



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:14 AM UTC

PDB ID : 1R0V / pdb_00001r0v
Title : Structure Determination of the Dimeric Endonuclease in a Pseudo-face-centered P21212 space group
Authors : Li, H.; Zhang, Y.
Deposited on : 2003-09-23
Resolution : 2.00 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

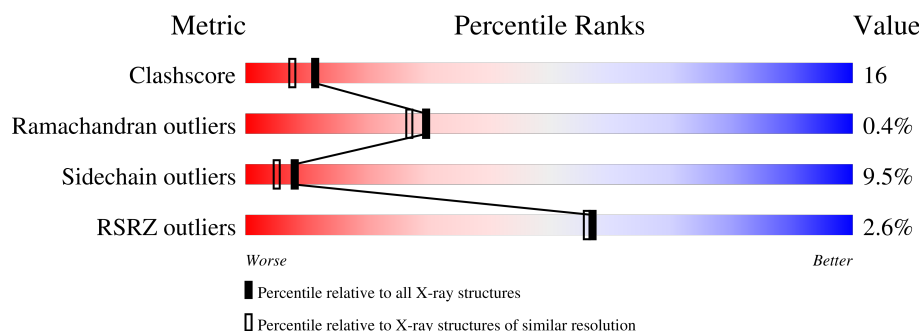
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	3% 41% 28% 9% • 20%
1	B	305	3% 38% 32% 8% • 20%
1	C	305	% 39% 32% 7% • 20%
1	D	305	% 45% 26% 7% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9073 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	244	Total	C	N	O	S	0	0	0
			2050	1309	351	385	5			
1	B	244	Total	C	N	O	S	0	0	0
			2050	1309	351	385	5			
1	C	244	Total	C	N	O	S	0	0	0
			2050	1309	351	385	5			
1	D	243	Total	C	N	O	S	0	0	0
			2042	1305	350	382	5			

There are 4 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
C	152	VAL	ILE	conflict	UNP O29362
D	152	VAL	ILE	conflict	UNP O29362

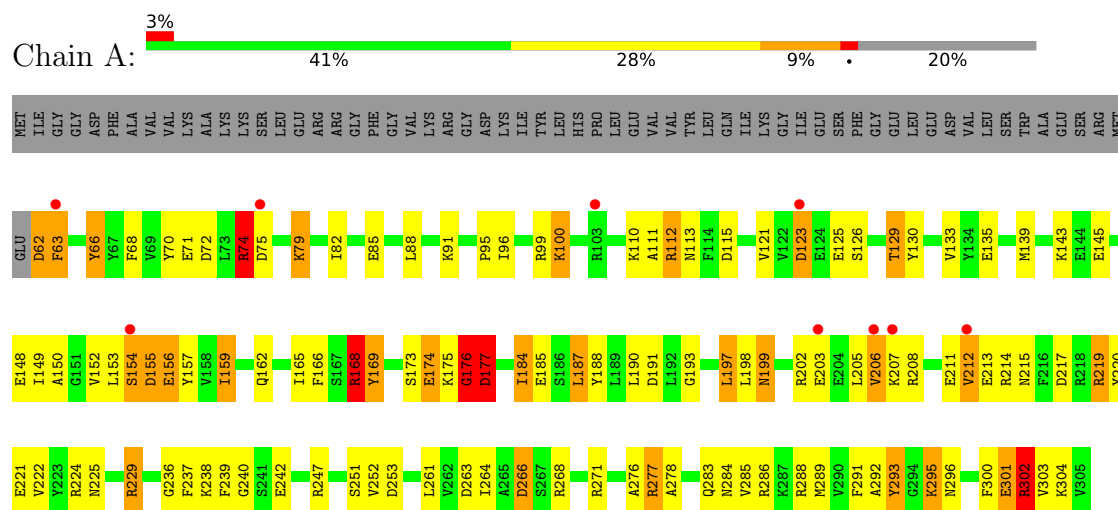
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	232	Total	O	0	0
			232	232		
2	B	215	Total	O	0	0
			215	215		
2	C	199	Total	O	0	0
			199	199		
2	D	235	Total	O	0	0
			235	235		

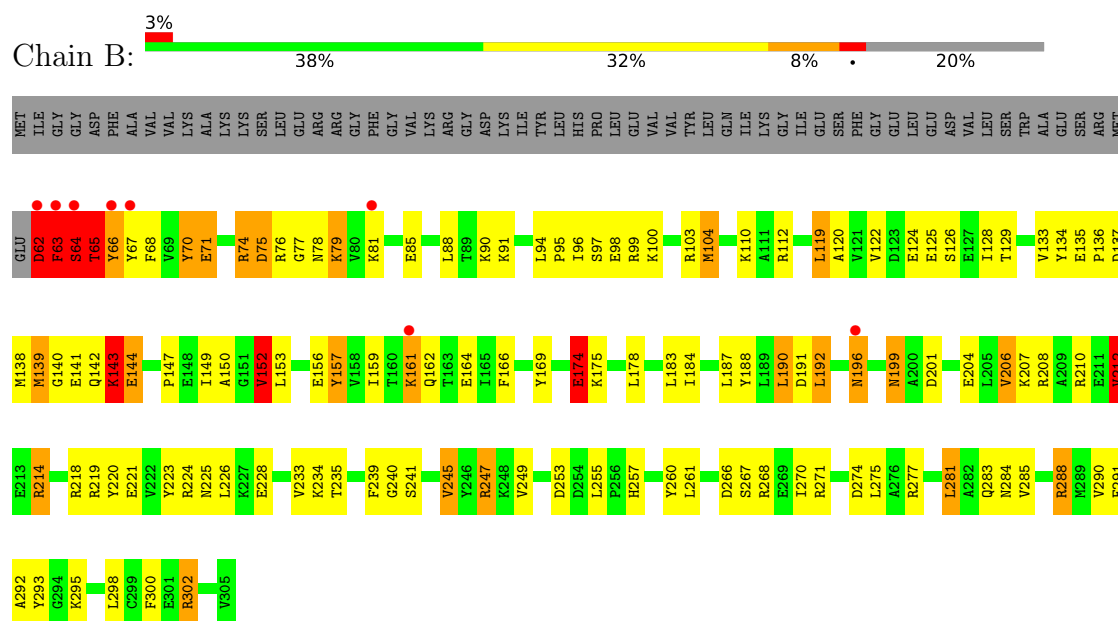
3 Residue-property plots

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

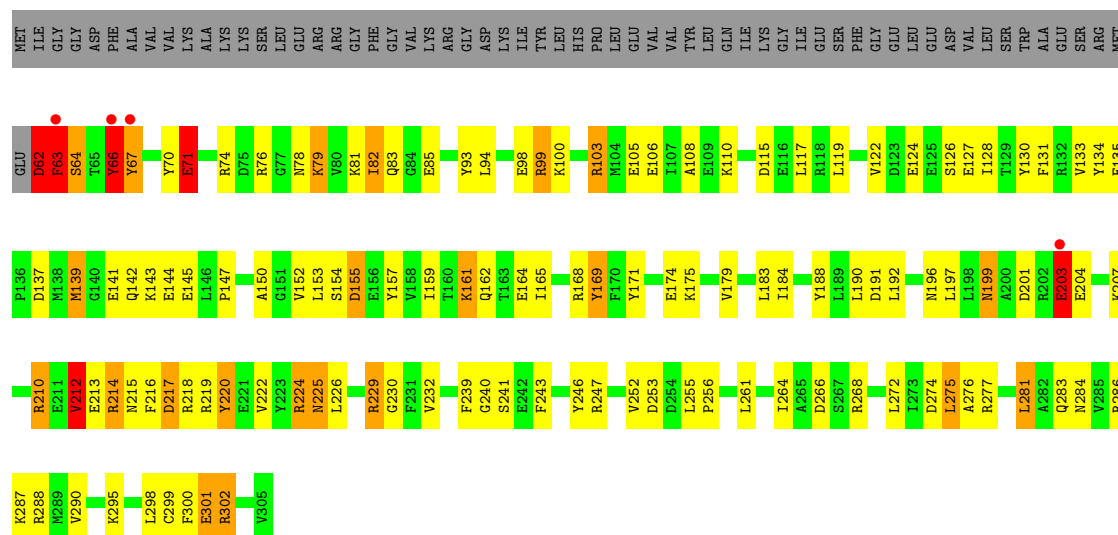


• Molecule 1: tRNA-intron endonuclease

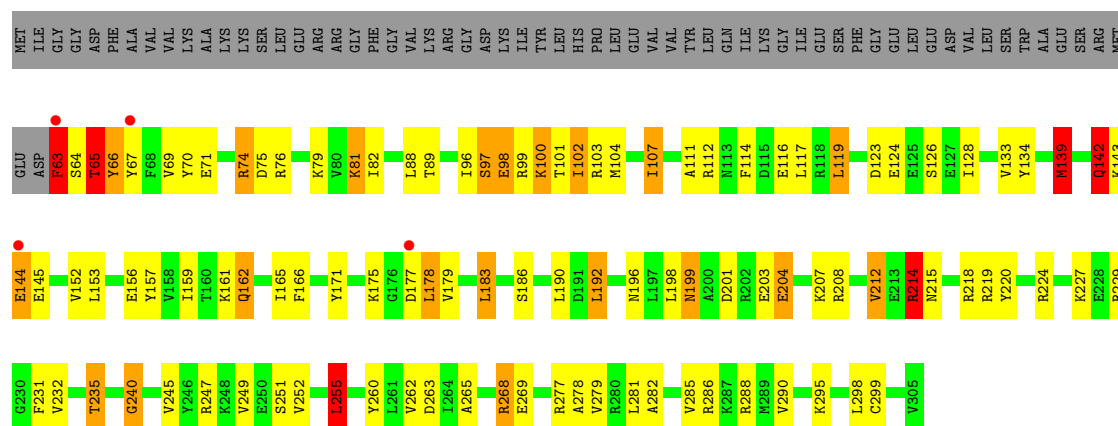


• Molecule 1: tRNA-intron endonuclease





• Molecule 1: tRNA-intron endonuclease



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.12Å 144.15Å 52.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.35 – 2.00 95.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (95.35-2.00) 92.7 (95.35-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.242 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9073	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4528e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	2.12	61/2085 (2.9%)	1.82	46/2798 (1.6%)
1	B	2.36	91/2085 (4.4%)	2.16	67/2798 (2.4%)
1	C	2.31	87/2085 (4.2%)	2.06	75/2798 (2.7%)
1	D	2.15	70/2077 (3.4%)	1.85	41/2787 (1.5%)
All	All	2.24	309/8332 (3.7%)	1.98	229/11181 (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	B	0	4
1	C	0	1
1	D	0	1
All	All	0	6

All (309) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	SER	CA-C	-15.18	1.32	1.52
1	C	268	ARG	CZ-NH2	-11.09	1.19	1.33
1	B	104	MET	SD-CE	10.94	2.06	1.79
1	D	214	ARG	C-O	-10.53	1.11	1.24
1	B	63	PHE	N-CA	10.38	1.59	1.46
1	D	64	SER	N-CA	-10.24	1.32	1.46
1	C	226	LEU	N-CA	10.21	1.59	1.46
1	C	64	SER	CA-C	-9.96	1.39	1.52
1	A	184	ILE	CA-CB	9.72	1.66	1.54
1	D	139	MET	SD-CE	9.38	2.02	1.79
1	C	63	PHE	CA-C	9.24	1.65	1.52
1	B	76	ARG	CZ-NH1	-9.24	1.19	1.32
1	C	284	ASN	CG-OD1	-9.16	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	PHE	C-N	-9.15	1.21	1.33
1	B	292	ALA	CA-CB	9.09	1.66	1.53
1	A	252	VAL	CA-CB	8.93	1.69	1.54
1	D	177	ASP	C-O	8.81	1.35	1.24
1	B	62	ASP	C-N	8.73	1.46	1.33
1	B	63	PHE	CB-CG	-8.68	1.30	1.50
1	B	285	VAL	CA-CB	8.64	1.66	1.54
1	C	252	VAL	CA-CB	8.60	1.67	1.54
1	B	62	ASP	CA-CB	8.59	1.70	1.53
1	C	142	GLN	C-O	-8.40	1.13	1.23
1	D	100	LYS	C-O	8.27	1.34	1.23
1	B	64	SER	CA-CB	-8.09	1.39	1.53
1	A	95	PRO	C-O	7.87	1.32	1.23
1	C	124	GLU	CD-OE2	-7.82	1.10	1.25
1	B	281	LEU	CG-CD1	-7.77	1.26	1.52
1	D	67	TYR	CB-CG	-7.68	1.34	1.51
1	B	266	ASP	CA-C	-7.55	1.46	1.53
1	C	64	SER	CA-CB	-7.52	1.41	1.53
1	C	67	TYR	CA-CB	-7.48	1.41	1.53
1	B	63	PHE	CA-C	-7.45	1.42	1.52
1	D	299	CYS	C-O	7.43	1.32	1.23
1	B	239	PHE	CG-CD2	-7.42	1.23	1.38
1	A	139	MET	CG-SD	-7.41	1.62	1.80
1	B	245	VAL	C-O	7.38	1.31	1.24
1	A	289	MET	CA-CB	7.25	1.63	1.53
1	D	178	LEU	CG-CD1	-7.24	1.28	1.52
1	D	144	GLU	CD-OE2	7.16	1.39	1.25
1	C	210	ARG	CZ-NH1	-7.14	1.22	1.32
1	B	255	LEU	CA-C	7.13	1.61	1.52
1	C	212	VAL	CA-CB	7.12	1.64	1.54
1	B	225	ASN	CG-OD1	-7.11	1.10	1.23
1	C	67	TYR	CB-CG	-7.11	1.36	1.51
1	B	144	GLU	CD-OE2	-7.10	1.11	1.25
1	C	131	PHE	CE1-CZ	-7.09	1.17	1.38
1	A	72	ASP	C-O	7.03	1.32	1.24
1	C	99	ARG	CZ-NH1	-7.00	1.23	1.32
1	D	76	ARG	CZ-NH2	-7.00	1.24	1.33
1	D	101	THR	CA-CB	-6.95	1.42	1.53
1	B	268	ARG	CZ-NH2	-6.94	1.24	1.33
1	B	283	GLN	CD-OE1	-6.93	1.10	1.23
1	A	96	ILE	CA-CB	6.86	1.65	1.55
1	B	62	ASP	N-CA	6.78	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	LYS	C-O	6.77	1.32	1.23
1	A	68	PHE	C-O	6.74	1.32	1.24
1	C	243	PHE	C-O	6.72	1.32	1.23
1	D	63	PHE	C-N	-6.71	1.24	1.33
1	C	255	LEU	C-O	-6.70	1.18	1.24
1	B	219	ARG	CZ-NH1	-6.69	1.23	1.32
1	C	137	ASP	C-O	-6.67	1.15	1.24
1	C	66	TYR	CA-CB	-6.66	1.43	1.53
1	C	212	VAL	CB-CG2	-6.64	1.30	1.52
1	D	218	ARG	CG-CD	6.64	1.72	1.52
1	B	119	LEU	CG-CD2	-6.62	1.30	1.52
1	D	299	CYS	CA-C	6.61	1.60	1.52
1	D	268	ARG	CZ-NH2	-6.59	1.24	1.33
1	A	157	TYR	CE1-CZ	-6.57	1.22	1.38
1	D	89	THR	CA-C	-6.56	1.44	1.52
1	B	62	ASP	CA-C	6.55	1.66	1.52
1	C	219	ARG	C-O	6.50	1.31	1.24
1	D	69	VAL	CA-CB	6.49	1.62	1.54
1	B	267	SER	N-CA	-6.48	1.37	1.46
1	C	82	ILE	CB-CG2	-6.47	1.31	1.52
1	D	71	GLU	C-O	-6.46	1.16	1.24
1	B	161	LYS	CD-CE	6.45	1.71	1.52
1	C	70	TYR	CE2-CZ	-6.45	1.22	1.38
1	B	68	PHE	C-N	6.44	1.41	1.33
1	C	144	GLU	CD-OE2	-6.43	1.13	1.25
1	B	138	MET	SD-CE	6.42	1.95	1.79
1	D	279	VAL	CA-CB	6.42	1.62	1.54
1	C	219	ARG	CZ-NH2	-6.41	1.25	1.33
1	A	277	ARG	C-O	6.39	1.31	1.24
1	B	206	VAL	C-O	6.37	1.31	1.24
1	C	76	ARG	CZ-NH2	-6.37	1.25	1.33
1	B	184	ILE	CA-CB	6.37	1.62	1.54
1	C	283	GLN	CD-OE1	-6.34	1.11	1.23
1	D	64	SER	CA-CB	-6.32	1.42	1.53
1	C	130	TYR	CG-CD1	-6.32	1.26	1.39
1	C	99	ARG	CZ-NH2	-6.32	1.25	1.33
1	B	70	TYR	CE2-CZ	-6.30	1.23	1.38
1	A	208	ARG	NE-CZ	6.29	1.40	1.33
1	B	63	PHE	C-N	-6.28	1.24	1.33
1	C	71	GLU	CA-CB	-6.26	1.43	1.53
1	C	142	GLN	CD-OE1	-6.26	1.11	1.23
1	B	284	ASN	CG-ND2	-6.26	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	ASP	CA-C	-6.26	1.44	1.52
1	C	299	CYS	CA-C	6.26	1.60	1.52
1	C	159	ILE	N-CA	6.24	1.53	1.46
1	D	65	THR	CB-CG2	-6.23	1.31	1.52
1	C	135	GLU	CD-OE2	-6.21	1.13	1.25
1	B	190	LEU	C-O	6.21	1.31	1.24
1	B	271	ARG	CZ-NH2	-6.19	1.25	1.33
1	B	75	ASP	CB-CG	-6.19	1.36	1.52
1	D	75	ASP	CA-C	6.18	1.61	1.52
1	B	290	VAL	CA-C	6.18	1.60	1.52
1	A	66	TYR	CB-CG	-6.16	1.38	1.51
1	C	247	ARG	CZ-NH2	-6.15	1.25	1.33
1	D	231	PHE	N-CA	6.15	1.53	1.45
1	C	78	ASN	CG-ND2	-6.15	1.20	1.33
1	B	234	LYS	CD-CE	6.12	1.70	1.52
1	C	212	VAL	CB-CG1	-6.12	1.32	1.52
1	D	107	ILE	C-O	6.12	1.32	1.24
1	D	114	PHE	CG-CD2	-6.11	1.26	1.38
1	D	285	VAL	C-O	6.11	1.31	1.24
1	B	66	TYR	CG-CD1	-6.09	1.26	1.39
1	B	78	ASN	CG-OD1	-6.09	1.11	1.23
1	A	188	TYR	CA-C	6.08	1.60	1.52
1	B	239	PHE	CE1-CZ	-6.08	1.20	1.38
1	A	121	VAL	CA-CB	-6.07	1.47	1.54
1	C	215	ASN	CG-OD1	6.03	1.35	1.23
1	D	260	TYR	N-CA	6.03	1.53	1.46
1	C	122	VAL	C-O	6.02	1.30	1.24
1	D	240	GLY	C-O	6.01	1.31	1.24
1	B	288	ARG	C-N	-6.00	1.25	1.33
1	B	128	ILE	C-O	-6.00	1.17	1.24
1	D	157	TYR	CE2-CZ	-5.99	1.23	1.38
1	B	76	ARG	CZ-NH2	-5.99	1.25	1.33
1	D	142	GLN	C-O	-5.97	1.16	1.23
1	C	239	PHE	CE1-CZ	-5.96	1.20	1.38
1	B	97	SER	CA-C	5.96	1.60	1.52
1	B	291	PHE	C-O	5.95	1.31	1.24
1	D	255	LEU	CG-CD2	-5.94	1.32	1.52
1	A	63	PHE	CA-C	-5.92	1.45	1.52
1	A	130	TYR	C-O	5.90	1.31	1.24
1	C	171	TYR	N-CA	5.89	1.53	1.45
1	A	165	ILE	CA-C	5.88	1.60	1.52
1	C	299	CYS	N-CA	5.87	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	ASN	CB-CG	-5.86	1.37	1.52
1	C	241	SER	CA-C	5.86	1.59	1.52
1	D	282	ALA	CA-CB	5.86	1.62	1.53
1	B	283	GLN	CD-NE2	-5.86	1.21	1.33
1	A	129	THR	C-O	-5.85	1.17	1.24
1	B	66	TYR	CB-CG	-5.84	1.38	1.51
1	A	221	GLU	N-CA	5.83	1.53	1.46
1	B	137	ASP	CG-OD2	-5.83	1.14	1.25
1	C	93	TYR	CD1-CE1	5.83	1.56	1.38
1	B	65	THR	CB-CG2	-5.83	1.33	1.52
1	B	71	GLU	CD-OE1	-5.82	1.14	1.25
1	C	70	TYR	CG-CD2	-5.80	1.27	1.39
1	C	108	ALA	CA-CB	5.79	1.62	1.53
1	D	134	TYR	C-O	5.79	1.30	1.23
1	A	300	PHE	C-N	-5.79	1.25	1.33
1	C	276	ALA	N-CA	5.78	1.53	1.46
1	A	139	MET	SD-CE	5.78	1.94	1.79
1	C	300	PHE	C-N	-5.78	1.25	1.33
1	B	70	TYR	CG-CD2	-5.78	1.27	1.39
1	B	241	SER	CA-CB	5.78	1.62	1.53
1	B	241	SER	CA-C	5.76	1.59	1.52
1	C	70	TYR	CG-CD1	-5.75	1.27	1.39
1	D	262	VAL	CA-CB	5.73	1.61	1.54
1	C	152	VAL	CB-CG2	-5.73	1.33	1.52
1	B	119	LEU	CB-CG	-5.72	1.42	1.53
1	D	162	GLN	CD-OE1	-5.72	1.12	1.23
1	C	94	LEU	CA-C	5.71	1.59	1.52
1	B	221	GLU	C-O	5.71	1.30	1.24
1	C	70	TYR	CE1-CZ	-5.71	1.24	1.38
1	D	278	ALA	CA-CB	5.70	1.62	1.53
1	B	226	LEU	N-CA	5.69	1.53	1.46
1	D	227	LYS	N-CA	5.69	1.53	1.46
1	B	159	ILE	N-CA	5.69	1.52	1.46
1	B	247	ARG	CD-NE	-5.67	1.38	1.46
1	D	165	ILE	C-O	5.67	1.31	1.24
1	C	283	GLN	CD-NE2	-5.66	1.21	1.33
1	D	265	ALA	N-CA	5.65	1.53	1.46
1	A	303	VAL	CA-CB	5.64	1.64	1.54
1	B	270	ILE	C-O	5.64	1.30	1.24
1	B	188	TYR	CA-C	5.63	1.59	1.52
1	D	64	SER	CA-C	-5.63	1.45	1.52
1	C	287	LYS	CA-C	-5.63	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	THR	C-O	5.62	1.30	1.23
1	C	281	LEU	CA-C	5.61	1.59	1.52
1	C	139	MET	SD-CE	5.61	1.93	1.79
1	C	284	ASN	CG-ND2	-5.61	1.21	1.33
1	C	184	ILE	CB-CG2	5.59	1.71	1.52
1	D	218	ARG	CB-CG	-5.58	1.35	1.52
1	B	300	PHE	C-O	-5.58	1.16	1.24
1	A	75	ASP	CA-CB	-5.57	1.43	1.53
1	A	263	ASP	N-CA	-5.57	1.39	1.45
1	A	283	GLN	C-O	5.56	1.30	1.24
1	C	264	ILE	CG1-CD1	5.56	1.73	1.51
1	B	157	TYR	CG-CD2	-5.55	1.27	1.39
1	C	165	ILE	CA-CB	5.55	1.64	1.54
1	A	221	GLU	CA-C	5.54	1.59	1.52
1	D	229	ARG	CA-C	5.54	1.60	1.52
1	D	290	VAL	CA-C	5.53	1.59	1.52
1	D	133	VAL	CA-C	-5.52	1.46	1.52
1	A	198	LEU	CA-C	-5.51	1.45	1.52
1	B	136	PRO	C-O	5.51	1.30	1.23
1	C	66	TYR	CB-CG	-5.51	1.39	1.51
1	A	111	ALA	CA-C	5.48	1.60	1.52
1	C	93	TYR	CA-C	5.47	1.59	1.52
1	D	255	LEU	C-O	-5.46	1.19	1.24
1	D	285	VAL	CA-CB	5.46	1.61	1.54
1	C	288	ARG	CB-CG	5.46	1.68	1.52
1	D	219	ARG	CG-CD	5.44	1.68	1.52
1	C	290	VAL	CA-C	5.43	1.59	1.52
1	A	205	LEU	CA-C	5.42	1.59	1.52
1	C	210	ARG	CZ-NH2	-5.41	1.26	1.33
1	C	272	LEU	C-O	-5.41	1.17	1.24
1	B	122	VAL	CA-C	-5.41	1.46	1.52
1	A	253	ASP	CG-OD1	-5.41	1.15	1.25
1	B	70	TYR	C-O	5.39	1.30	1.24
1	A	284	ASN	CG-OD1	-5.39	1.13	1.23
1	C	157	TYR	CE1-CZ	-5.39	1.25	1.38
1	C	70	TYR	N-CA	-5.38	1.39	1.46
1	C	241	SER	N-CA	-5.38	1.39	1.45
1	A	242	GLU	CD-OE1	-5.36	1.15	1.25
1	A	238	LYS	C-O	-5.36	1.17	1.24
1	D	282	ALA	C-O	-5.35	1.18	1.24
1	D	81	LYS	CD-CE	5.35	1.68	1.52
1	A	113	ASN	CA-CB	5.34	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	VAL	C-O	5.34	1.31	1.24
1	C	98	GLU	CD-OE1	-5.33	1.15	1.25
1	C	266	ASP	C-O	5.33	1.29	1.24
1	B	157	TYR	CE2-CZ	-5.33	1.25	1.38
1	C	188	TYR	CA-C	5.31	1.59	1.52
1	D	186	SER	N-CA	5.30	1.52	1.46
1	C	239	PHE	CD1-CE1	5.29	1.54	1.38
1	A	296	ASN	N-CA	-5.29	1.38	1.45
1	A	293	TYR	C-O	5.29	1.30	1.23
1	B	70	TYR	CA-C	5.29	1.59	1.52
1	D	255	LEU	CA-C	5.29	1.59	1.52
1	C	225	ASN	CG-ND2	-5.28	1.22	1.33
1	C	302	ARG	CZ-NH1	5.28	1.40	1.32
1	D	288	ARG	C-O	5.27	1.29	1.23
1	D	245	VAL	N-CA	5.26	1.52	1.46
1	A	121	VAL	CB-CG1	5.26	1.70	1.52
1	A	291	PHE	C-O	5.26	1.30	1.24
1	D	166	PHE	CA-CB	5.26	1.62	1.53
1	A	88	LEU	CA-C	5.24	1.58	1.52
1	B	112	ARG	C-O	5.24	1.30	1.23
1	D	214	ARG	C-N	-5.24	1.26	1.33
1	A	285	VAL	N-CA	5.24	1.52	1.46
1	B	94	LEU	CA-C	5.24	1.58	1.52
1	D	171	TYR	CA-C	5.24	1.59	1.52
1	A	154	SER	C-O	5.22	1.30	1.23
1	C	230	GLY	C-O	-5.22	1.17	1.24
1	C	246	TYR	CA-C	-5.22	1.46	1.52
1	A	135	GLU	CD-OE1	-5.22	1.15	1.25
1	D	128	ILE	CA-CB	5.21	1.60	1.54
1	D	190	LEU	C-O	5.21	1.30	1.24
1	C	222	VAL	CA-CB	5.20	1.60	1.54
1	A	289	MET	SD-CE	-5.20	1.66	1.79
1	B	63	PHE	CA-CB	-5.19	1.44	1.53
1	C	117	LEU	CA-C	5.19	1.59	1.52
1	A	185	GLU	C-O	5.18	1.30	1.24
1	C	255	LEU	CA-C	5.18	1.59	1.52
1	B	137	ASP	C-O	-5.18	1.18	1.24
1	B	147	PRO	CA-C	5.18	1.58	1.52
1	B	124	GLU	CD-OE2	-5.18	1.15	1.25
1	B	140	GLY	CA-C	-5.18	1.46	1.52
1	B	271	ARG	CZ-NH1	-5.18	1.25	1.32
1	A	149	ILE	CB-CG2	5.17	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	124	GLU	CD-OE1	-5.17	1.15	1.25
1	A	283	GLN	CA-CB	5.17	1.61	1.53
1	D	67	TYR	N-CA	-5.16	1.40	1.46
1	A	187	LEU	N-CA	5.15	1.52	1.46
1	C	93	TYR	CG-CD1	-5.15	1.28	1.39
1	B	275	LEU	C-O	5.14	1.30	1.24
1	B	218	ARG	N-CA	-5.13	1.40	1.46
1	A	276	ALA	N-CA	5.13	1.52	1.46
1	A	251	SER	C-O	5.13	1.29	1.23
1	A	125	GLU	N-CA	-5.13	1.39	1.46
1	A	165	ILE	N-CA	-5.13	1.40	1.46
1	A	166	PHE	C-O	-5.13	1.18	1.24
1	D	126	SER	CA-CB	5.13	1.61	1.53
1	A	247	ARG	CD-NE	-5.11	1.39	1.46
1	D	282	ALA	CA-C	5.11	1.59	1.52
1	B	233	VAL	CA-CB	-5.11	1.47	1.54
1	A	229	ARG	N-CA	5.10	1.52	1.46
1	B	120	ALA	C-O	5.10	1.29	1.23
1	A	278	ALA	CA-CB	5.10	1.61	1.53
1	C	174	GLU	C-O	5.10	1.30	1.23
1	A	66	TYR	CE2-CZ	-5.08	1.26	1.38
1	A	112	ARG	C-O	5.08	1.29	1.23
1	B	143	LYS	CA-C	-5.08	1.46	1.52
1	B	220	TYR	CA-C	5.08	1.59	1.52
1	A	292	ALA	CA-C	5.08	1.59	1.52
1	B	103	ARG	CA-C	-5.08	1.46	1.52
1	B	100	LYS	N-CA	-5.08	1.39	1.45
1	A	91	LYS	CE-NZ	-5.07	1.34	1.49
1	C	268	ARG	NE-CZ	-5.06	1.27	1.33
1	C	217	ASP	CG-OD2	-5.05	1.15	1.25
1	B	141	GLU	N-CA	5.05	1.51	1.46
1	B	225	ASN	CG-ND2	-5.05	1.22	1.33
1	D	102	ILE	CA-CB	5.05	1.63	1.55
1	D	66	TYR	CB-CG	-5.05	1.40	1.51
1	D	104	MET	C-O	-5.04	1.18	1.24
1	B	169	TYR	N-CA	-5.04	1.39	1.46
1	B	212	VAL	CB-CG2	-5.04	1.35	1.52
1	D	82	ILE	CA-C	5.04	1.58	1.52
1	C	229	ARG	C-O	5.03	1.30	1.24
1	A	222	VAL	C-O	-5.03	1.18	1.24
1	B	228	GLU	CD-OE1	-5.03	1.15	1.25
1	D	265	ALA	C-O	-5.03	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	281	LEU	CG-CD2	-5.01	1.36	1.52
1	A	219	ARG	CG-CD	5.01	1.67	1.52

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	PHE	CA-C-N	-25.00	73.79	121.54
1	B	63	PHE	C-N-CA	-25.00	73.79	121.54
1	B	63	PHE	N-CA-C	-24.21	59.24	110.80
1	C	268	ARG	NE-CZ-NH1	14.99	136.50	121.50
1	C	63	PHE	CA-C-N	-14.89	93.94	122.53
1	C	63	PHE	C-N-CA	-14.89	93.94	122.53
1	B	64	SER	N-CA-CB	-12.75	88.94	110.49
1	C	268	ARG	NE-CZ-NH2	-12.33	108.10	119.20
1	B	64	SER	CA-CB-OG	-12.20	86.69	111.10
1	D	64	SER	N-CA-CB	-11.22	91.53	110.49
1	B	261	LEU	CD1-CG-CD2	-10.77	87.11	110.80
1	B	62	ASP	CA-C-N	9.79	140.25	121.54
1	B	62	ASP	C-N-CA	9.79	140.25	121.54
1	B	119	LEU	CD1-CG-CD2	-9.53	89.83	110.80
1	D	268	ARG	NE-CZ-NH1	9.52	131.02	121.50
1	C	183	LEU	CD1-CG-CD2	-9.45	90.00	110.80
1	C	261	LEU	CD1-CG-CD2	-9.38	90.15	110.80
1	B	63	PHE	N-CA-CB	-9.34	94.71	110.49
1	C	210	ARG	NE-CZ-NH2	9.32	127.59	119.20
1	B	63	PHE	O-C-N	-9.07	110.52	122.59
1	B	64	SER	CB-CA-C	9.03	128.39	110.42
1	C	62	ASP	CA-C-N	-8.98	105.42	120.68
1	C	62	ASP	C-N-CA	-8.98	105.42	120.68
1	C	103	ARG	NE-CZ-NH2	8.90	127.21	119.20
1	C	214	ARG	NE-CZ-NH2	8.86	127.18	119.20
1	B	62	ASP	CA-C-O	-8.82	105.80	120.80
1	C	64	SER	N-CA-C	8.72	124.02	113.12
1	C	63	PHE	N-CA-C	8.71	123.20	112.23
1	D	214	ARG	O-C-N	-8.52	113.09	122.12
1	C	119	LEU	CD1-CG-CD2	-8.40	92.31	110.80
1	B	66	TYR	CB-CA-C	-8.36	96.64	110.85
1	C	74	ARG	CG-CD-NE	-8.36	93.61	112.00
1	C	71	GLU	CB-CG-CD	-8.35	98.41	112.60
1	C	214	ARG	NE-CZ-NH1	-8.31	113.19	121.50
1	D	212	VAL	CB-CA-C	-8.23	101.56	111.94
1	C	67	TYR	N-CA-CB	-8.20	98.07	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	LEU	CD1-CG-CD2	-8.04	93.11	110.80
1	C	71	GLU	N-CA-C	8.01	122.32	112.23
1	B	133	VAL	CB-CA-C	-7.99	98.66	110.81
1	B	64	SER	N-CA-C	-7.98	93.81	110.80
1	A	133	VAL	CB-CA-C	-7.91	99.05	110.83
1	C	63	PHE	O-C-N	-7.84	111.82	122.33
1	C	99	ARG	NE-CZ-NH2	7.84	126.26	119.20
1	B	152	VAL	CA-CB-CG1	7.80	123.66	110.40
1	A	176	GLY	O-C-N	-7.77	112.60	122.70
1	B	137	ASP	OD1-CG-OD2	-7.71	104.39	122.90
1	B	271	ARG	NE-CZ-NH2	7.65	126.09	119.20
1	A	208	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	A	214	ARG	NE-CZ-NH2	7.47	125.92	119.20
1	B	74	ARG	NE-CZ-NH2	7.46	125.91	119.20
1	B	219	ARG	NE-CZ-NH2	7.44	125.89	119.20
1	A	193	GLY	N-CA-C	-7.40	104.55	115.72
1	D	214	ARG	CA-C-N	-7.37	107.46	121.54
1	D	214	ARG	C-N-CA	-7.37	107.46	121.54
1	B	76	ARG	NE-CZ-NH2	7.32	125.79	119.20
1	D	214	ARG	N-CA-C	7.24	120.09	111.33
1	C	63	PHE	CA-CB-CG	-7.24	106.56	113.80
1	B	219	ARG	NH1-CZ-NH2	-7.20	109.95	119.30
1	B	214	ARG	CD-NE-CZ	7.18	134.46	124.40
1	C	274	ASP	OD1-CG-OD2	-7.14	105.75	122.90
1	D	214	ARG	NE-CZ-NH2	-7.12	112.80	119.20
1	B	288	ARG	CA-C-O	-7.11	112.91	120.80
1	A	66	TYR	N-CA-CB	-7.11	99.64	110.16
1	C	224	ARG	N-CA-C	7.06	118.98	111.28
1	B	271	ARG	NH1-CZ-NH2	-7.06	110.12	119.30
1	B	253	ASP	OD1-CG-OD2	-7.03	106.02	122.90
1	C	212	VAL	CG1-CB-CG2	-7.01	95.37	110.80
1	A	174	GLU	CA-C-N	7.01	132.19	122.79
1	A	174	GLU	C-N-CA	7.01	132.19	122.79
1	D	218	ARG	CG-CD-NE	-7.00	96.60	112.00
1	C	63	PHE	CA-C-O	6.96	128.00	119.79
1	A	268	ARG	NE-CZ-NH1	-6.96	114.54	121.50
1	C	82	ILE	CG1-CB-CG2	-6.87	90.09	110.70
1	C	127	GLU	CA-C-N	-6.85	114.70	123.19
1	C	127	GLU	C-N-CA	-6.85	114.70	123.19
1	D	178	LEU	CD1-CG-CD2	-6.84	95.76	110.80
1	A	214	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	C	71	GLU	CA-CB-CG	6.79	127.68	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	GLU	CA-CB-CG	6.78	127.66	114.10
1	B	212	VAL	CG1-CB-CG2	-6.75	95.95	110.80
1	B	210	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	D	63	PHE	CA-C-N	-6.71	108.72	121.54
1	D	63	PHE	C-N-CA	-6.71	108.72	121.54
1	A	168	ARG	CB-CA-C	6.68	121.04	109.15
1	C	137	ASP	OD1-CG-OD2	-6.61	107.05	122.90
1	A	239	PHE	N-CA-C	-6.59	104.47	113.30
1	D	133	VAL	CB-CA-C	-6.58	100.82	110.81
1	D	251	SER	CB-CA-C	-6.57	98.13	110.16
1	B	64	SER	O-C-N	6.53	131.28	122.59
1	B	268	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	B	76	ARG	NH1-CZ-NH2	-6.51	110.83	119.30
1	B	214	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	A	301	GLU	CB-CA-C	6.50	121.03	109.65
1	C	301	GLU	CB-CA-C	6.50	121.02	109.65
1	A	202	ARG	NE-CZ-NH2	6.48	125.04	119.20
1	C	218	ARG	CG-CD-NE	-6.48	97.75	112.00
1	B	65	THR	OG1-CB-CG2	-6.45	96.40	109.30
1	C	67	TYR	CB-CA-C	-6.44	100.10	110.79
1	A	247	ARG	CG-CD-NE	-6.44	97.84	112.00
1	C	137	ASP	CB-CG-OD2	6.40	133.13	118.40
1	B	90	LYS	N-CA-C	-6.38	105.50	113.28
1	C	191	ASP	OD1-CG-OD2	-6.38	107.59	122.90
1	A	148	GLU	CA-C-O	-6.37	113.76	120.58
1	C	64	SER	CA-CB-OG	-6.36	98.37	111.10
1	C	214	ARG	CD-NE-CZ	6.35	133.29	124.40
1	A	215	ASN	CB-CA-C	6.34	121.05	111.80
1	C	268	ARG	CD-NE-CZ	-6.32	115.55	124.40
1	C	74	ARG	CD-NE-CZ	6.31	133.24	124.40
1	D	69	VAL	N-CA-C	6.30	117.08	110.72
1	B	210	ARG	NH1-CZ-NH2	-6.25	111.18	119.30
1	D	177	ASP	CB-CA-C	-6.25	97.52	109.95
1	C	103	ARG	CD-NE-CZ	6.25	133.15	124.40
1	C	222	VAL	N-CA-C	6.23	116.40	110.42
1	D	159	ILE	CB-CA-C	6.22	119.88	110.62
1	C	203	GLU	CA-CB-CG	-6.18	101.74	114.10
1	A	63	PHE	N-CA-CB	6.17	119.02	110.07
1	B	300	PHE	CA-C-O	-6.17	114.04	120.70
1	C	99	ARG	NH1-CZ-NH2	-6.17	111.28	119.30
1	B	135	GLU	OE1-CD-OE2	-6.15	108.14	122.90
1	D	67	TYR	N-CA-CB	-6.14	101.10	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASP	CA-C-N	-6.14	113.47	122.86
1	A	266	ASP	C-N-CA	-6.14	113.47	122.86
1	A	152	VAL	CB-CA-C	6.13	119.93	110.50
1	B	152	VAL	CB-CA-C	6.12	119.92	110.50
1	A	126	SER	N-CA-C	6.08	120.28	112.86
1	C	64	SER	CB-CA-C	6.07	119.58	109.56
1	D	119	LEU	CB-CA-C	-6.07	100.33	110.29
1	B	77	GLY	N-CA-C	-6.07	106.78	115.64
1	A	271	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	74	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	D	67	TYR	N-CA-C	6.04	117.54	111.07
1	D	192	LEU	N-CA-C	-6.03	105.68	113.16
1	D	281	LEU	CD1-CG-CD2	-6.02	97.56	110.80
1	D	268	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	A	71	GLU	N-CA-C	5.97	117.79	111.28
1	C	66	TYR	N-CA-C	5.95	117.44	111.07
1	A	159	ILE	CB-CA-C	5.90	119.90	110.82
1	D	218	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	C	64	SER	N-CA-CB	-5.89	101.41	110.42
1	A	295	LYS	CB-CA-C	-5.87	101.56	111.02
1	A	206	VAL	O-C-N	5.87	127.56	121.87
1	C	253	ASP	OD1-CG-OD2	-5.86	108.83	122.90
1	C	76	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	A	62	ASP	CA-C-N	5.86	128.41	120.44
1	A	62	ASP	C-N-CA	5.86	128.41	120.44
1	A	74	ARG	CG-CD-NE	-5.85	99.12	112.00
1	C	274	ASP	CB-CG-OD2	5.84	131.83	118.40
1	B	218	ARG	CG-CD-NE	-5.82	99.19	112.00
1	B	266	ASP	N-CA-C	5.82	117.16	108.31
1	A	206	VAL	CB-CA-C	5.81	119.98	112.14
1	C	124	GLU	OE1-CD-OE2	-5.79	109.00	122.90
1	C	62	ASP	N-CA-C	-5.74	94.94	111.00
1	A	212	VAL	CB-CA-C	5.73	119.91	112.24
1	D	183	LEU	CB-CG-CD1	5.72	127.85	110.70
1	D	112	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	D	107	ILE	CA-C-N	5.69	127.84	120.44
1	D	107	ILE	C-N-CA	5.69	127.84	120.44
1	B	293	TYR	CB-CA-C	5.69	118.90	110.14
1	A	68	PHE	CA-C-O	5.67	126.56	120.55
1	A	251	SER	N-CA-CB	-5.67	102.77	111.56
1	C	169	TYR	N-CA-C	5.67	120.36	113.38
1	A	217	ASP	N-CA-C	5.66	117.91	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	VAL	CB-CA-C	-5.65	102.41	110.83
1	B	152	VAL	N-CA-CB	-5.62	102.23	111.44
1	B	247	ARG	CG-CD-NE	-5.61	99.66	112.00
1	B	62	ASP	N-CA-C	5.61	126.70	111.00
1	B	62	ASP	CB-CA-C	5.61	120.75	110.10
1	D	74	ARG	CA-CB-CG	-5.58	102.93	114.10
1	B	95	PRO	CA-C-O	-5.58	114.61	121.31
1	B	206	VAL	CB-CA-C	5.58	119.92	112.22
1	D	104	MET	N-CA-C	-5.57	105.29	111.36
1	B	191	ASP	OD1-CG-OD2	-5.56	109.55	122.90
1	A	74	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	B	95	PRO	CB-CA-C	-5.54	103.84	111.21
1	D	240	GLY	CA-C-N	-5.52	113.15	123.03
1	D	240	GLY	C-N-CA	-5.52	113.15	123.03
1	C	256	PRO	CB-CA-C	-5.52	103.11	111.44
1	C	103	ARG	CG-CD-NE	-5.50	99.91	112.00
1	C	218	ARG	N-CA-CB	-5.49	102.03	110.16
1	D	177	ASP	CA-C-O	-5.47	112.10	119.11
1	B	99	ARG	N-CA-C	5.47	119.80	113.18
1	C	275	LEU	CD1-CG-CD2	-5.43	98.85	110.80
1	A	264	ILE	N-CA-CB	-5.39	104.66	111.46
1	D	263	ASP	N-CA-C	-5.38	101.34	109.85
1	B	71	GLU	CB-CA-C	-5.37	101.71	110.85
1	C	219	ARG	NH1-CZ-NH2	-5.37	112.32	119.30
1	D	214	ARG	CD-NE-CZ	5.37	131.91	124.40
1	B	98	GLU	OE1-CD-OE2	-5.33	110.10	122.90
1	A	208	ARG	NH1-CZ-NH2	-5.33	112.38	119.30
1	B	71	GLU	CG-CD-OE2	5.30	130.59	118.40
1	D	116	GLU	N-CA-C	5.29	119.29	112.41
1	D	214	ARG	CG-CD-NE	-5.28	100.38	112.00
1	C	70	TYR	CA-C-N	-5.25	111.75	120.68
1	C	70	TYR	C-N-CA	-5.25	111.75	120.68
1	B	91	LYS	CD-CE-NZ	5.23	128.64	111.90
1	B	192	LEU	N-CA-C	-5.23	106.85	113.18
1	D	97	SER	N-CA-C	-5.23	102.74	110.48
1	B	214	ARG	N-CA-C	-5.19	102.81	110.48
1	A	191	ASP	OD1-CG-OD2	-5.18	110.47	122.90
1	C	63	PHE	CB-CA-C	5.18	120.94	110.38
1	C	216	PHE	N-CA-C	5.17	117.32	111.11
1	B	214	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	B	285	VAL	CA-CB-CG2	5.17	119.18	110.40
1	A	169	TYR	N-CA-C	5.16	119.73	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	VAL	N-CA-C	-5.16	105.68	110.53
1	B	201	ASP	OD1-CG-OD2	-5.16	110.52	122.90
1	A	268	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	B	223	TYR	N-CA-C	-5.14	105.68	111.28
1	B	137	ASP	CB-CG-OD1	5.14	130.21	118.40
1	C	220	TYR	N-CA-C	-5.13	105.77	111.36
1	A	302	ARG	CA-CB-CG	-5.11	103.87	114.10
1	B	261	LEU	N-CA-C	-5.11	101.07	109.40
1	B	255	LEU	N-CA-C	5.10	120.40	113.16
1	C	184	ILE	CB-CG1-CD1	-5.09	103.11	113.80
1	A	253	ASP	OD1-CG-OD2	-5.09	110.69	122.90
1	B	274	ASP	OD1-CG-OD2	-5.08	110.70	122.90
1	D	235	THR	OG1-CB-CG2	-5.08	99.14	109.30
1	C	232	VAL	N-CA-C	-5.08	101.10	108.36
1	C	217	ASP	N-CA-C	5.08	116.81	111.28
1	C	179	VAL	CA-C-N	-5.07	115.72	122.72
1	C	179	VAL	C-N-CA	-5.07	115.72	122.72
1	D	75	ASP	N-CA-C	-5.07	105.88	111.71
1	C	161	LYS	N-CA-C	-5.07	107.15	113.38
1	C	106	GLU	CB-CA-C	-5.05	102.26	110.85
1	C	105	GLU	CA-C-O	-5.04	114.41	120.10
1	C	128	ILE	CA-C-N	-5.04	116.05	123.00
1	C	128	ILE	C-N-CA	-5.04	116.05	123.00
1	D	201	ASP	OD1-CG-OD2	-5.04	110.81	122.90
1	A	286	ARG	CG-CD-NE	-5.02	100.95	112.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	62	ASP	Mainchain,Peptide
1	B	63	PHE	Mainchain,Peptide
1	C	63	PHE	Peptide
1	D	63	PHE	Peptide

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	2050	0	2055	82	1
1	B	2050	0	2054	88	2
1	C	2050	0	2054	77	3
1	D	2042	0	2051	62	3
2	A	232	0	0	23	2
2	B	215	0	0	25	1
2	C	199	0	0	32	1
2	D	235	0	0	21	1
All	All	9073	0	8214	264	7

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 16.

All (264) 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:D:139:MET:SD	1:D:139:MET:CE	2.03	1.46
1:B:104:MET:SD	1:B:104:MET:CE	2.06	1.40
1:B:175:LYS:HG2	2:B:492:HOH:O	1.12	1.26
1:B:175:LYS:HB2	2:B:506:HOH:O	1.13	1.26
1:D:175:LYS:HG2	2:D:526:HOH:O	1.34	1.22
1:A:173:SER:HB2	2:A:534:HOH:O	1.05	1.22
1:A:212:VAL:CG2	2:B:507:HOH:O	1.86	1.22
1:B:152:VAL:HG21	1:C:63:PHE:CE1	1.80	1.16
1:D:63:PHE:CE2	2:D:460:HOH:O	2.00	1.14
1:A:212:VAL:HB	2:B:507:HOH:O	1.51	1.11
1:A:176:GLY:O	1:A:177:ASP:HB3	1.40	1.11
1:D:286:ARG:HG2	2:D:446:HOH:O	1.49	1.11
1:B:143:LYS:CE	2:B:518:HOH:O	1.98	1.10
1:B:161:LYS:HD2	1:C:67:TYR:CE2	1.67	1.10
1:D:269:GLU:OE2	2:D:447:HOH:O	1.65	1.10
1:A:207:LYS:HG2	2:A:408:HOH:O	1.48	1.10
1:D:144:GLU:OE1	2:D:351:HOH:O	1.67	1.09
1:D:204:GLU:HG3	2:D:513:HOH:O	1.53	1.07
1:A:115:ASP:HB3	2:A:536:HOH:O	1.55	1.07
1:C:154:SER:HB3	2:C:499:HOH:O	1.61	1.01
1:C:164:GLU:OE2	2:C:458:HOH:O	1.78	1.01
1:B:62:ASP:N	1:B:67:TYR:CD2	2.27	1.01
1:C:67:TYR:HD1	2:C:412:HOH:O	1.44	1.00
1:B:143:LYS:HE3	2:B:518:HOH:O	1.59	1.00
1:B:161:LYS:CD	1:C:67:TYR:CE2	2.45	0.98
1:A:79:LYS:HB2	1:A:79:LYS:HZ2	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:TYR:CD1	2:C:412:HOH:O	2.13	0.97
1:C:66:TYR:CE1	2:C:415:HOH:O	2.19	0.95
1:B:152:VAL:CG2	1:C:63:PHE:CE1	2.50	0.95
1:D:153:LEU:H	1:D:199:ASN:HD21	1.15	0.94
1:A:207:LYS:NZ	2:A:344:HOH:O	2.00	0.94
1:A:79:LYS:NZ	1:A:79:LYS:CB	2.32	0.91
1:C:302:ARG:NE	2:C:369:HOH:O	1.95	0.90
1:D:63:PHE:CZ	2:D:460:HOH:O	2.17	0.90
2:A:510:HOH:O	1:B:64:SER:HB2	1.71	0.90
1:B:161:LYS:HD2	1:C:67:TYR:HE2	1.14	0.89
1:C:134:TYR:CB	2:C:494:HOH:O	2.21	0.89
1:A:79:LYS:HZ2	1:A:79:LYS:CB	1.85	0.88
1:C:62:ASP:N	2:C:464:HOH:O	2.06	0.87
1:B:152:VAL:HG11	1:C:63:PHE:CE1	2.11	0.86
1:B:174:GLU:OE1	2:B:399:HOH:O	1.92	0.85
1:C:190:LEU:HD23	2:C:401:HOH:O	1.76	0.85
1:D:220:TYR:CZ	1:D:224:ARG:HD3	2.12	0.85
1:C:199:ASN:H	1:C:199:ASN:HD22	1.26	0.84
1:D:224:ARG:NH1	2:D:530:HOH:O	2.08	0.84
1:C:115:ASP:OD2	2:C:491:HOH:O	1.94	0.84
1:C:134:TYR:HB3	2:C:494:HOH:O	1.75	0.83
1:A:176:GLY:O	1:A:177:ASP:CB	2.16	0.83
1:C:201:ASP:OD1	2:C:471:HOH:O	1.96	0.82
1:A:115:ASP:CB	2:A:536:HOH:O	2.18	0.82
1:D:199:ASN:HD22	1:D:199:ASN:H	1.28	0.82
1:B:190:LEU:C	1:B:190:LEU:HD23	2.06	0.81
1:A:63:PHE:HZ	1:D:152:VAL:HG12	1.46	0.80
1:B:81:LYS:HE2	1:B:88:LEU:HD12	1.64	0.79
1:C:281:LEU:HD13	1:C:281:LEU:C	2.08	0.79
1:D:224:ARG:HD2	2:D:530:HOH:O	1.84	0.78
1:B:152:VAL:CG1	1:C:63:PHE:HE1	1.96	0.78
1:A:66:TYR:OH	2:A:359:HOH:O	2.01	0.78
1:A:63:PHE:HZ	1:D:152:VAL:CG1	1.96	0.78
1:C:220:TYR:CZ	1:C:224:ARG:HD2	2.19	0.78
1:B:161:LYS:NZ	1:C:67:TYR:CE1	2.50	0.77
1:B:175:LYS:CG	2:B:492:HOH:O	1.86	0.77
1:C:66:TYR:HE1	2:C:415:HOH:O	1.60	0.77
1:B:152:VAL:HG11	1:C:63:PHE:HE1	1.45	0.77
1:B:85:GLU:OE1	1:B:110:LYS:NZ	2.17	0.76
1:B:153:LEU:H	1:B:199:ASN:HD21	1.30	0.76
1:C:63:PHE:CA	1:C:64:SER:OG	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LYS:O	2:C:346:HOH:O	2.05	0.75
1:D:144:GLU:OE1	2:D:424:HOH:O	2.05	0.74
1:A:211:GLU:OE2	2:A:530:HOH:O	2.05	0.74
1:A:212:VAL:CB	2:B:507:HOH:O	1.98	0.74
1:A:199:ASN:H	1:A:199:ASN:HD22	1.35	0.73
1:C:153:LEU:H	1:C:199:ASN:HD21	1.36	0.73
1:B:144:GLU:CD	2:B:460:HOH:O	2.32	0.73
1:B:175:LYS:CG	2:B:506:HOH:O	2.25	0.73
1:A:159:ILE:HD13	1:B:62:ASP:HB2	1.71	0.72
1:A:115:ASP:CG	2:A:536:HOH:O	2.33	0.72
1:B:139:MET:HE3	2:B:452:HOH:O	1.89	0.72
1:D:142:GLN:HE22	1:D:249:VAL:H	1.38	0.72
1:D:208:ARG:O	1:D:212:VAL:HG23	1.89	0.72
1:B:70:TYR:HE1	1:B:74:ARG:HH21	1.38	0.72
1:A:145:GLU:OE1	2:A:475:HOH:O	2.08	0.71
1:B:161:LYS:CD	1:C:67:TYR:HE2	1.92	0.71
1:A:70:TYR:HE2	1:A:74:ARG:NH2	1.88	0.71
1:B:175:LYS:CB	2:B:506:HOH:O	1.87	0.71
1:C:161:LYS:HE3	2:C:500:HOH:O	1.90	0.70
1:C:168:ARG:HD3	1:C:169:TYR:CZ	2.26	0.70
1:A:63:PHE:CZ	1:D:152:VAL:HG12	2.27	0.70
1:B:166:PHE:CD2	1:B:174:GLU:HG2	2.25	0.70
1:A:79:LYS:NZ	1:A:79:LYS:HB3	2.07	0.70
1:B:152:VAL:CB	1:C:63:PHE:HE1	2.04	0.69
1:C:302:ARG:NH2	2:C:369:HOH:O	2.26	0.69
1:C:71:GLU:OE2	2:C:490:HOH:O	2.11	0.68
1:C:217:ASP:OD1	2:C:503:HOH:O	2.10	0.68
1:A:153:LEU:H	1:A:199:ASN:HD21	1.38	0.68
1:A:212:VAL:HG21	2:B:507:HOH:O	1.63	0.68
1:B:161:LYS:NZ	2:B:463:HOH:O	2.26	0.67
1:B:175:LYS:HG3	2:B:506:HOH:O	1.91	0.67
1:A:220:TYR:CZ	1:A:224:ARG:HD2	2.29	0.66
1:C:175:LYS:HG2	2:D:537:HOH:O	1.95	0.66
1:D:102:ILE:HB	1:D:107:ILE:HD12	1.76	0.66
1:B:63:PHE:CD2	1:B:67:TYR:HD1	2.14	0.65
1:B:178:LEU:HD12	2:B:456:HOH:O	1.95	0.65
1:C:63:PHE:N	1:C:64:SER:OG	2.29	0.65
1:A:82:ILE:CD1	1:D:198:LEU:HD21	2.27	0.65
1:A:74:ARG:NH1	1:D:161:LYS:HD2	2.11	0.65
1:A:85:GLU:OE1	1:A:110:LYS:NZ	2.29	0.65
1:A:63:PHE:CZ	1:D:152:VAL:CG1	2.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:HB3	1:A:79:LYS:HZ3	1.62	0.64
1:B:150:ALA:H	1:B:162:GLN:NE2	1.96	0.64
1:D:144:GLU:CD	2:D:424:HOH:O	2.41	0.64
1:A:277:ARG:HB2	1:B:240:GLY:HA3	1.79	0.63
1:D:204:GLU:CD	2:D:471:HOH:O	2.41	0.63
1:B:152:VAL:CB	1:C:63:PHE:CE1	2.81	0.63
2:B:463:HOH:O	1:C:67:TYR:CE1	2.50	0.63
1:C:204:GLU:HB2	2:C:497:HOH:O	1.99	0.63
1:B:142:GLN:HE22	1:B:249:VAL:H	1.47	0.62
1:C:63:PHE:HD2	1:C:67:TYR:HB2	1.63	0.62
1:D:204:GLU:CG	2:D:471:HOH:O	2.48	0.62
1:C:190:LEU:CD2	2:C:401:HOH:O	2.40	0.62
1:A:175:LYS:HE2	1:B:126:SER:OG	2.01	0.61
1:A:207:LYS:CG	2:A:408:HOH:O	2.25	0.61
1:C:85:GLU:OE1	1:C:110:LYS:NZ	2.28	0.61
1:A:150:ALA:H	1:A:162:GLN:NE2	1.98	0.61
1:D:268:ARG:HD3	2:D:529:HOH:O	1.99	0.61
1:A:82:ILE:HD11	1:D:198:LEU:HD21	1.83	0.60
1:B:63:PHE:CD2	1:B:67:TYR:CD1	2.89	0.60
1:D:88:LEU:HD13	2:D:536:HOH:O	2.00	0.60
1:A:79:LYS:CB	1:A:79:LYS:HZ3	2.14	0.60
1:B:143:LYS:HE2	2:B:518:HOH:O	1.84	0.60
1:A:199:ASN:HD22	1:A:199:ASN:N	2.00	0.59
1:B:164:GLU:CD	2:B:475:HOH:O	2.45	0.59
1:C:147:PRO:HG3	2:C:458:HOH:O	2.03	0.59
1:B:79:LYS:HZ2	1:B:79:LYS:HB2	1.66	0.59
1:D:98:GLU:HG2	1:D:123:ASP:HA	1.85	0.59
1:A:150:ALA:H	1:A:162:GLN:HE21	1.48	0.59
1:C:281:LEU:HD13	1:C:281:LEU:O	2.03	0.59
1:A:240:GLY:HA3	1:B:277:ARG:HB2	1.85	0.58
2:A:468:HOH:O	1:B:214:ARG:HG3	2.02	0.58
1:A:175:LYS:O	1:A:176:GLY:C	2.46	0.58
1:A:70:TYR:CE2	1:A:74:ARG:NH2	2.70	0.58
1:B:143:LYS:CD	2:B:518:HOH:O	2.44	0.58
1:B:152:VAL:CG2	1:C:63:PHE:CZ	2.86	0.58
1:B:152:VAL:HG21	1:C:63:PHE:CZ	2.38	0.58
1:A:159:ILE:CD1	1:B:62:ASP:HB2	2.35	0.57
1:B:199:ASN:HD22	1:B:199:ASN:H	1.52	0.57
1:A:190:LEU:HD23	1:A:190:LEU:C	2.28	0.57
1:B:62:ASP:N	1:B:67:TYR:HD2	1.95	0.57
1:C:281:LEU:C	1:C:281:LEU:CD1	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:HD2	1:A:169:TYR:CE1	2.40	0.56
1:B:152:VAL:CG1	1:C:63:PHE:CE1	2.80	0.56
1:A:74:ARG:HH12	1:D:161:LYS:HD2	1.69	0.56
1:B:79:LYS:CB	1:B:79:LYS:NZ	2.69	0.55
1:D:286:ARG:CD	2:D:446:HOH:O	2.53	0.55
1:D:286:ARG:CG	2:D:446:HOH:O	2.25	0.55
1:C:199:ASN:HD22	1:C:199:ASN:N	1.96	0.55
1:B:63:PHE:HD2	1:B:67:TYR:HB2	1.72	0.55
1:B:257:HIS:HD2	2:B:450:HOH:O	1.89	0.55
1:D:102:ILE:CG2	1:D:107:ILE:HD11	2.36	0.55
1:A:155:ASP:OD1	1:B:64:SER:CB	2.55	0.54
1:A:62:ASP:OD1	2:A:498:HOH:O	2.18	0.54
1:B:142:GLN:NE2	1:B:249:VAL:H	2.06	0.54
1:C:63:PHE:CD2	1:C:67:TYR:CG	2.96	0.54
1:B:96:ILE:HG21	1:B:119:LEU:HD22	1.90	0.53
1:D:96:ILE:HG21	1:D:119:LEU:HD22	1.90	0.53
2:A:510:HOH:O	1:B:65:THR:HG22	2.07	0.53
1:A:159:ILE:HD13	1:B:62:ASP:CB	2.38	0.53
1:B:164:GLU:OE2	2:B:475:HOH:O	2.19	0.53
1:C:286:ARG:NH1	2:C:368:HOH:O	2.41	0.53
1:C:225:ASN:HD21	1:C:229:ARG:HE	1.57	0.53
1:A:63:PHE:CD2	1:D:199:ASN:HB3	2.44	0.52
1:A:173:SER:CB	2:A:534:HOH:O	1.91	0.52
1:D:81:LYS:HE2	1:D:88:LEU:HD12	1.92	0.52
1:A:302:ARG:CZ	2:A:535:HOH:O	2.58	0.51
1:B:129:THR:HG23	1:B:302:ARG:HD2	1.93	0.51
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.76	0.51
1:A:220:TYR:CE2	1:A:224:ARG:HD2	2.46	0.51
1:D:247:ARG:HD3	2:D:388:HOH:O	2.10	0.50
1:D:70:TYR:CE1	1:D:74:ARG:HD3	2.45	0.50
1:A:129:THR:HG23	1:A:302:ARG:HD2	1.93	0.50
1:C:220:TYR:CE2	1:C:224:ARG:HD2	2.46	0.50
1:A:168:ARG:HD3	1:A:169:TYR:CZ	2.47	0.50
1:D:199:ASN:HD22	1:D:199:ASN:N	2.02	0.50
1:A:62:ASP:N	2:A:421:HOH:O	2.44	0.49
1:C:99:ARG:HG2	1:D:212:VAL:HG12	1.94	0.49
1:A:63:PHE:CZ	1:D:152:VAL:HG11	2.47	0.49
1:D:224:ARG:CD	2:D:530:HOH:O	2.51	0.49
1:C:63:PHE:CD2	1:C:67:TYR:CD2	3.00	0.49
1:B:190:LEU:HD23	1:B:190:LEU:O	2.12	0.49
1:C:214:ARG:HG3	2:C:498:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASP:OD1	1:B:64:SER:HB2	2.13	0.49
1:A:213:GLU:OE1	1:A:219:ARG:NH2	2.46	0.49
1:C:277:ARG:HB2	1:D:240:GLY:HA3	1.94	0.49
1:A:266:ASP:HA	1:A:293:TYR:HA	1.95	0.48
1:B:129:THR:CG2	1:B:302:ARG:HD2	2.43	0.48
1:B:134:TYR:OH	1:B:288:ARG:HD3	2.14	0.48
1:C:240:GLY:HA3	1:D:277:ARG:HB2	1.96	0.48
1:C:79:LYS:CB	1:C:79:LYS:NZ	2.77	0.48
1:C:134:TYR:HB2	2:C:494:HOH:O	1.99	0.48
1:B:152:VAL:HG11	1:C:63:PHE:CD1	2.47	0.48
1:B:152:VAL:HB	1:C:63:PHE:HE1	1.78	0.48
1:B:208:ARG:O	1:B:212:VAL:HG12	2.14	0.48
1:D:65:THR:HG21	1:D:97:SER:HB2	1.95	0.48
1:D:102:ILE:CG2	1:D:107:ILE:CD1	2.91	0.48
1:B:71:GLU:O	1:B:75:ASP:HB2	2.14	0.47
1:B:190:LEU:C	1:B:190:LEU:CD2	2.82	0.47
1:A:70:TYR:HE2	1:A:74:ARG:HH21	1.58	0.47
1:B:187:LEU:HD22	1:B:206:VAL:HG22	1.95	0.47
1:C:115:ASP:CG	2:C:491:HOH:O	2.51	0.47
1:A:155:ASP:OD1	1:B:64:SER:HB3	2.14	0.47
1:A:203:GLU:HG2	2:A:377:HOH:O	2.13	0.47
1:C:79:LYS:CB	1:C:79:LYS:HZ2	2.27	0.47
1:A:225:ASN:HD21	1:A:229:ARG:HE	1.63	0.47
1:A:184:ILE:CD1	1:A:219:ARG:HG2	2.45	0.47
1:D:156:GLU:OE2	2:D:352:HOH:O	2.20	0.46
1:B:143:LYS:HD3	2:B:518:HOH:O	2.12	0.46
1:C:210:ARG:NE	2:C:503:HOH:O	2.14	0.46
1:A:159:ILE:HD13	1:B:62:ASP:CG	2.41	0.46
1:A:288:ARG:HG2	2:A:532:HOH:O	2.15	0.46
1:C:212:VAL:HG23	1:C:213:GLU:HG3	1.97	0.46
1:B:156:GLU:HG3	1:B:157:TYR:CE1	2.50	0.46
1:C:115:ASP:HA	2:C:494:HOH:O	2.15	0.46
1:A:236:GLY:O	1:A:237:PHE:C	2.57	0.45
1:B:247:ARG:NH2	1:B:260:TYR:OH	2.50	0.45
1:C:150:ALA:H	1:C:162:GLN:NE2	2.14	0.45
1:A:168:ARG:CB	1:A:168:ARG:HH11	2.30	0.45
1:A:63:PHE:CE2	1:D:199:ASN:HB3	2.52	0.45
1:A:62:ASP:CG	2:A:498:HOH:O	2.60	0.45
1:A:100:LYS:O	2:A:321:HOH:O	2.20	0.44
1:A:123:ASP:OD2	1:B:235:THR:HG21	2.17	0.44
1:C:164:GLU:CD	2:C:474:HOH:O	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLU:HG3	1:D:99:ARG:HD2	1.98	0.44
1:A:63:PHE:HZ	1:D:152:VAL:HG11	1.76	0.43
1:A:207:LYS:O	1:A:211:GLU:HG3	2.19	0.43
1:D:142:GLN:NE2	1:D:249:VAL:H	2.10	0.43
1:B:245:VAL:HB	1:B:260:TYR:HB2	2.00	0.43
1:C:190:LEU:HD23	1:C:190:LEU:C	2.43	0.43
1:C:71:GLU:HB2	2:C:490:HOH:O	2.18	0.43
1:A:155:ASP:HB3	1:A:156:GLU:H	1.60	0.42
1:A:187:LEU:HD22	1:A:206:VAL:HG12	2.00	0.42
2:A:534:HOH:O	1:B:125:GLU:HB3	2.18	0.42
1:C:81:LYS:HE3	1:C:83:GLN:OE1	2.20	0.42
1:C:175:LYS:NZ	2:C:384:HOH:O	2.52	0.42
1:B:150:ALA:H	1:B:162:GLN:HE21	1.65	0.42
1:A:154:SER:O	1:A:155:ASP:CB	2.68	0.42
1:A:190:LEU:HD12	1:A:197:LEU:HD22	2.02	0.42
1:B:79:LYS:HB2	1:B:79:LYS:NZ	2.30	0.42
1:D:102:ILE:HG21	1:D:107:ILE:CD1	2.49	0.42
1:B:149:ILE:HB	1:B:162:GLN:HE21	1.85	0.42
1:D:178:LEU:N	1:D:178:LEU:HD12	2.34	0.42
1:D:214:ARG:HE	1:D:214:ARG:HB2	1.39	0.42
1:D:220:TYR:CE2	1:D:224:ARG:HD3	2.53	0.42
2:A:340:HOH:O	1:B:65:THR:CG2	2.67	0.41
1:C:126:SER:OG	1:D:175:LYS:HE3	2.19	0.41
1:A:63:PHE:CG	1:D:199:ASN:HB3	2.55	0.41
1:D:102:ILE:CB	1:D:107:ILE:HD12	2.49	0.41
1:C:302:ARG:CZ	2:C:369:HOH:O	2.43	0.41
1:D:111:ALA:HB2	1:D:117:LEU:HD23	2.02	0.41
1:B:81:LYS:CE	1:B:88:LEU:HD12	2.42	0.41
1:B:204:GLU:HB2	2:B:413:HOH:O	2.21	0.41
1:D:252:VAL:HA	1:D:255:LEU:HD22	2.03	0.41
1:B:302:ARG:HH11	1:B:302:ARG:HD3	1.75	0.40
1:C:164:GLU:HB2	2:C:317:HOH:O	2.20	0.40
1:D:96:ILE:CG2	1:D:119:LEU:HD22	2.52	0.40

All (7) 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:224:ARG:NE	1:C:203:GLU:OE1[3_545]	1.97	0.23
1:D:224:ARG:NH2	2:A:413:HOH:O[3_556]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:OE2	1:D:224:ARG:NH2[3_546]	2.06	0.14
1:C:210:ARG:NH2	2:B:517:HOH:O[3_555]	2.07	0.13
1:D:269:GLU:OE2	2:A:529:HOH:O[3_556]	2.13	0.07
1:B:224:ARG:CD	1:C:203:GLU:OE1[3_545]	2.13	0.07
2:C:429:HOH:O	2:D:423:HOH:O[2_565]	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	242/305 (79%)	233 (96%)	6 (2%)	3 (1%)	10	6
1	B	242/305 (79%)	233 (96%)	9 (4%)	0	100	100
1	C	242/305 (79%)	234 (97%)	7 (3%)	1 (0%)	30	27
1	D	241/305 (79%)	234 (97%)	7 (3%)	0	100	100
All	All	967/1220 (79%)	934 (97%)	29 (3%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLY
1	A	177	ASP
1	A	155	ASP
1	C	155	ASP

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	222/273 (81%)	205 (92%)	17 (8%)	12	8
1	B	222/273 (81%)	202 (91%)	20 (9%)	9	6
1	C	222/273 (81%)	200 (90%)	22 (10%)	7	4
1	D	221/273 (81%)	196 (89%)	25 (11%)	5	3
All	All	887/1092 (81%)	803 (90%)	84 (10%)	8	5

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	79	LYS
1	A	99	ARG
1	A	100	LYS
1	A	123	ASP
1	A	143	LYS
1	A	156	GLU
1	A	168	ARG
1	A	174	GLU
1	A	177	ASP
1	A	197	LEU
1	A	199	ASN
1	A	261	LEU
1	A	295	LYS
1	A	301	GLU
1	A	302	ARG
1	A	304	LYS
1	B	62	ASP
1	B	63	PHE
1	B	64	SER
1	B	65	THR
1	B	66	TYR
1	B	79	LYS
1	B	139	MET
1	B	143	LYS
1	B	152	VAL
1	B	174	GLU
1	B	183	LEU
1	B	192	LEU
1	B	196	ASN
1	B	199	ASN
1	B	207	LYS
1	B	212	VAL

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Mol	Chain	Res	Type
1	B	281	LEU
1	B	295	LYS
1	B	298	LEU
1	B	302	ARG
1	C	62	ASP
1	C	66	TYR
1	C	71	GLU
1	C	79	LYS
1	C	82	ILE
1	C	103	ARG
1	C	139	MET
1	C	141	GLU
1	C	143	LYS
1	C	145	GLU
1	C	155	ASP
1	C	192	LEU
1	C	196	ASN
1	C	197	LEU
1	C	199	ASN
1	C	203	GLU
1	C	207	LYS
1	C	212	VAL
1	C	275	LEU
1	C	295	LYS
1	C	298	LEU
1	C	301	GLU
1	D	65	THR
1	D	66	TYR
1	D	79	LYS
1	D	98	GLU
1	D	100	LYS
1	D	103	ARG
1	D	139	MET
1	D	142	GLN
1	D	143	LYS
1	D	145	GLU
1	D	162	GLN
1	D	179	VAL
1	D	183	LEU
1	D	192	LEU
1	D	196	ASN
1	D	199	ASN

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Mol	Chain	Res	Type
1	D	203	GLU
1	D	204	GLU
1	D	207	LYS
1	D	214	ARG
1	D	215	ASN
1	D	235	THR
1	D	255	LEU
1	D	295	LYS
1	D	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	162	GLN
1	A	196	ASN
1	A	199	ASN
1	A	225	ASN
1	A	257	HIS
1	A	283	GLN
1	B	142	GLN
1	B	162	GLN
1	B	199	ASN
1	C	78	ASN
1	C	162	GLN
1	C	199	ASN
1	C	225	ASN
1	C	284	ASN
1	D	142	GLN
1	D	162	GLN
1	D	199	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	244/305 (80%)	0.22	9 (3%) 45 44	19, 27, 38, 50	0
1	B	244/305 (80%)	0.21	8 (3%) 49 48	19, 27, 38, 52	0
1	C	244/305 (80%)	0.24	4 (1%) 70 70	19, 27, 38, 50	0
1	D	243/305 (79%)	0.11	4 (1%) 70 70	18, 27, 38, 51	0
All	All	975/1220 (79%)	0.20	25 (2%) 57 56	18, 27, 38, 52	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	PHE	11.4
1	B	63	PHE	5.8
1	C	67	TYR	5.2
1	D	63	PHE	4.9
1	C	66	TYR	4.2
1	A	63	PHE	3.9
1	B	64	SER	3.4
1	B	67	TYR	3.3
1	A	207	LYS	3.1
1	B	66	TYR	3.0
1	A	154	SER	2.9
1	B	62	ASP	2.8
1	D	67	TYR	2.8
1	C	203	GLU	2.4
1	B	196	ASN	2.3
1	D	177	ASP	2.3
1	A	206	VAL	2.2
1	A	212	VAL	2.2
1	B	81	LYS	2.2
1	A	123	ASP	2.2
1	D	144	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	161	LYS	2.1
1	A	203	GLU	2.0
1	A	75	ASP	2.0
1	A	103	ARG	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.