



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:52 PM GMT

PDB ID : 1R11
Title : Structure Determination of the Dimeric Endonuclease in a Pseudo-face-centered P21 space group
Authors : Li, H.; Zhang, Y.
Deposited on : 2003-09-23
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

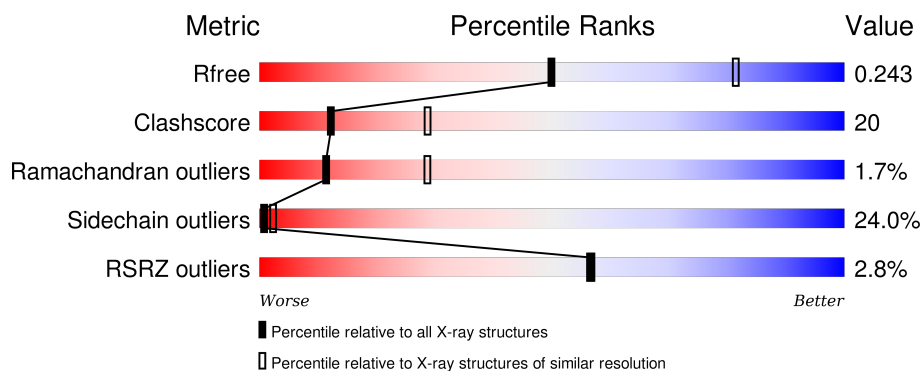
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

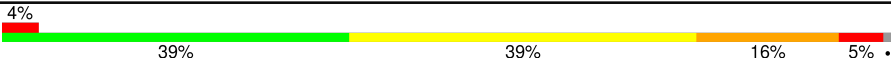
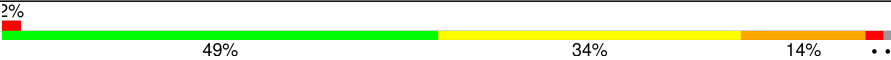
The reported resolution of this entry is 2.70 Å.

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	305	 4% 39% 39% 16% 5% .
1	B	305	 2% 49% 34% 14% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5042 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 tRNA-intron endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	11	0	0
			2521	1612	432	471	6			
1	B	303	Total	C	N	O	S	13	0	0
			2521	1612	432	471	6			

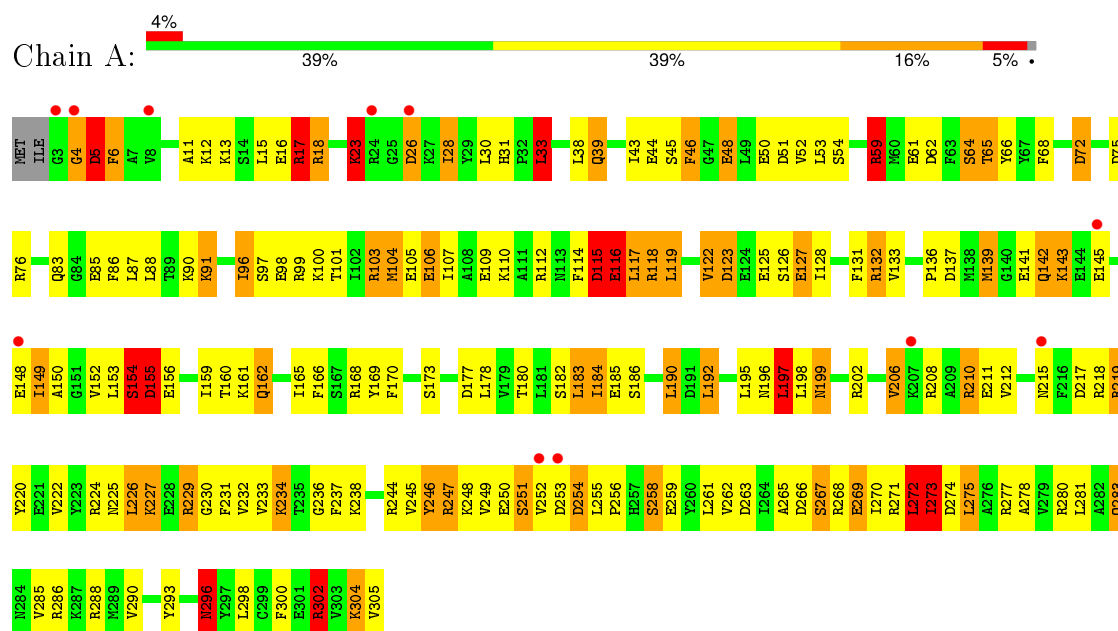
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	VAL	ILE	CONFLICT	UNP O29362
B	152	VAL	ILE	CONFLICT	UNP O29362

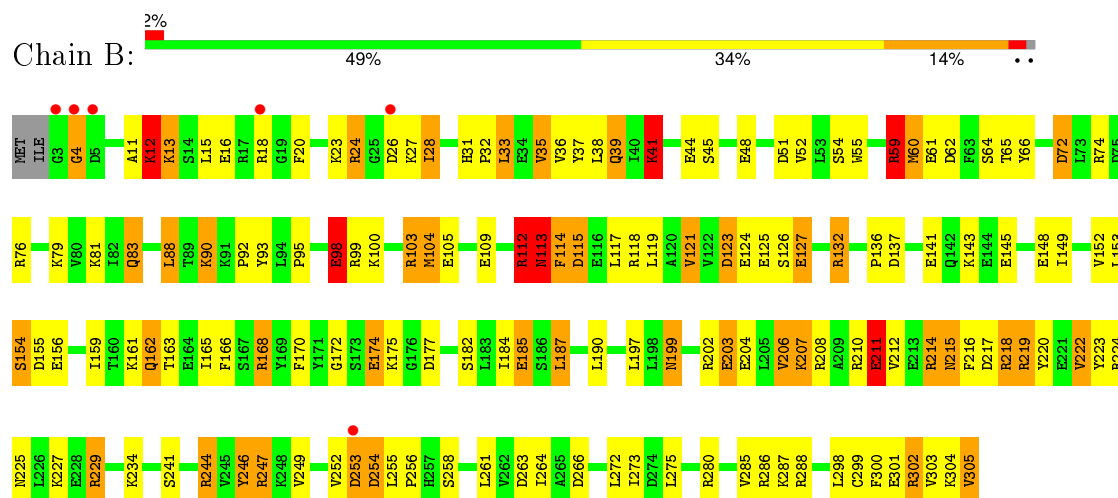
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: tRNA-intron endonuclease



• Molecule 1: tRNA-intron endonuclease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.41Å 74.17Å 84.86Å 90.00° 106.13° 90.00°	Depositor
Resolution (Å)	26.66 – 2.70 26.65 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.66-2.70) 77.2 (26.65-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.293 0.247 , 0.243	Depositor DCC
R_{free} test set	633 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 24.8	EDS
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14075 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5042	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.47	31/2565 (1.2%)	1.74	72/3440 (2.1%)
1	B	1.47	19/2565 (0.7%)	1.61	45/3440 (1.3%)
All	All	1.47	50/5130 (1.0%)	1.68	117/6880 (1.7%)

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	1	9
1	B	2	1
All	All	3	10

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ARG	CZ-NH1	24.80	1.65	1.33
1	A	4	GLY	C-N	18.99	1.77	1.34
1	B	41	LYS	CE-NZ	-18.96	1.01	1.49
1	B	137	ASP	CB-CG	-13.52	1.23	1.51
1	A	115	ASP	C-N	12.02	1.61	1.34
1	A	117	LEU	C-N	-10.60	1.09	1.34
1	A	83	GLN	C-N	10.09	1.51	1.33
1	A	206	VAL	CB-CG2	-9.81	1.32	1.52
1	A	23	LYS	C-N	9.67	1.56	1.34
1	A	141	GLU	C-N	9.46	1.55	1.34
1	A	127	GLU	CD-OE2	9.37	1.35	1.25
1	A	258	SER	C-N	9.05	1.54	1.34
1	B	15	LEU	C-N	9.02	1.54	1.34
1	A	116	GLU	CD-OE2	-8.96	1.15	1.25
1	A	114	PHE	C-N	8.47	1.53	1.34
1	A	206	VAL	CB-CG1	-7.99	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	PHE	C-N	7.85	1.52	1.34
1	A	197	LEU	CB-CG	-7.73	1.30	1.52
1	A	118	ARG	C-N	-7.58	1.16	1.34
1	B	206	VAL	CB-CG1	-7.54	1.37	1.52
1	A	252	VAL	C-N	7.49	1.51	1.34
1	B	223	TYR	C-N	7.21	1.50	1.34
1	A	272	LEU	C-N	-7.13	1.17	1.34
1	A	15	LEU	CG-CD2	-7.12	1.25	1.51
1	A	267	SER	C-N	7.05	1.50	1.34
1	B	246	TYR	C-N	6.86	1.49	1.34
1	B	301	GLU	CD-OE1	6.66	1.32	1.25
1	B	13	LYS	C-N	6.62	1.49	1.34
1	B	121	VAL	CB-CG2	-6.56	1.39	1.52
1	B	61	GLU	C-N	6.56	1.49	1.34
1	A	106	GLU	C-N	6.51	1.49	1.34
1	A	178	LEU	CG-CD2	-6.50	1.27	1.51
1	B	206	VAL	CB-CG2	-6.29	1.39	1.52
1	A	269	GLU	CG-CD	-6.23	1.42	1.51
1	B	305	VAL	CB-CG1	-6.23	1.39	1.52
1	A	302	ARG	CG-CD	-6.10	1.36	1.51
1	A	45	SER	C-N	-6.05	1.20	1.34
1	B	286	ARG	NE-CZ	-6.05	1.25	1.33
1	A	177	ASP	C-N	5.97	1.47	1.34
1	A	109	GLU	CD-OE2	-5.94	1.19	1.25
1	A	126	SER	C-N	-5.84	1.20	1.34
1	B	224	ARG	C-N	5.70	1.47	1.34
1	B	121	VAL	CB-CG1	-5.67	1.41	1.52
1	A	296	ASN	C-N	5.53	1.46	1.34
1	B	203	GLU	CD-OE2	5.48	1.31	1.25
1	A	128	ILE	C-N	5.37	1.46	1.34
1	B	215	ASN	CG-OD1	5.34	1.35	1.24
1	A	127	GLU	C-N	5.24	1.46	1.34
1	B	148	GLU	CD-OE2	-5.16	1.20	1.25
1	A	288	ARG	CG-CD	-5.15	1.39	1.51

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ARG	NE-CZ-NH1	25.75	133.17	120.30
1	A	247	ARG	NE-CZ-NH1	25.48	133.04	120.30
1	A	127	GLU	OE1-CD-OE2	-20.03	99.27	123.30
1	B	41	LYS	CD-CE-NZ	19.40	156.31	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ARG	NE-CZ-NH2	19.14	129.87	120.30
1	B	132	ARG	NH1-CZ-NH2	-13.68	104.35	119.40
1	A	5	ASP	CB-CG-OD2	13.61	130.55	118.30
1	A	127	GLU	CG-CD-OE2	-12.24	93.82	118.30
1	A	247	ARG	NH1-CZ-NH2	-12.01	106.19	119.40
1	A	215	ASN	CB-CA-C	11.91	134.22	110.40
1	A	59	ARG	NE-CZ-NH2	10.66	125.63	120.30
1	A	206	VAL	CG1-CB-CG2	-10.65	93.87	110.90
1	A	285	VAL	CG1-CB-CG2	-9.88	95.09	110.90
1	A	154	SER	CB-CA-C	9.59	128.32	110.10
1	A	123	ASP	CB-CG-OD2	9.16	126.54	118.30
1	A	115	ASP	CB-CG-OD1	-9.06	110.15	118.30
1	A	272	LEU	C-N-CA	9.06	144.34	121.70
1	A	112	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	B	247	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	B	121	VAL	CB-CA-C	8.66	127.85	111.40
1	A	155	ASP	CB-CG-OD1	8.57	126.01	118.30
1	B	302	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	72	ASP	CB-CG-OD2	8.35	125.82	118.30
1	A	253	ASP	CB-CG-OD2	8.27	125.74	118.30
1	B	13	LYS	CD-CE-NZ	-8.17	92.91	111.70
1	A	15	LEU	CB-CG-CD2	8.11	124.79	111.00
1	B	137	ASP	CB-CG-OD1	7.97	125.48	118.30
1	A	5	ASP	CB-CG-OD1	-7.91	111.18	118.30
1	B	273	ILE	CG1-CB-CG2	-7.90	94.02	111.40
1	A	178	LEU	CB-CG-CD2	7.89	124.42	111.00
1	B	4	GLY	C-N-CA	-7.74	102.34	121.70
1	A	217	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	5	ASP	CA-C-N	-7.68	100.31	117.20
1	B	103	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	137	ASP	CA-CB-CG	7.65	130.22	113.40
1	B	229	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	109	GLU	CB-CA-C	7.58	125.56	110.40
1	A	272	LEU	O-C-N	-7.47	110.75	122.70
1	A	112	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	247	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	6	PHE	CA-C-N	-7.14	101.50	117.20
1	B	286	ARG	NH1-CZ-NH2	-7.13	111.56	119.40
1	A	198	LEU	CD1-CG-CD2	-7.11	89.16	110.50
1	B	286	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	B	219	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	112	ARG	NE-CZ-NH2	7.02	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ASP	CB-CA-C	7.01	124.43	110.40
1	A	23	LYS	CB-CA-C	6.99	124.38	110.40
1	A	4	GLY	CA-C-N	-6.93	101.96	117.20
1	A	263	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	178	LEU	CB-CG-CD1	6.87	122.67	111.00
1	A	117	LEU	C-N-CA	6.77	138.63	121.70
1	B	177	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	302	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	128	ILE	CB-CG1-CD1	6.74	132.78	113.90
1	A	274	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	115	ASP	CA-C-N	-6.64	102.60	117.20
1	A	123	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	B	253	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	85	GLU	CA-C-N	-6.47	102.97	117.20
1	B	211	GLU	OE1-CD-OE2	-6.42	115.60	123.30
1	B	59	ARG	CA-CB-CG	6.32	127.31	113.40
1	B	60	MET	C-N-CA	-6.31	105.92	121.70
1	A	26	ASP	O-C-N	6.28	132.74	122.70
1	B	288	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	33	LEU	CB-CG-CD2	6.23	121.59	111.00
1	B	159	ILE	CG1-CB-CG2	-6.20	97.75	111.40
1	B	266	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	152	VAL	CB-CA-C	6.17	123.12	111.40
1	A	75	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	263	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	143	LYS	CD-CE-NZ	6.04	125.58	111.70
1	A	17	ARG	CB-CA-C	6.04	122.47	110.40
1	B	74	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	A	272	LEU	CA-C-N	5.98	130.36	117.20
1	A	269	GLU	OE1-CD-OE2	5.96	130.46	123.30
1	A	115	ASP	C-N-CA	-5.94	106.85	121.70
1	A	51	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	175	LYS	O-C-N	-5.84	113.28	123.20
1	B	254	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	6	PHE	O-C-N	5.80	131.98	122.70
1	A	127	GLU	C-N-CA	-5.79	107.22	121.70
1	A	127	GLU	CA-C-N	-5.79	104.47	117.20
1	B	113	ASN	CB-CA-C	5.78	121.97	110.40
1	A	6	PHE	CB-CA-C	-5.75	98.90	110.40
1	B	218	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	72	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	62	ASP	CB-CG-OD2	5.72	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	O-C-N	5.70	131.82	122.70
1	B	12	LYS	CG-CD-CE	-5.67	94.90	111.90
1	B	215	ASN	CB-CA-C	5.66	121.72	110.40
1	B	62	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	33	LEU	CB-CG-CD2	5.63	120.58	111.00
1	A	46	PHE	N-CA-CB	5.62	120.72	110.60
1	A	137	ASP	CB-CG-OD2	5.61	123.34	118.30
1	B	121	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	A	103	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	26	ASP	CA-C-N	-5.59	104.91	117.20
1	A	115	ASP	O-C-N	5.53	131.54	122.70
1	A	109	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	A	141	GLU	CB-CA-C	5.45	121.30	110.40
1	A	280	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	16	GLU	O-C-N	-5.43	114.02	122.70
1	B	118	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	254	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	218	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	266	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	45	SER	C-N-CA	5.24	134.80	121.70
1	A	246	TYR	O-C-N	-5.24	114.32	122.70
1	A	288	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	103	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	273	ILE	CG1-CB-CG2	-5.11	100.15	111.40
1	A	229	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	253	ASP	OD1-CG-OD2	-5.06	113.68	123.30
1	A	285	VAL	CA-CB-CG1	5.03	118.44	110.90
1	A	139	MET	CG-SD-CE	5.01	108.22	100.20
1	B	13	LYS	CB-CG-CD	-5.01	98.57	111.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	46	PHE	CA
1	B	113	ASN	CA
1	B	115	ASP	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASP	Sidechain
1	A	116	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	A	117	LEU	Mainchain
1	A	119	LEU	Mainchain
1	A	127	GLU	Sidechain
1	A	197	LEU	Mainchain
1	A	247	ARG	Sidechain
1	A	272	LEU	Peptide
1	A	5	ASP	Mainchain
1	B	215	ASN	Sidechain

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	2521	0	2529	112	3
1	B	2521	0	2534	98	6
All	All	5042	0	5063	199	6

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 20.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLY:C	1:A:5:ASP:N	1.77	1.36
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.06	1.20
1:B:12:LYS:HE3	1:B:12:LYS:CA	1.75	1.10
1:B:12:LYS:HA	1:B:12:LYS:CE	1.79	1.08
1:A:48:GLU:HA	1:A:48:GLU:OE2	1.54	1.08
1:A:190:LEU:HD12	1:A:197:LEU:HD13	1.42	1.01
1:B:12:LYS:HA	1:B:12:LYS:HE3	0.96	0.96
1:A:104:MET:HE1	1:A:300:PHE:HE1	1.32	0.91
1:B:199:ASN:HD22	1:B:199:ASN:H	1.20	0.88
1:A:43:ILE:O	1:A:44:GLU:HG2	1.73	0.87
1:B:104:MET:CE	1:B:300:PHE:CE1	2.57	0.86
1:A:149:ILE:HB	1:A:162:GLN:HG3	1.58	0.84
1:A:199:ASN:HD22	1:A:199:ASN:H	1.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:MET:CE	1:B:300:PHE:HE1	1.91	0.82
1:A:11:ALA:HA	1:A:28:ILE:HD12	1.64	0.80
1:A:104:MET:HE1	1:A:300:PHE:CE1	2.15	0.80
1:A:104:MET:HE2	1:A:298:LEU:HD12	1.64	0.80
1:A:17:ARG:HG2	1:A:17:ARG:HH21	1.45	0.80
1:B:168:ARG:NH1	1:B:168:ARG:HG2	1.86	0.79
1:A:6:PHE:HD1	1:A:30:LEU:O	1.64	0.79
1:B:149:ILE:HB	1:B:162:GLN:HG3	1.62	0.79
1:B:104:MET:HE1	1:B:300:PHE:CE1	2.17	0.78
1:B:55:TRP:NE1	1:B:59:ARG:NH1	2.31	0.78
1:B:153:LEU:H	1:B:199:ASN:HD21	1.31	0.78
1:B:98:GLU:HG2	1:B:99:ARG:HG3	1.65	0.78
1:B:81:LYS:HB3	1:B:88:LEU:HD12	1.66	0.78
1:B:207:LYS:O	1:B:211:GLU:HG2	1.85	0.76
1:A:238:LYS:NZ	1:B:127:GLU:HG2	2.01	0.75
1:A:219:ARG:NH2	1:B:124:GLU:OE1	2.19	0.75
1:A:199:ASN:HD22	1:A:199:ASN:N	1.83	0.74
1:B:182:SER:OG	1:B:185:GLU:HG2	1.88	0.74
1:B:168:ARG:CG	1:B:168:ARG:HH11	1.95	0.73
1:A:17:ARG:CG	1:A:17:ARG:HH21	2.01	0.72
1:A:180:THR:HG21	1:B:126:SER:HB3	1.74	0.70
1:A:13:LYS:HB2	1:A:13:LYS:NZ	2.07	0.69
1:A:11:ALA:HA	1:A:28:ILE:CD1	2.21	0.69
1:A:206:VAL:HG12	1:A:210:ARG:HE	1.56	0.69
1:A:91:LYS:HG2	1:A:116:GLU:HG2	1.75	0.69
1:B:112:ARG:HB3	1:B:112:ARG:HH11	1.56	0.68
1:A:64:SER:HB3	1:B:155:ASP:OD2	1.93	0.68
1:B:258:SER:OG	1:B:287:LYS:HE3	1.93	0.68
1:A:4:GLY:CA	1:A:5:ASP:N	2.58	0.67
1:B:39:GLN:HE21	1:B:52:VAL:HG21	1.59	0.66
1:A:17:ARG:NH2	1:A:17:ARG:HG2	2.06	0.66
1:A:150:ALA:H	1:A:162:GLN:HE21	1.43	0.65
1:A:238:LYS:HZ1	1:B:127:GLU:HG2	1.62	0.65
1:B:72:ASP:O	1:B:76:ARG:HG3	1.97	0.65
1:A:156:GLU:HG2	1:A:212:VAL:HG11	1.78	0.64
1:A:250:GLU:O	1:A:251:SER:HB3	1.98	0.64
1:B:55:TRP:CD1	1:B:59:ARG:NH1	2.66	0.64
1:A:123:ASP:HB3	1:A:125:GLU:H	1.62	0.63
1:B:121:VAL:HG21	1:B:272:LEU:HD13	1.80	0.63
1:B:104:MET:HE3	1:B:298:LEU:HD23	1.81	0.63
1:B:55:TRP:HE1	1:B:59:ARG:NH1	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PHE:CD1	1:A:30:LEU:O	2.51	0.62
1:A:182:SER:OG	1:A:185:GLU:HG2	2.00	0.62
1:B:104:MET:HE3	1:B:300:PHE:CE1	2.34	0.62
1:B:285:VAL:HG12	1:B:287:LYS:HD2	1.82	0.62
1:A:231:PHE:CD2	1:A:245:VAL:CG1	2.83	0.62
1:B:31:HIS:CE1	1:B:33:LEU:HD12	2.36	0.60
1:B:149:ILE:HB	1:B:162:GLN:CG	2.30	0.60
1:B:90:LYS:HB3	1:B:90:LYS:NZ	2.17	0.58
1:A:250:GLU:HG2	1:A:254:ASP:OD2	2.03	0.58
1:A:43:ILE:C	1:A:44:GLU:HG2	2.23	0.58
1:B:55:TRP:HE1	1:B:59:ARG:HH11	1.49	0.58
1:A:104:MET:CE	1:A:300:PHE:CE1	2.86	0.58
1:B:199:ASN:HD22	1:B:199:ASN:N	1.88	0.57
1:B:37:TYR:CZ	1:B:41:LYS:HD3	2.40	0.57
1:A:4:GLY:O	1:A:59:ARG:NE	2.35	0.57
1:A:104:MET:CE	1:A:298:LEU:HD12	2.35	0.57
1:B:182:SER:OG	1:B:185:GLU:CG	2.53	0.57
1:B:302:ARG:HG2	1:B:303:VAL:N	2.20	0.57
1:B:214:ARG:NE	1:B:214:ARG:HA	2.18	0.56
1:B:109:GLU:HA	1:B:109:GLU:OE2	2.03	0.56
1:A:33:LEU:HD21	1:A:66:TYR:HB3	1.86	0.56
1:B:225:ASN:OD1	1:B:229:ARG:HD2	2.05	0.56
1:B:187:LEU:HD23	1:B:220:TYR:CZ	2.40	0.56
1:A:153:LEU:H	1:A:199:ASN:HD21	1.54	0.56
1:A:249:VAL:HG13	1:A:254:ASP:HB2	1.86	0.56
1:B:37:TYR:CE1	1:B:41:LYS:HD3	2.41	0.55
1:A:118:ARG:NH2	1:A:132:ARG:HD3	2.21	0.55
1:A:4:GLY:C	1:A:5:ASP:CA	2.73	0.55
1:B:39:GLN:NE2	1:B:52:VAL:HG21	2.22	0.55
1:B:214:ARG:HA	1:B:214:ARG:HE	1.72	0.55
1:B:90:LYS:HB3	1:B:90:LYS:HZ3	1.72	0.54
1:A:271:ARG:HB3	1:A:273:ILE:HD13	1.89	0.54
1:B:199:ASN:ND2	1:B:199:ASN:H	1.99	0.54
1:A:6:PHE:HD1	1:A:30:LEU:C	2.11	0.54
1:B:121:VAL:CG2	1:B:272:LEU:HD13	2.37	0.53
1:B:249:VAL:HG13	1:B:254:ASP:HB2	1.91	0.53
1:B:104:MET:HE3	1:B:300:PHE:CZ	2.45	0.52
1:A:166:PHE:O	1:A:170:PHE:N	2.42	0.52
1:A:169:TYR:C	1:A:170:PHE:CD1	2.83	0.52
1:A:199:ASN:N	1:A:199:ASN:ND2	2.55	0.52
1:B:222:VAL:HG11	1:B:264:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ALA:HA	1:B:28:ILE:HD12	1.91	0.52
1:B:104:MET:CE	1:B:300:PHE:CZ	2.93	0.52
1:A:238:LYS:HZ2	1:B:127:GLU:HG2	1.73	0.51
1:A:160:THR:OG1	1:A:162:GLN:HG2	2.11	0.51
1:A:184:ILE:HD11	1:A:220:TYR:HA	1.93	0.51
1:B:136:PRO:HG3	1:B:299:CYS:HB2	1.91	0.51
1:A:244:ARG:HD2	1:A:246:TYR:OH	2.10	0.51
1:A:149:ILE:HB	1:A:162:GLN:CG	2.33	0.51
1:A:31:HIS:ND1	1:A:33:LEU:HB2	2.26	0.51
1:B:156:GLU:HG2	1:B:212:VAL:HG11	1.93	0.51
1:A:97:SER:HA	1:A:122:VAL:HG23	1.92	0.50
1:A:12:LYS:O	1:A:16:GLU:HG3	2.10	0.50
1:B:168:ARG:NH1	1:B:168:ARG:CG	2.64	0.50
1:A:13:LYS:HZ3	1:A:13:LYS:HB2	1.76	0.50
1:B:199:ASN:N	1:B:199:ASN:ND2	2.56	0.49
1:A:155:ASP:HB2	1:B:64:SER:HB3	1.94	0.49
1:B:123:ASP:HB3	1:B:125:GLU:H	1.76	0.49
1:B:285:VAL:CG1	1:B:287:LYS:HD2	2.42	0.49
1:B:255:LEU:N	1:B:256:PRO:CD	2.75	0.49
1:A:224:ARG:O	1:A:225:ASN:C	2.48	0.49
1:B:206:VAL:O	1:B:210:ARG:HG3	2.13	0.49
1:A:48:GLU:OE2	1:A:48:GLU:CA	2.41	0.48
1:A:118:ARG:HA	1:A:131:PHE:O	2.12	0.48
1:A:250:GLU:O	1:A:251:SER:CB	2.61	0.48
1:A:149:ILE:HG13	1:A:195:LEU:CD1	2.44	0.48
1:A:149:ILE:HG13	1:A:195:LEU:HD13	1.95	0.48
1:A:226:LEU:HB3	1:A:233:VAL:HG21	1.96	0.48
1:A:142:GLN:HB3	1:A:230:GLY:O	2.14	0.47
1:A:265:ALA:O	1:A:268:ARG:HB2	2.13	0.47
1:B:216:PHE:O	1:B:217:ASP:C	2.49	0.47
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.70	0.47
1:A:190:LEU:CD1	1:A:197:LEU:HD13	2.30	0.47
1:A:262:VAL:HG22	1:A:290:VAL:HB	1.96	0.47
1:B:92:PRO:O	1:B:117:LEU:HD12	2.15	0.47
1:A:293:TYR:CZ	1:A:296:ASN:HB2	2.50	0.47
1:B:149:ILE:CB	1:B:162:GLN:HG3	2.41	0.47
1:A:304:LYS:HE3	1:A:304:LYS:HB3	1.51	0.47
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.72	0.47
1:B:112:ARG:C	1:B:114:PHE:H	2.18	0.46
1:B:31:HIS:CG	1:B:32:PRO:HD2	2.50	0.46
1:A:65:THR:HB	1:A:122:VAL:HG21	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:HB3	1:A:125:GLU:N	2.30	0.46
1:A:149:ILE:CB	1:A:162:GLN:HG3	2.38	0.46
1:A:225:ASN:OD1	1:A:229:ARG:HD2	2.16	0.46
1:A:190:LEU:HD12	1:A:197:LEU:CD1	2.29	0.46
1:A:154:SER:HB3	1:A:159:ILE:HD13	1.96	0.46
1:A:275:LEU:HD11	1:A:300:PHE:CD2	2.52	0.46
1:A:202:ARG:O	1:A:206:VAL:HG23	2.16	0.46
1:A:283:GLN:HE21	1:A:283:GLN:HB3	1.50	0.46
1:A:150:ALA:N	1:A:162:GLN:HE21	2.13	0.45
1:B:35:VAL:O	1:B:38:LEU:HB2	2.16	0.45
1:A:104:MET:CE	1:A:298:LEU:CD1	2.94	0.45
1:B:166:PHE:O	1:B:170:PHE:N	2.50	0.45
1:B:166:PHE:CE2	1:B:174:GLU:HG2	2.51	0.45
1:A:23:LYS:HB2	1:A:28:ILE:HG13	1.99	0.45
1:A:64:SER:O	1:A:68:PHE:CD1	2.70	0.45
1:A:255:LEU:N	1:A:256:PRO:CD	2.79	0.45
1:A:103:ARG:HD2	1:A:269:GLU:OE1	2.17	0.45
1:A:18:ARG:HA	1:A:18:ARG:HD2	1.44	0.45
1:B:66:TYR:CD2	1:B:95:PRO:HG2	2.52	0.45
1:A:227:LYS:HD2	1:A:227:LYS:HA	1.51	0.45
1:B:197:LEU:HA	1:B:197:LEU:HD12	1.81	0.44
1:B:225:ASN:O	1:B:229:ARG:HG3	2.17	0.44
1:B:227:LYS:HD2	1:B:227:LYS:HA	1.74	0.44
1:B:244:ARG:HD2	1:B:246:TYR:OH	2.17	0.44
1:B:18:ARG:HB3	1:B:20:PHE:CD1	2.53	0.44
1:A:96:ILE:HG12	1:A:272:LEU:HD11	1.99	0.44
1:A:106:GLU:O	1:A:110:LYS:HG3	2.17	0.44
1:A:277:ARG:NH2	1:B:241:SER:HB2	2.33	0.44
1:A:125:GLU:HG2	1:B:172:GLY:HA2	1.99	0.44
1:A:11:ALA:CA	1:A:28:ILE:HD12	2.41	0.43
1:B:4:GLY:O	1:B:59:ARG:CD	2.66	0.43
1:A:302:ARG:HD2	1:A:302:ARG:HH11	1.61	0.43
1:B:12:LYS:HB3	1:B:12:LYS:HE2	1.37	0.43
1:A:91:LYS:HG2	1:A:116:GLU:CG	2.46	0.43
1:A:39:GLN:NE2	1:A:52:VAL:HG21	2.33	0.43
1:B:184:ILE:HG23	1:B:185:GLU:N	2.33	0.43
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.67	0.42
1:B:93:TYR:OH	1:B:305:VAL:OXT	2.22	0.42
1:A:107:ILE:HD13	1:A:107:ILE:HA	1.85	0.42
1:B:252:VAL:O	1:B:255:LEU:HB2	2.20	0.42
1:A:104:MET:HE2	1:A:298:LEU:CD1	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.84	0.41
1:A:76:ARG:HH12	1:A:304:LYS:NZ	2.18	0.41
1:A:231:PHE:CD2	1:A:245:VAL:HG13	2.55	0.41
1:A:277:ARG:O	1:A:278:ALA:C	2.57	0.41
1:A:87:LEU:O	1:A:88:LEU:HD23	2.20	0.41
1:A:183:LEU:HA	1:A:183:LEU:HD12	1.80	0.41
1:B:182:SER:OG	1:B:184:ILE:HG22	2.21	0.41
1:B:32:PRO:O	1:B:36:VAL:HG23	2.20	0.41
1:A:232:VAL:HB	1:A:246:TYR:HB2	2.03	0.41
1:B:18:ARG:HB3	1:B:20:PHE:CE1	2.55	0.41
1:B:104:MET:HE1	1:B:300:PHE:CZ	2.55	0.41
1:B:98:GLU:HG2	1:B:99:ARG:N	2.35	0.41
1:A:155:ASP:HB2	1:B:64:SER:CB	2.50	0.41
1:A:281:LEU:HD11	1:B:280:ARG:HG2	2.02	0.41
1:B:4:GLY:O	1:B:59:ARG:HD2	2.21	0.40
1:A:206:VAL:O	1:A:210:ARG:HG3	2.21	0.40
1:A:118:ARG:HH22	1:A:132:ARG:HD3	1.86	0.40
1:B:166:PHE:O	1:B:170:PHE:HA	2.21	0.40
1:A:97:SER:C	1:A:99:ARG:H	2.24	0.40
1:A:236:GLY:O	1:A:237:PHE:C	2.58	0.40
1:A:38:LEU:HD13	1:A:44:GLU:HG3	2.03	0.40
1:A:234:LYS:HZ2	1:A:234:LYS:HG2	1.51	0.40

All (6) 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:B:12:LYS:NZ	1:B:204:GLU:CD[1_554]	1.70	0.50
1:B:12:LYS:NZ	1:B:204:GLU:OE1[1_554]	1.75	0.45
1:A:43:ILE:O	1:B:103:ARG:NH1[2_656]	1.86	0.34
1:B:12:LYS:NZ	1:B:204:GLU:OE2[1_554]	2.05	0.15
1:A:192:LEU:O	1:B:24:ARG:NH1[1_455]	2.08	0.12
1:A:136:PRO:O	1:B:113:ASN:CB[1_455]	2.18	0.02

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	301/305 (99%)	272 (90%)	25 (8%)	4 (1%)	15	37
1	B	301/305 (99%)	267 (89%)	28 (9%)	6 (2%)	9	24
All	All	602/610 (99%)	539 (90%)	53 (9%)	10 (2%)	11	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	SER
1	A	273	ILE
1	B	113	ASN
1	A	104	MET
1	B	154	SER
1	A	154	SER
1	B	98	GLU
1	B	83	GLN
1	B	123	ASP
1	B	35	VAL

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	271/273 (99%)	200 (74%)	71 (26%)	0	2
1	B	271/273 (99%)	212 (78%)	59 (22%)	1	3
All	All	542/546 (99%)	412 (76%)	130 (24%)	1	2

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	17	ARG

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Mol	Chain	Res	Type
1	A	18	ARG
1	A	23	LYS
1	A	26	ASP
1	A	28	ILE
1	A	33	LEU
1	A	39	GLN
1	A	46	PHE
1	A	48	GLU
1	A	50	GLU
1	A	53	LEU
1	A	54	SER
1	A	59	ARG
1	A	61	GLU
1	A	64	SER
1	A	65	THR
1	A	72	ASP
1	A	90	LYS
1	A	91	LYS
1	A	96	ILE
1	A	98	GLU
1	A	100	LYS
1	A	101	THR
1	A	105	GLU
1	A	115	ASP
1	A	119	LEU
1	A	122	VAL
1	A	132	ARG
1	A	133	VAL
1	A	139	MET
1	A	142	GLN
1	A	143	LYS
1	A	145	GLU
1	A	148	GLU
1	A	149	ILE
1	A	152	VAL
1	A	155	ASP
1	A	161	LYS
1	A	162	GLN
1	A	165	ILE
1	A	168	ARG
1	A	173	SER
1	A	183	LEU

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Mol	Chain	Res	Type
1	A	184	ILE
1	A	186	SER
1	A	190	LEU
1	A	192	LEU
1	A	196	ASN
1	A	199	ASN
1	A	208	ARG
1	A	210	ARG
1	A	211	GLU
1	A	218	ARG
1	A	219	ARG
1	A	222	VAL
1	A	226	LEU
1	A	227	LYS
1	A	234	LYS
1	A	248	LYS
1	A	258	SER
1	A	259	GLU
1	A	267	SER
1	A	270	ILE
1	A	275	LEU
1	A	283	GLN
1	A	286	ARG
1	A	296	ASN
1	A	302	ARG
1	A	304	LYS
1	A	305	VAL
1	B	12	LYS
1	B	13	LYS
1	B	23	LYS
1	B	24	ARG
1	B	26	ASP
1	B	27	LYS
1	B	28	ILE
1	B	39	GLN
1	B	41	LYS
1	B	44	GLU
1	B	45	SER
1	B	48	GLU
1	B	51	ASP
1	B	54	SER
1	B	59	ARG

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Mol	Chain	Res	Type
1	B	60	MET
1	B	65	THR
1	B	79	LYS
1	B	83	GLN
1	B	88	LEU
1	B	90	LYS
1	B	98	GLU
1	B	100	LYS
1	B	104	MET
1	B	105	GLU
1	B	112	ARG
1	B	114	PHE
1	B	115	ASP
1	B	127	GLU
1	B	132	ARG
1	B	141	GLU
1	B	143	LYS
1	B	145	GLU
1	B	154	SER
1	B	161	LYS
1	B	162	GLN
1	B	163	THR
1	B	165	ILE
1	B	168	ARG
1	B	174	GLU
1	B	185	GLU
1	B	187	LEU
1	B	190	LEU
1	B	199	ASN
1	B	202	ARG
1	B	203	GLU
1	B	207	LYS
1	B	208	ARG
1	B	211	GLU
1	B	214	ARG
1	B	218	ARG
1	B	219	ARG
1	B	222	VAL
1	B	234	LYS
1	B	244	ARG
1	B	247	ARG
1	B	253	ASP

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Mol	Chain	Res	Type
1	B	275	LEU
1	B	304	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	142	GLN
1	A	162	GLN
1	A	199	ASN
1	A	215	ASN
1	B	39	GLN
1	B	83	GLN
1	B	199	ASN
1	B	284	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 carbohydrates 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 ⓘ

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	303/305 (99%)	0.11	11 (3%) 46 46	26, 27, 27, 28	9 (2%)
1	B	303/305 (99%)	0.03	6 (1%) 68 69	26, 27, 27, 28	8 (2%)
All	All	606/610 (99%)	0.07	17 (2%) 56 57	26, 27, 27, 28	17 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	4.4
1	B	4	GLY	3.6
1	A	4	GLY	3.0
1	B	5	ASP	2.9
1	B	26	ASP	2.7
1	A	8	VAL	2.6
1	A	215	ASN	2.4
1	B	18	ARG	2.2
1	A	253	ASP	2.2
1	A	207	LYS	2.2
1	A	148	GLU	2.2
1	A	26	ASP	2.1
1	B	3	GLY	2.1
1	A	252	VAL	2.0
1	A	145	GLU	2.0
1	B	253	ASP	2.0
1	A	24	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.