



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 1R11 / pdb_00001r11
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

<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

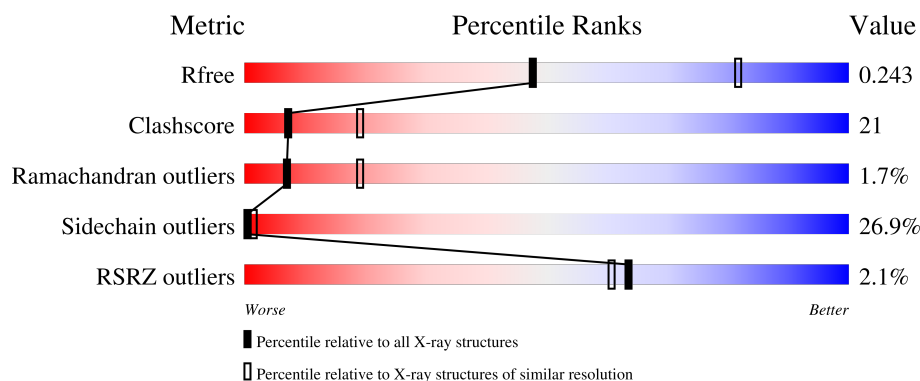
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	305	2% 36% 41% 18% 5%
1	B	305	3% 42% 41% 13% ...

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			

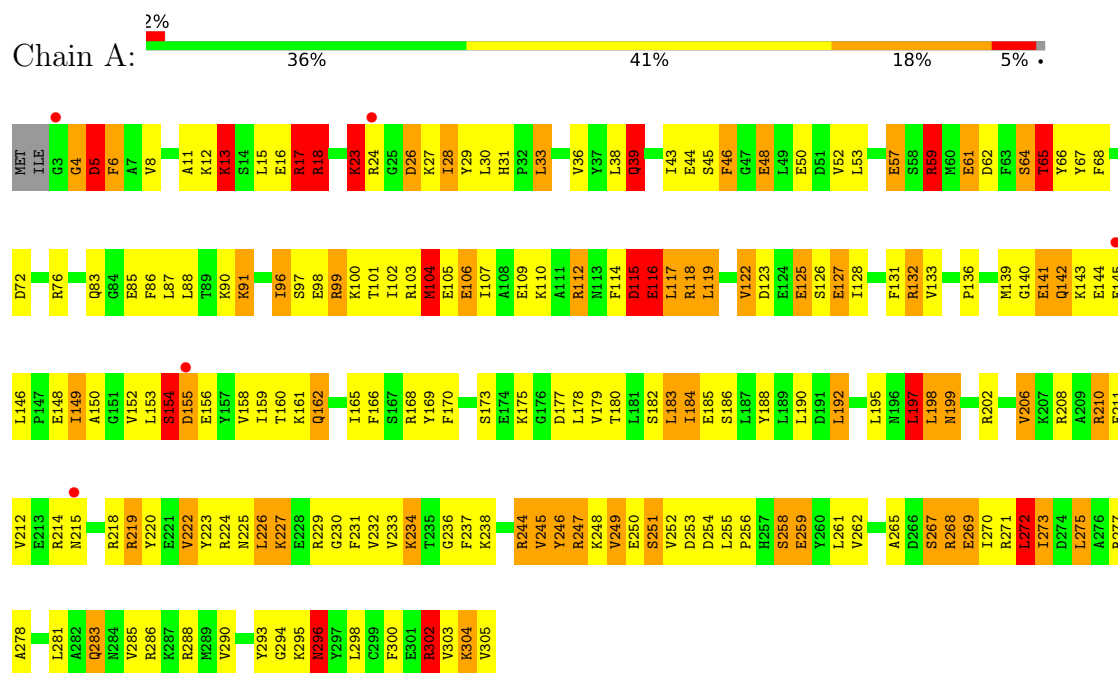
There are 2 discrepancies between the modelled and reference sequences:

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

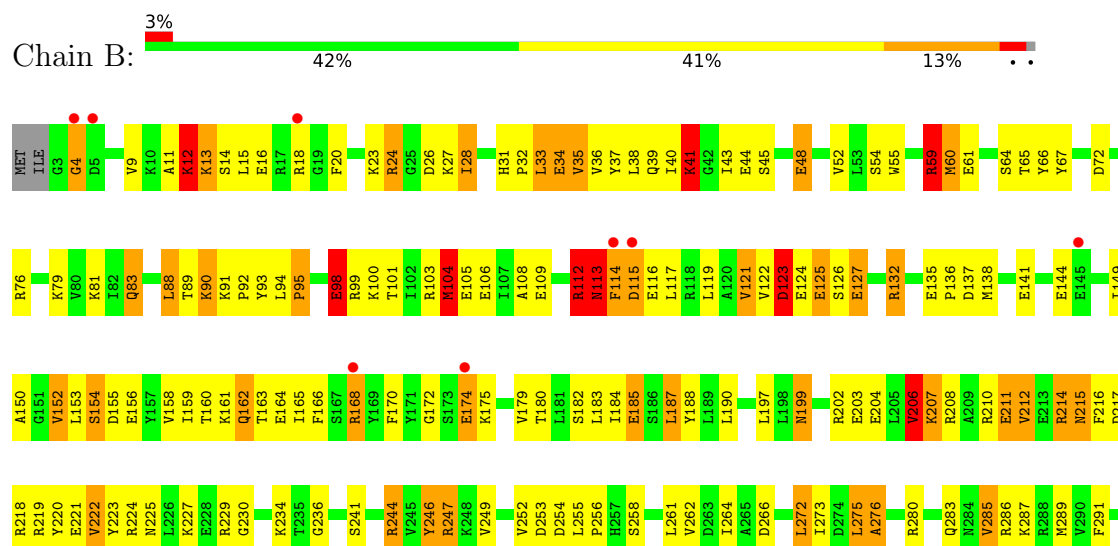
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: tRNA-intron endonuclease



• Molecule 1: tRNA-intron endonuclease



L298	C299	F300	F301	R302	V303	K304	V305
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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 26.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.66-2.70) 76.8 (26.66-2.70)	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	655 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	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, 0.333 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	1.94	44/2565 (1.7%)	1.90	89/3440 (2.6%)
1	B	1.69	29/2565 (1.1%)	1.77	48/3440 (1.4%)
All	All	1.82	73/5130 (1.4%)	1.84	137/6880 (2.0%)

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 (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLY	C-N	28.18	1.77	1.34
1	B	132	ARG	CZ-NH1	23.25	1.65	1.32
1	A	23	LYS	C-N	18.68	1.56	1.33
1	A	117	LEU	C-N	-18.55	1.09	1.33
1	A	115	ASP	C-N	18.49	1.61	1.33
1	A	141	GLU	C-N	16.88	1.55	1.33
1	B	15	LEU	C-N	16.72	1.54	1.33
1	B	41	LYS	CE-NZ	-15.90	1.01	1.49
1	A	258	SER	C-N	13.64	1.54	1.33
1	A	86	PHE	C-N	13.57	1.52	1.33
1	A	114	PHE	C-N	13.11	1.53	1.33
1	A	252	VAL	C-N	13.06	1.51	1.33
1	B	223	TYR	C-N	12.83	1.50	1.33
1	A	267	SER	C-N	12.73	1.50	1.33
1	A	106	GLU	C-N	12.28	1.49	1.33
1	A	118	ARG	C-N	-12.27	1.16	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLU	C-N	12.16	1.49	1.33
1	A	83	GLN	C-N	12.13	1.51	1.33
1	A	272	LEU	C-N	-11.75	1.17	1.33
1	B	246	TYR	C-N	11.69	1.49	1.33
1	A	197	LEU	CB-CG	-11.65	1.30	1.53
1	B	137	ASP	CB-CG	-11.48	1.23	1.52
1	B	224	ARG	C-N	10.46	1.47	1.33
1	B	13	LYS	C-N	10.41	1.49	1.33
1	A	127	GLU	C-N	10.02	1.46	1.33
1	B	104	MET	SD-CE	-10.02	1.54	1.79
1	A	126	SER	C-N	-9.84	1.20	1.33
1	A	128	ILE	C-N	9.73	1.46	1.33
1	A	177	ASP	C-N	9.43	1.47	1.33
1	A	45	SER	C-N	-9.40	1.20	1.33
1	A	296	ASN	C-N	9.23	1.46	1.33
1	A	249	VAL	C-N	8.91	1.45	1.33
1	A	15	LEU	CG-CD2	-8.20	1.25	1.52
1	A	303	VAL	CA-CB	7.82	1.63	1.55
1	A	246	TYR	C-N	-7.77	1.23	1.33
1	A	253	ASP	C-N	7.54	1.44	1.33
1	A	178	LEU	CG-CD2	-7.50	1.27	1.52
1	A	128	ILE	CG1-CD1	-7.46	1.22	1.51
1	A	29	TYR	C-N	-7.21	1.23	1.33
1	B	286	ARG	NE-CZ	-7.15	1.25	1.33
1	A	259	GLU	C-N	-7.08	1.22	1.33
1	A	27	LYS	C-N	7.03	1.42	1.33
1	A	6	PHE	C-N	6.98	1.43	1.33
1	A	102	ILE	C-N	6.94	1.43	1.33
1	B	14	SER	C-N	-6.68	1.24	1.33
1	A	99	ARG	C-N	-6.64	1.24	1.33
1	B	60	MET	C-N	-6.61	1.24	1.33
1	B	215	ASN	CG-OD1	6.40	1.35	1.23
1	B	60	MET	SD-CE	-6.40	1.63	1.79
1	A	206	VAL	CB-CG2	-6.15	1.32	1.52
1	A	62	ASP	C-N	-6.15	1.26	1.33
1	B	138	MET	SD-CE	-6.14	1.64	1.79
1	B	289	MET	SD-CE	-5.76	1.65	1.79
1	B	121	VAL	C-N	5.74	1.41	1.33
1	B	206	VAL	CA-CB	5.73	1.61	1.54
1	A	127	GLU	CD-OE2	5.58	1.35	1.25
1	B	4	GLY	C-N	5.57	1.41	1.33
1	A	24	ARG	CA-CB	-5.51	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	GLU	C-O	-5.44	1.17	1.24
1	B	291	PHE	C-O	-5.39	1.17	1.23
1	A	104	MET	SD-CE	-5.39	1.66	1.79
1	B	175	LYS	CA-C	-5.38	1.46	1.53
1	B	33	LEU	CG-CD1	-5.35	1.34	1.52
1	B	95	PRO	C-O	-5.34	1.18	1.23
1	A	223	TYR	CA-C	5.30	1.59	1.52
1	B	247	ARG	C-N	-5.27	1.26	1.33
1	A	302	ARG	CG-CD	-5.25	1.36	1.52
1	B	276	ALA	CA-CB	-5.22	1.45	1.53
1	A	116	GLU	N-CA	-5.19	1.40	1.46
1	B	123	ASP	N-CA	5.15	1.52	1.46
1	B	188	TYR	N-CA	-5.08	1.40	1.46
1	A	140	GLY	C-N	5.07	1.39	1.33
1	A	116	GLU	CD-OE2	-5.03	1.15	1.25

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ASP	CA-CB-CG	17.62	130.22	112.60
1	B	41	LYS	CD-CE-NZ	13.88	156.31	111.90
1	B	121	VAL	CB-CA-C	13.66	127.85	110.91
1	A	215	ASN	CB-CA-C	13.31	134.22	111.46
1	A	127	GLU	CA-C-N	-12.88	107.22	123.19
1	A	127	GLU	C-N-CA	-12.88	107.22	123.19
1	A	272	LEU	CA-C-N	12.43	144.34	121.97
1	A	272	LEU	C-N-CA	12.43	144.34	121.97
1	B	4	GLY	CA-C-N	-12.24	102.34	122.54
1	B	4	GLY	C-N-CA	-12.24	102.34	122.54
1	B	215	ASN	OD1-CG-ND2	-12.13	110.47	122.60
1	B	286	ARG	NE-CZ-NH2	11.86	129.87	119.20
1	B	132	ARG	NE-CZ-NH1	11.67	133.17	121.50
1	A	247	ARG	NE-CZ-NH1	11.54	133.04	121.50
1	B	132	ARG	NH1-CZ-NH2	-11.50	104.35	119.30
1	A	117	LEU	CA-C-N	11.25	138.63	122.77
1	A	117	LEU	C-N-CA	11.25	138.63	122.77
1	A	272	LEU	O-C-N	-10.73	110.75	122.12
1	A	127	GLU	CG-CD-OE2	-10.69	93.82	118.40
1	A	247	ARG	NH1-CZ-NH2	-10.09	106.19	119.30
1	A	127	GLU	OE1-CD-OE2	-9.85	99.27	122.90
1	A	198	LEU	CD1-CG-CD2	-9.84	89.16	110.80
1	B	144	GLU	N-CA-C	9.77	122.16	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ASP	CA-C-N	-9.58	106.85	122.08
1	A	115	ASP	C-N-CA	-9.58	106.85	122.08
1	B	60	MET	CA-C-N	-9.32	105.92	121.39
1	B	60	MET	C-N-CA	-9.32	105.92	121.39
1	A	140	GLY	CA-C-N	-9.16	110.55	123.20
1	A	140	GLY	C-N-CA	-9.16	110.55	123.20
1	A	128	ILE	CB-CG1-CD1	9.04	132.78	113.80
1	A	154	SER	CB-CA-C	8.99	128.32	110.42
1	A	23	LYS	CB-CA-C	8.83	124.38	109.72
1	A	247	ARG	O-C-N	8.48	131.82	122.15
1	A	6	PHE	O-C-N	8.40	131.98	122.99
1	B	152	VAL	CB-CA-C	8.39	123.12	110.62
1	B	266	ASP	CB-CA-C	-8.38	105.82	115.79
1	B	115	ASP	CB-CA-C	8.09	124.43	109.54
1	A	109	GLU	CB-CA-C	8.07	125.56	110.63
1	A	85	GLU	CA-C-N	-7.97	110.29	122.81
1	A	85	GLU	C-N-CA	-7.97	110.29	122.81
1	A	26	ASP	O-C-N	7.93	132.74	122.04
1	A	115	ASP	O-C-N	7.92	131.54	122.20
1	B	16	GLU	O-C-N	-7.76	114.02	122.09
1	A	206	VAL	CG1-CB-CG2	-7.70	93.87	110.80
1	A	246	TYR	O-C-N	-7.58	114.32	123.19
1	A	45	SER	CA-C-N	7.43	134.80	122.54
1	A	45	SER	C-N-CA	7.43	134.80	122.54
1	B	4	GLY	N-CA-C	7.16	120.86	111.70
1	A	59	ARG	NE-CZ-NH2	7.14	125.63	119.20
1	A	285	VAL	CG1-CB-CG2	-7.14	95.09	110.80
1	B	12	LYS	CG-CD-CE	-7.13	94.90	111.30
1	A	46	PHE	N-CA-CB	6.91	120.72	110.49
1	B	180	THR	N-CA-C	6.81	119.38	108.41
1	A	85	GLU	O-C-N	6.77	130.31	122.25
1	B	59	ARG	CA-CB-CG	6.61	127.31	114.10
1	A	45	SER	O-C-N	-6.50	115.60	123.27
1	A	141	GLU	CB-CA-C	6.49	121.30	111.70
1	A	67	TYR	N-CA-C	6.46	117.98	111.07
1	A	6	PHE	CB-CA-C	-6.31	98.90	111.91
1	A	188	TYR	N-CA-C	-6.31	103.93	111.69
1	A	17	ARG	CB-CA-C	6.29	122.47	110.27
1	A	128	ILE	CB-CA-C	6.29	120.20	110.83
1	A	83	GLN	O-C-N	-6.28	115.99	123.28
1	A	295	LYS	CA-C-N	-6.26	111.82	123.03
1	A	295	LYS	C-N-CA	-6.26	111.82	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	LYS	CA-C-N	6.26	129.18	120.29
1	A	13	LYS	C-N-CA	6.26	129.18	120.29
1	A	127	GLU	O-C-N	6.25	130.50	122.81
1	B	89	THR	N-CA-C	-6.24	97.51	110.80
1	A	117	LEU	O-C-N	-6.17	115.28	122.87
1	A	36	VAL	N-CA-C	6.00	116.74	110.62
1	A	144	GLU	N-CA-C	5.98	118.36	108.49
1	B	286	ARG	NH1-CZ-NH2	-5.95	111.56	119.30
1	A	247	ARG	CA-C-N	-5.95	110.20	121.63
1	A	247	ARG	C-N-CA	-5.95	110.20	121.63
1	B	13	LYS	CD-CE-NZ	-5.93	92.91	111.90
1	B	60	MET	O-C-N	5.92	130.47	122.59
1	A	5	ASP	O-C-N	5.84	130.26	122.26
1	A	5	ASP	CA-C-N	-5.83	112.42	122.10
1	A	5	ASP	C-N-CA	-5.83	112.42	122.10
1	B	272	LEU	CA-C-N	5.82	128.43	120.46
1	B	272	LEU	C-N-CA	5.82	128.43	120.46
1	B	113	ASN	CB-CA-C	5.80	121.97	110.42
1	A	6	PHE	CA-C-N	-5.79	113.72	122.81
1	A	6	PHE	C-N-CA	-5.79	113.72	122.81
1	A	65	THR	CA-CB-OG1	5.74	118.21	109.60
1	A	269	GLU	N-CA-C	5.74	117.41	109.15
1	B	101	THR	N-CA-C	-5.73	100.79	109.85
1	A	104	MET	CA-C-N	5.71	128.50	120.28
1	A	104	MET	C-N-CA	5.71	128.50	120.28
1	B	9	VAL	CA-C-N	-5.68	113.38	121.50
1	B	9	VAL	C-N-CA	-5.68	113.38	121.50
1	B	215	ASN	CB-CA-C	5.68	121.72	110.42
1	A	85	GLU	CA-C-O	5.67	126.28	119.59
1	A	112	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	48	GLU	CB-CA-C	5.61	119.01	109.80
1	A	106	GLU	O-C-N	5.60	129.99	122.49
1	A	146	LEU	N-CA-C	5.58	117.99	110.29
1	A	8	VAL	CA-C-N	-5.58	116.18	122.48
1	A	8	VAL	C-N-CA	-5.58	116.18	122.48
1	B	273	ILE	CG1-CB-CG2	-5.56	94.02	110.70
1	B	13	LYS	CB-CG-CD	-5.53	98.57	111.30
1	A	178	LEU	CA-C-N	-5.53	115.90	123.14
1	A	178	LEU	C-N-CA	-5.53	115.90	123.14
1	B	95	PRO	CA-C-O	-5.52	114.69	121.31
1	A	132	ARG	CB-CA-C	5.50	118.69	109.89
1	A	29	TYR	CA-C-N	-5.48	114.98	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	TYR	C-N-CA	-5.48	114.98	122.93
1	A	214	ARG	CA-C-N	-5.46	114.02	123.25
1	A	214	ARG	C-N-CA	-5.46	114.02	123.25
1	B	283	GLN	N-CA-C	5.39	117.16	111.28
1	A	268	ARG	CA-C-N	-5.36	113.29	121.66
1	A	268	ARG	C-N-CA	-5.36	113.29	121.66
1	A	222	VAL	CB-CA-C	5.35	119.61	112.22
1	A	46	PHE	N-CA-C	5.35	119.91	113.17
1	A	112	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	5	ASP	CB-CG-OD2	5.28	130.55	118.40
1	B	262	VAL	N-CA-C	5.28	115.45	107.75
1	B	112	ARG	CA-C-N	5.26	131.59	121.54
1	B	112	ARG	C-N-CA	5.26	131.59	121.54
1	A	245	VAL	N-CA-C	5.24	115.41	107.75
1	A	61	GLU	O-C-N	5.24	128.88	122.96
1	B	116	GLU	O-C-N	-5.20	116.31	121.88
1	A	269	GLU	CA-CB-CG	-5.20	103.70	114.10
1	A	39	GLN	CB-CA-C	5.14	118.88	110.96
1	B	183	LEU	N-CA-C	-5.13	105.86	111.82
1	B	112	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	18	ARG	CB-CA-C	5.12	118.15	109.55
1	B	137	ASP	N-CA-CB	5.12	117.60	109.51
1	A	296	ASN	O-C-N	5.11	130.25	122.94
1	B	212	VAL	N-CA-C	5.11	116.21	111.81
1	B	67	TYR	N-CA-C	5.09	117.22	111.02
1	B	94	LEU	CB-CA-C	5.08	115.52	110.33
1	A	27	LYS	CA-C-N	-5.05	116.92	123.19
1	A	27	LYS	C-N-CA	-5.05	116.92	123.19
1	B	115	ASP	N-CA-C	5.04	117.61	110.50
1	B	230	GLY	CA-C-O	-5.03	112.99	119.13

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

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Mol	Chain	Res	Type	Group
1	A	116	GLU	Sidechain
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 [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	2521	0	2530	118	3
1	B	2521	0	2534	101	6
All	All	5042	0	5064	208	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 21.

All (208) 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	1.42
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:A:48:GLU:HA	1:A:48:GLU:OE2	1.54	1.08
1:B:12:LYS:HA	1:B:12:LYS:CE	1.79	1.08
1:A:190:LEU:HD12	1:A:197:LEU:HD13	1.42	1.01
1:A:104:MET:HE1	1:A:300:PHE:CE1	1.99	0.97
1:B:12:LYS:HE3	1:B:12:LYS:HA	0.96	0.96
1:B:104:MET:HE1	1:B:300:PHE:CE1	2.03	0.93
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ILE:HB	1:A:162:GLN:HG3	1.58	0.84
1:A:199:ASN:H	1:A:199:ASN:HD22	1.27	0.83
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:17:ARG:HH21	1:A:17:ARG:HG2	1.45	0.80
1:B:168:ARG:HG2	1:B:168:ARG:NH1	1.86	0.79
1:A:6:PHE:HD1	1:A:30:LEU:O	1.64	0.79
1:B:104:MET:HE1	1:B:300:PHE:CZ	2.17	0.79
1:B:149:ILE:HB	1:B:162:GLN:HG3	1.62	0.79
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:104:MET:HE1	1:A:300:PHE:CZ	2.20	0.76
1:A:238:LYS:NZ	1:B:127:GLU:HG2	2.01	0.75
1:A:104:MET:HE1	1:A:300:PHE:HE1	1.48	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:HH11	1:B:168:ARG:CG	1.95	0.73
1:A:17:ARG:HH21	1:A:17:ARG:CG	2.01	0.72
1:B:55:TRP:NE1	1:B:59:ARG:HH11	1.88	0.72
1:A:180:THR:HG21	1:B:126:SER:HB3	1.74	0.70
1:A:13:LYS:NZ	1:A:13:LYS:HB2	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:HH11	1:B:112:ARG:HB3	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:104:MET:HE3	1:A:104:MET:HA	1.76	0.67
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:HG2	1:A:17:ARG:NH2	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:B:55:TRP:CD1	1:B:59:ARG:NH1	2.66	0.64
1:A:250:GLU:O	1:A:251:SER:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:43:ILE:C	1:A:44:GLU:HG2	2.23	0.63
1:B:55:TRP:HE1	1:B:59:ARG:NH1	1.97	0.62
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: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:A:4:GLY:C	1:A:5:ASP:CA	2.73	0.59
1:A:104:MET:HE3	1:A:298:LEU:HD12	1.84	0.59
1:B:90:LYS:HB3	1:B:90:LYS:NZ	2.17	0.58
1:A:6:PHE:HD1	1:A:30:LEU:C	2.11	0.58
1:A:250:GLU:HG2	1:A:254:ASP:OD2	2.03	0.58
1:B:55:TRP:HE1	1:B:59:ARG:HH11	1.49	0.58
1:B:104:MET:HE3	1:B:298:LEU:HD23	1.85	0.58
1:B:199:ASN:HD22	1:B:199:ASN:N	1.88	0.57
1:A:169:TYR:C	1:A:170:PHE:CD1	2.83	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:A:104:MET:CE	1:A:300:PHE:HE1	2.15	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:HA	1:B:214:ARG:NE	2.18	0.56
1:A:33:LEU:HD21	1:A:66:TYR:HB3	1.86	0.56
1:B:109:GLU:HA	1:B:109:GLU:OE2	2.03	0.56
1:B:187:LEU:HD23	1:B:220:TYR:CZ	2.40	0.56
1:B:225:ASN:OD1	1:B:229:ARG:HD2	2.05	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:A:118:ARG:NH2	1:A:132:ARG:HD3	2.21	0.55
1:B:37:TYR:CE1	1:B:41:LYS:HD3	2.41	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:H	1:B:199:ASN:ND2	1.99	0.54
1:B:121:VAL:CG2	1:B:272:LEU:HD13	2.37	0.53
1:A:224:ARG:O	1:A:225:ASN:C	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HG13	1:B:254:ASP:HB2	1.91	0.53
1:A:166:PHE:O	1:A:170:PHE:N	2.42	0.52
1:B:125:GLU:O	1:B:126:SER:OG	2.25	0.52
1:B:216:PHE:O	1:B:217:ASP:C	2.49	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
1:B:11:ALA:HA	1:B:28:ILE:HD12	1.91	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:112:ARG:C	1:B:114:PHE:H	2.18	0.51
1:A:244:ARG:HD2	1:A:246:TYR:OH	2.10	0.51
1:B:136:PRO:HG3	1:B:299:CYS:HB2	1.91	0.51
1:A:31:HIS:ND1	1:A:33:LEU:HB2	2.26	0.51
1:A:149:ILE:HB	1:A:162:GLN:CG	2.33	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:HB2	1:A:13:LYS:HZ3	1.76	0.50
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: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: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:A:293:TYR:CZ	1:A:296:ASN:HB2	2.50	0.47
1:B:92:PRO:O	1:B:117:LEU:HD12	2.15	0.47
1:A:304:LYS:HB3	1:A:304:LYS:HE3	1.51	0.47
1:B:149:ILE:CB	1:B:162:GLN:HG3	2.41	0.47
1:B:261:LEU:HA	1:B:261:LEU:HD23	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:277:ARG:O	1:A:278:ALA:C	2.57	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:202:ARG:O	1:A:206:VAL:HG23	2.16	0.46
1:A:275:LEU:HD11	1:A:300:PHE:CD2	2.52	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:A:97:SER:C	1:A:99:ARG:H	2.24	0.45
1:A:236:GLY:O	1:A:237:PHE:C	2.58	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:18:ARG:HA	1:A:18:ARG:HD2	1.44	0.45
1:A:103:ARG:HD2	1:A:269:GLU:OE1	2.17	0.45
1:A:255:LEU:N	1:A:256:PRO:CD	2.79	0.45
1:B:108:ALA:O	1:B:109:GLU:C	2.57	0.45
1:A:227:LYS:HA	1:A:227:LYS:HD2	1.51	0.45
1:B:66:TYR:CD2	1:B:95:PRO:HG2	2.52	0.45
1:B:93:TYR:OH	1:B:305:VAL:OXT	2.22	0.45
1:B:197:LEU:HD12	1:B:197:LEU:HA	1.81	0.44
1:A:237:PHE:C	1:A:237:PHE:CD2	2.96	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: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:B:18:ARG:HB3	1:B:20:PHE:CD1	2.53	0.44
1:B:244:ARG:HD2	1:B:246:TYR:OH	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:A:302:ARG:HH11	1:A:302:ARG:HD2	1.61	0.43
1:B:4:GLY:O	1:B:59:ARG:CD	2.66	0.43
1:B:34:GLU:O	1:B:35:VAL:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:HB3	1:B:12:LYS:HE2	1.37	0.43
1:A:39:GLN:NE2	1:A:52:VAL:HG21	2.33	0.43
1:A:91:LYS:HG2	1:A:116:GLU:CG	2.46	0.43
1:A:293:TYR:O	1:A:294:GLY:C	2.61	0.43
1:B:184:ILE:HG23	1:B:185:GLU:N	2.33	0.43
1:B:119:LEU:HA	1:B:119:LEU:HD12	1.67	0.42
1:B:275:LEU:O	1:B:276:ALA:C	2.60	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: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: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:150:ALA:O	1:B:160:THR:OG1	2.26	0.41
1:A:232:VAL:HB	1:A:246:TYR:HB2	2.03	0.41
1:B:32:PRO:O	1:B:36:VAL:HG23	2.20	0.41
1:B:182:SER:OG	1:B:184:ILE:HG22	2.21	0.41
1:A:110:LYS:C	1:A:112:ARG:H	2.28	0.41
1:B:18:ARG:HB3	1:B:20:PHE:CE1	2.55	0.41
1:A:57:GLU:C	1:A:59:ARG:H	2.29	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:98:GLU:HG2	1:B:99:ARG:N	2.35	0.41
1:A:206:VAL:O	1:A:210:ARG:HG3	2.21	0.40
1:B:4:GLY:O	1:B:59:ARG:HD2	2.21	0.40
1:A:97:SER:C	1:A:99:ARG:N	2.78	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: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
1:B:236:GLY:C	1:B:241:SER:O	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	301/305 (99%)	272 (90%)	25 (8%)	4 (1%)	9	25
1	B	301/305 (99%)	267 (89%)	28 (9%)	6 (2%)	6	16
All	All	602/610 (99%)	539 (90%)	53 (9%)	10 (2%)	7	19

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 [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	271/273 (99%)	195 (72%)	76 (28%)	0	1
1	B	271/273 (99%)	201 (74%)	70 (26%)	0	2
All	All	542/546 (99%)	396 (73%)	146 (27%)	0	1

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	17	ARG
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	57	GLU
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	125	GLU
1	A	133	VAL
1	A	139	MET
1	A	141	GLU
1	A	142	GLN

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Mol	Chain	Res	Type
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	158	VAL
1	A	161	LYS
1	A	162	GLN
1	A	165	ILE
1	A	168	ARG
1	A	173	SER
1	A	175	LYS
1	A	179	VAL
1	A	183	LEU
1	A	184	ILE
1	A	186	SER
1	A	192	LEU
1	A	198	LEU
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	244	ARG
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	288	ARG
1	A	296	ASN
1	A	302	ARG
1	A	304	LYS

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Mol	Chain	Res	Type
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	34	GLU
1	B	40	ILE
1	B	41	LYS
1	B	43	ILE
1	B	44	GLU
1	B	45	SER
1	B	48	GLU
1	B	54	SER
1	B	59	ARG
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	91	LYS
1	B	98	GLU
1	B	100	LYS
1	B	104	MET
1	B	105	GLU
1	B	106	GLU
1	B	112	ARG
1	B	114	PHE
1	B	115	ASP
1	B	122	VAL
1	B	125	GLU
1	B	127	GLU
1	B	132	ARG
1	B	141	GLU
1	B	152	VAL
1	B	154	SER
1	B	158	VAL
1	B	159	ILE
1	B	161	LYS

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Mol	Chain	Res	Type
1	B	162	GLN
1	B	163	THR
1	B	164	GLU
1	B	165	ILE
1	B	168	ARG
1	B	174	GLU
1	B	179	VAL
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	206	VAL
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	221	GLU
1	B	222	VAL
1	B	234	LYS
1	B	244	ARG
1	B	247	ARG
1	B	253	ASP
1	B	275	LEU
1	B	285	VAL
1	B	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	162	GLN
1	A	199	ASN
1	A	257	HIS
1	B	39	GLN
1	B	83	GLN
1	B	199	ASN
1	B	215	ASN
1	B	257	HIS

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Mol	Chain	Res	Type
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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4:GLY	C	5:ASP	N	1.77
1	A	115:ASP	C	116:GLU	N	1.61
1	A	45:SER	C	46:PHE	N	1.20
1	A	272:LEU	C	273:ILE	N	1.17
1	A	118:ARG	C	119:LEU	N	1.16
1	A	117:LEU	C	118:ARG	N	1.09

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	303/305 (99%)	0.26	5 (1%) 69 67	23, 27, 27, 28	9 (2%)
1	B	303/305 (99%)	0.32	8 (2%) 57 54	17, 27, 27, 28	8 (2%)
All	All	606/610 (99%)	0.29	13 (2%) 63 61	17, 27, 27, 28	17 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	GLY	4.1
1	B	18	ARG	3.3
1	B	115	ASP	3.1
1	B	114	PHE	2.8
1	B	145	GLU	2.6
1	A	3	GLY	2.6
1	A	24	ARG	2.4
1	B	5	ASP	2.3
1	B	174	GLU	2.3
1	A	145	GLU	2.2
1	A	155	ASP	2.2
1	B	168	ARG	2.0
1	A	215	ASN	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.