.24	1.00
2:D:232:LEU:O	2:D:236:THR:HG22	1.63	0.99
1:C:158:LEU:O	1:C:159:ASP:HB2	1.69	0.92
2:D:265:ALA:O	2:D:275:ASN:ND2	2.02	0.92
2:D:296:GLU:OE1	2:D:296:GLU:HA	1.66	0.92
2:D:255:VAL:HG12	2:D:256:ARG:H	1.36	0.90
2:D:269:ARG:O	2:D:272:GLY:N	2.05	0.90
1:A:40:LYS:NZ	3:A:2005:HOH:O	1.58	0.90
2:D:340:ALA:C	2:D:341:ARG:HG2	1.96	0.90
2:D:296:GLU:C	2:D:298:ARG:H	1.81	0.87
2:D:282:MET:HE2	2:D:286:LYS:HB2	1.56	0.87
2:D:255:VAL:HG12	2:D:256:ARG:N	1.91	0.86
2:D:283:VAL:HB	2:D:286:LYS:HD2	1.55	0.86
1:C:84:GLN:O	1:C:84:GLN:HG3	1.70	0.85
1:A:37:ILE:HD12	1:A:59:ARG:NH1	1.91	0.85
2:D:327:ARG:HG3	2:D:327:ARG:HH11	1.41	0.85
1:B:130:ARG:HH11	1:B:130:ARG:CG	1.90	0.83
2:D:220:LYS:NZ	2:D:341:ARG:HD3	1.95	0.81
2:D:296:GLU:O	2:D:298:ARG:N	2.13	0.81
1:C:14:GLU:OE1	1:C:14:GLU:HA	1.79	0.80
2:D:318:SER:O	2:D:319:HIS:HD2	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:232:LEU:O	2:D:236:THR:CG2	2.29	0.79
2:D:296:GLU:OE1	2:D:296:GLU:CA	2.30	0.79
2:D:294:LEU:HA	2:D:299:VAL:HG12	1.63	0.78
2:D:368:GLU:HB2	2:D:369:GLU:OE1	1.83	0.78
1:A:37:ILE:CD1	1:A:59:ARG:NH1	2.48	0.77
2:D:367:ILE:O	2:D:368:GLU:C	2.27	0.75
1:A:79:ALA:O	1:A:83:VAL:CG2	2.33	0.75
1:C:14:GLU:OE1	1:C:14:GLU:CA	2.30	0.74
2:D:264:LEU:HA	2:D:267:TRP:HE3	1.52	0.74
1:B:130:ARG:HG2	1:B:130:ARG:NH1	1.93	0.74
2:D:313:ASP:C	2:D:313:ASP:OD1	2.30	0.74
1:A:158:LEU:O	1:A:159:ASP:HB2	1.88	0.73
2:D:275:ASN:OD1	2:D:275:ASN:C	2.30	0.73
1:A:76:ALA:H	1:A:98:GLN:HE21	1.35	0.72
1:B:158:LEU:O	1:B:159:ASP:HB2	1.88	0.72
2:D:318:SER:O	2:D:319:HIS:CD2	2.42	0.72
2:D:258:ARG:HG3	2:D:258:ARG:HH11	1.54	0.71
2:D:264:LEU:HA	2:D:267:TRP:CE3	2.25	0.71
2:D:288:ASN:HA	2:D:291:ILE:HG22	1.72	0.71
2:D:222:ILE:HD12	2:D:336:ILE:HD12	1.73	0.71
2:D:293:ARG:O	2:D:296:GLU:O	2.11	0.69
2:D:282:MET:CE	2:D:286:LYS:HB2	2.22	0.68
1:C:2:LYS:O	1:C:2:LYS:HD3	1.93	0.68
2:D:249:THR:HG22	2:D:250:ARG:N	2.09	0.68
2:D:258:ARG:HG3	2:D:258:ARG:NH1	2.07	0.67
1:B:53:GLU:HG3	1:B:81:LEU:HD21	1.76	0.66
2:D:220:LYS:HZ1	2:D:341:ARG:HD3	1.60	0.66
2:D:313:ASP:OD1	2:D:314:ILE:N	2.30	0.65
2:D:282:MET:CE	2:D:286:LYS:CB	2.74	0.65
2:D:325:MET:HE2	2:D:360:LEU:HA	1.77	0.65
1:A:75:ASP:C	1:A:75:ASP:OD1	2.39	0.65
2:D:369:GLU:OE1	2:D:369:GLU:N	2.30	0.65
2:D:245:GLN:HB3	2:D:247:GLU:OE1	1.97	0.64
1:A:54:GLN:HE21	2:D:307:VAL:HG12	1.63	0.64
2:D:300:ASN:OD1	2:D:300:ASN:N	2.30	0.63
2:D:359:LEU:HG	3:D:2003:HOH:O	1.98	0.63
1:A:117:VAL:CG2	1:B:18:VAL:HG21	2.29	0.63
1:C:79:ALA:O	1:C:83:VAL:HG23	1.97	0.63
2:D:296:GLU:C	2:D:298:ARG:N	2.45	0.62
2:D:283:VAL:HB	2:D:286:LYS:CD	2.29	0.62
1:B:12:TYR:O	1:B:13:GLN:C	2.42	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:O	1:C:85:ASN:ND2	2.32	0.62
2:D:220:LYS:HZ3	2:D:341:ARG:HD3	1.63	0.61
2:D:369:GLU:O	2:D:369:GLU:HG2	1.90	0.61
2:D:258:ARG:HG2	2:D:279:GLU:OE2	2.02	0.60
1:C:158:LEU:O	1:C:159:ASP:CB	2.46	0.60
2:D:327:ARG:HG3	2:D:327:ARG:NH1	2.08	0.60
1:A:35:GLN:HE21	1:A:141:GLY:HA2	1.66	0.59
1:C:16:VAL:HG11	1:C:152:ILE:HD12	1.83	0.59
2:D:340:ALA:O	2:D:341:ARG:CB	2.47	0.59
1:A:12:TYR:O	1:A:13:GLN:C	2.42	0.58
2:D:255:VAL:CG1	2:D:256:ARG:N	2.62	0.58
2:D:255:VAL:CG1	2:D:256:ARG:H	2.11	0.58
2:D:269:ARG:O	2:D:270:GLU:C	2.46	0.58
2:D:230:ASP:OD1	2:D:383:THR:OG1	2.19	0.58
2:D:341:ARG:C	2:D:343:GLY:H	2.12	0.58
1:C:72:ALA:HB3	1:C:97:ARG:HD3	1.87	0.57
1:C:89:GLY:HA2	1:C:107:ILE:HG12	1.85	0.57
2:D:294:LEU:HD22	2:D:302:LEU:HB2	1.86	0.57
1:C:154:SER:OG	1:C:156:ASP:O	2.22	0.57
2:D:275:ASN:HA	2:D:301:VAL:HB	1.87	0.56
1:A:97:ARG:NH1	1:B:6:SER:HB3	2.20	0.56
2:D:278:LEU:O	2:D:278:LEU:HG	2.06	0.56
1:B:130:ARG:HD2	1:B:139:PHE:CZ	2.40	0.56
1:A:117:VAL:HG22	1:B:18:VAL:HG21	1.88	0.55
1:B:156:ASP:N	1:B:156:ASP:OD1	2.31	0.55
1:B:13:GLN:OE1	1:B:13:GLN:HA	2.06	0.55
1:C:18:VAL:HG22	1:C:152:ILE:HG22	1.89	0.55
1:B:57:ARG:CZ	1:B:86:GLU:OE1	2.53	0.55
2:D:309:ALA:O	2:D:338:ARG:NH2	2.40	0.55
1:C:129:VAL:O	1:C:129:VAL:HG23	2.07	0.54
1:A:132:ASN:O	1:A:133:PHE:HB3	2.06	0.54
2:D:282:MET:HE1	2:D:286:LYS:HB3	1.89	0.54
2:D:341:ARG:C	2:D:343:GLY:N	2.64	0.54
1:A:37:ILE:HD12	1:A:59:ARG:HH11	1.72	0.54
1:B:135:GLY:N	3:B:2008:HOH:O	2.25	0.54
1:B:91:VAL:HG21	1:B:144:LEU:HD11	1.90	0.53
2:D:282:MET:CE	2:D:286:LYS:HB3	2.38	0.53
1:A:72:ALA:CB	1:A:97:ARG:HB2	2.39	0.53
1:B:39:VAL:HG11	1:B:48:LEU:HD21	1.90	0.53
3:A:2010:HOH:O	2:D:328:SER:HA	2.08	0.52
1:B:19:VAL:HG23	1:B:151:ILE:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:NE2	1:A:141:GLY:HA2	2.24	0.52
2:D:339:THR:O	2:D:340:ALA:HB3	2.11	0.51
2:D:268:LEU:O	2:D:269:ARG:C	2.47	0.51
2:D:288:ASN:O	2:D:291:ILE:HG22	2.09	0.51
1:A:74:VAL:HB	1:A:96:VAL:HG22	1.91	0.51
2:D:233:GLU:N	3:D:2001:HOH:O	2.28	0.51
1:B:55:ASN:HA	1:B:85:ASN:HB3	1.92	0.51
1:A:97:ARG:HH11	1:B:6:SER:HB3	1.76	0.50
1:A:37:ILE:HD11	1:A:59:ARG:NH1	2.25	0.50
2:D:265:ALA:C	2:D:275:ASN:HD21	2.19	0.50
2:D:275:ASN:O	2:D:275:ASN:CG	2.53	0.50
1:B:131:VAL:CG2	1:B:138:PHE:HB2	2.41	0.50
2:D:275:ASN:OD1	2:D:275:ASN:O	2.29	0.50
1:C:132:ASN:O	1:C:133:PHE:HB3	2.12	0.50
2:D:266:ASN:O	2:D:267:TRP:C	2.54	0.50
1:B:42:PHE:CE1	1:B:68:SER:HB2	2.46	0.50
2:D:295:THR:O	2:D:296:GLU:OE1	2.30	0.50
2:D:318:SER:C	2:D:319:HIS:HD2	2.19	0.50
1:A:25:ASN:ND2	1:A:148:ASN:OD1	2.39	0.49
2:D:278:LEU:HD11	2:D:287:ARG:HG3	1.94	0.49
2:D:255:VAL:HG13	2:D:324:ASP:OD2	2.11	0.49
2:D:299:VAL:C	2:D:300:ASN:OD1	2.55	0.49
1:B:154:SER:OG	1:B:156:ASP:O	2.29	0.49
1:A:115:ILE:HD13	1:B:21:PRO:HD3	1.94	0.49
1:C:19:VAL:HG12	1:C:20:GLU:N	2.26	0.49
2:D:315:PRO:O	2:D:316:ASP:C	2.55	0.49
2:D:276:CYS:O	2:D:302:LEU:HA	2.13	0.49
1:B:56:GLY:O	1:B:87:TRP:HA	2.11	0.48
2:D:340:ALA:C	2:D:341:ARG:CG	2.63	0.48
1:C:76:ALA:H	1:C:98:GLN:NE2	2.10	0.48
1:A:31:SER:HB2	1:A:146:ALA:O	2.13	0.48
1:B:23:PHE:HE1	1:B:92:ILE:O	1.97	0.48
1:C:100:ASP:O	1:C:103:GLU:HG2	2.14	0.48
1:C:76:ALA:H	1:C:98:GLN:HE21	1.61	0.48
2:D:297:GLY:O	2:D:298:ARG:C	2.56	0.48
2:D:258:ARG:HH11	2:D:258:ARG:CG	2.24	0.47
2:D:376:ILE:O	2:D:379:LEU:O	2.31	0.47
1:B:130:ARG:CG	1:B:130:ARG:NH1	2.59	0.47
1:C:147:ASP:C	1:C:147:ASP:OD1	2.57	0.47
1:C:4:ASP:HB3	1:C:7:GLU:HB2	1.96	0.47
1:B:135:GLY:CA	3:B:2008:HOH:O	2.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ALA:HB3	1:A:97:ARG:HD3	1.97	0.46
1:A:96:VAL:HG13	1:A:97:ARG:N	2.30	0.46
1:C:28:GLY:HA3	1:C:105:LEU:O	2.16	0.46
2:D:233:GLU:HB2	3:D:2001:HOH:O	1.88	0.46
2:D:263:GLU:O	2:D:264:LEU:C	2.57	0.46
1:B:32:PHE:CD1	1:B:108:GLY:HA3	2.51	0.46
1:B:117:VAL:HG22	1:C:18:VAL:HG21	1.96	0.46
2:D:257:LYS:HA	2:D:257:LYS:HD3	1.55	0.46
2:D:314:ILE:HA	2:D:315:PRO:HD3	1.45	0.46
2:D:364:GLY:O	2:D:367:ILE:O	2.34	0.46
2:D:318:SER:C	2:D:319:HIS:CD2	2.94	0.46
1:B:8:LEU:HD13	1:B:158:LEU:HD23	1.97	0.46
2:D:307:VAL:O	2:D:309:ALA:N	2.49	0.46
2:D:231:ASP:HB3	3:D:2001:HOH:O	2.15	0.46
2:D:327:ARG:HA	2:D:359:LEU:HD22	1.98	0.45
1:C:130:ARG:CZ	1:C:139:PHE:HB2	2.47	0.45
1:B:74:VAL:HB	1:B:96:VAL:HG12	1.98	0.45
1:B:75:ASP:HB3	1:B:97:ARG:HE	1.82	0.45
1:C:30:ALA:O	1:C:147:ASP:HA	2.17	0.45
1:C:32:PHE:CD2	1:C:108:GLY:HA3	2.51	0.45
2:D:269:ARG:O	2:D:271:ALA:N	2.50	0.45
1:B:130:ARG:HB2	1:B:139:PHE:CE2	2.52	0.45
1:B:79:ALA:O	1:B:82:ALA:HB3	2.17	0.45
2:D:282:MET:HE2	2:D:282:MET:HB3	1.48	0.45
2:D:247:GLU:H	2:D:247:GLU:CD	2.24	0.45
2:D:327:ARG:NH1	2:D:327:ARG:CG	2.76	0.45
1:B:67:GLY:HA2	1:B:112:MET:CE	2.48	0.44
1:A:12:TYR:CE2	1:A:158:LEU:HG	2.52	0.44
2:D:279:GLU:O	2:D:281:GLU:N	2.48	0.44
2:D:279:GLU:O	2:D:282:MET:HG3	2.16	0.44
2:D:288:ASN:CA	2:D:291:ILE:HG22	2.45	0.44
2:D:369:GLU:O	2:D:369:GLU:CG	2.60	0.44
1:C:46:GLY:HA3	1:C:123:GLY:HA2	2.00	0.43
1:A:90:LEU:N	1:A:108:GLY:O	2.48	0.43
1:B:107:ILE:HG12	1:B:108:GLY:N	2.33	0.43
1:C:2:LYS:HD3	1:C:2:LYS:C	2.43	0.43
1:B:76:ALA:O	1:B:77:GLU:C	2.60	0.43
1:A:54:GLN:NE2	2:D:307:VAL:HG12	2.31	0.43
1:A:12:TYR:O	1:A:14:GLU:N	2.52	0.43
1:B:98:GLN:O	1:B:99:VAL:C	2.62	0.43
1:C:36:ILE:HA	1:C:60:VAL:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:ARG:NH2	2:D:381:PRO:HB2	2.33	0.43
2:D:250:ARG:HB3	2:D:317:VAL:HA	2.00	0.43
1:B:67:GLY:HA2	1:B:112:MET:HE2	2.01	0.42
1:C:130:ARG:HH11	1:C:137:THR:CG2	2.32	0.42
2:D:281:GLU:O	2:D:282:MET:C	2.62	0.42
1:B:72:ALA:HB3	1:B:97:ARG:HD3	2.00	0.42
2:D:380:ARG:HA	2:D:381:PRO:HD3	1.85	0.42
1:B:132:ASN:OD1	1:B:137:THR:HB	2.19	0.42
2:D:249:THR:O	2:D:300:ASN:HB3	2.19	0.42
1:C:84:GLN:O	1:C:84:GLN:CG	2.54	0.42
2:D:255:VAL:HG11	2:D:260:ARG:HB3	2.02	0.42
1:A:97:ARG:HD2	1:A:116:PRO:O	2.20	0.42
1:B:35:GLN:O	1:B:59:ARG:HA	2.20	0.42
2:D:243:LEU:HA	2:D:243:LEU:HD23	1.82	0.42
1:B:2:LYS:HE2	1:B:2:LYS:HB3	1.79	0.41
1:C:130:ARG:HH11	1:C:137:THR:HG22	1.86	0.41
1:C:19:VAL:CG1	1:C:20:GLU:N	2.83	0.41
1:A:59:ARG:NH2	2:D:307:VAL:HG23	2.35	0.41
1:A:132:ASN:HD22	1:A:132:ASN:C	2.28	0.41
1:B:130:ARG:CD	1:B:139:PHE:CZ	3.03	0.41
2:D:223:HIS:HB2	2:D:347:THR:HG23	2.02	0.41
1:B:155:GLU:C	1:B:156:ASP:OD1	2.63	0.41
1:C:6:SER:OG	3:C:2001:HOH:O	2.16	0.41
1:A:72:ALA:CB	1:A:97:ARG:HD3	2.51	0.41
1:A:74:VAL:HB	1:A:96:VAL:CG2	2.51	0.41
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.94	0.41
1:B:52:LEU:HD23	1:B:87:TRP:CE2	2.55	0.41
1:B:53:GLU:C	1:B:54:GLN:O	2.58	0.41
1:C:81:LEU:HD12	1:C:85:ASN:HD21	1.84	0.41
1:A:76:ALA:H	1:A:98:GLN:NE2	2.09	0.40
1:B:158:LEU:O	1:B:159:ASP:CB	2.64	0.40
1:A:89:GLY:CA	1:A:108:GLY:O	2.69	0.40
2:D:227:TYR:CD1	2:D:227:TYR:N	2.89	0.40
2:D:256:ARG:HG2	2:D:257:LYS:N	2.32	0.40
1:A:57:ARG:HA	1:A:86:GLU:O	2.21	0.40
1:B:12:TYR:CE2	1:B:158:LEU:HG	2.57	0.40
1:C:112:MET:O	1:C:113:ALA:HB2	2.22	0.40

All (3) 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:C:156:ASP:OD2	2:D:226:TYR:OH[3_555]	2.00	0.20
2:D:344:ARG:NH1	2:D:355:HIS:N[4_455]	2.15	0.05
2:D:344:ARG:NH1	2:D:355:HIS:CB[4_455]	2.16	0.04

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	156/161 (97%)	149 (96%)	7 (4%)	0	100	100
1	B	156/161 (97%)	142 (91%)	14 (9%)	0	100	100
1	C	156/161 (97%)	147 (94%)	9 (6%)	0	100	100
2	D	168/170 (99%)	154 (92%)	12 (7%)	2 (1%)	10	34
All	All	636/653 (97%)	592 (93%)	42 (7%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	308	ALA
2	D	220	LYS

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	125/128 (98%)	112 (90%)	13 (10%)	7	23
1	B	125/128 (98%)	111 (89%)	14 (11%)	6	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	125/128 (98%)	117 (94%)	8 (6%)	16	44
2	D	144/144 (100%)	114 (79%)	30 (21%)	1	4
All	All	519/528 (98%)	454 (88%)	65 (12%)	4	15

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	57	ARG
1	A	59	ARG
1	A	81	LEU
1	A	83	VAL
1	A	92	ILE
1	A	96	VAL
1	A	97	ARG
1	A	104	GLU
1	A	117	VAL
1	A	132	ASN
1	A	137	THR
1	A	159	ASP
1	B	2	LYS
1	B	19	VAL
1	B	24	SER
1	B	71	ARG
1	B	92	ILE
1	B	117	VAL
1	B	122	GLU
1	B	126	GLU
1	B	130	ARG
1	B	137	THR
1	B	144	LEU
1	B	154	SER
1	B	156	ASP
1	B	158	LEU
1	C	6	SER
1	C	7	GLU
1	C	14	GLU
1	C	24	SER
1	C	51	LEU
1	C	84	GLN
1	C	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	127	SER
2	D	221	LYS
2	D	233	GLU
2	D	236	THR
2	D	240	VAL
2	D	246	PRO
2	D	249	THR
2	D	251	SER
2	D	257	LYS
2	D	258	ARG
2	D	259	GLU
2	D	263	GLU
2	D	275	ASN
2	D	278	LEU
2	D	286	LYS
2	D	291	ILE
2	D	292	LYS
2	D	296	GLU
2	D	299	VAL
2	D	300	ASN
2	D	302	LEU
2	D	310	ARG
2	D	313	ASP
2	D	314	ILE
2	D	344	ARG
2	D	347	THR
2	D	352	VAL
2	D	353	GLU
2	D	360	LEU
2	D	371	ILE
2	D	384	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	54	GLN
1	A	55	ASN
1	A	98	GLN
1	A	132	ASN
1	C	35	GLN
1	C	85	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	98	GLN
1	C	110	GLN
2	D	241	HIS
2	D	284	GLN
2	D	319	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	158/161 (98%)	-0.52	0 100 100	20, 30, 46, 52	0
1	B	158/161 (98%)	-0.53	0 100 100	20, 31, 45, 52	0
1	C	158/161 (98%)	-0.51	0 100 100	21, 30, 44, 49	0
2	D	170/170 (100%)	0.35	5 (2%) 53 45	25, 56, 81, 85	0
All	All	644/653 (98%)	-0.29	5 (0%) 82 77	20, 34, 74, 85	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	340	ALA	2.6
2	D	342	ALA	2.5
2	D	220	LYS	2.3
2	D	341	ARG	2.3
2	D	387	SER	2.2

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.