



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:22 AM UTC

PDB ID : 1DOF / pdb_00001dof
Title : THE CRYSTAL STRUCTURE OF ADENYLOSUCCINATE LYASE FROM
PYROBACULUM AEROPHILUM: INSIGHTS INTO THERMAL STABIL-
ITY AND HUMAN PATHOLOGY
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Deposited on : 1999-12-20
Resolution : 2.10 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

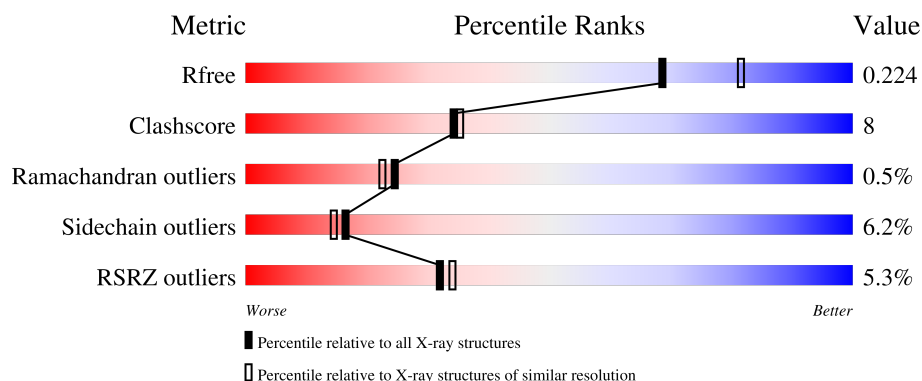
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	403	4% 74% 17% • •
1	B	403	7% 69% 22% • • •
1	C	403	4% 69% 21% 5% • •
1	D	403	5% 68% 22% • • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12664 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 ADENYLOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2977	1900	522	543	12			
1	B	385	Total	C	N	O	S	0	0	0
			2961	1890	520	539	12			
1	C	385	Total	C	N	O	S	0	0	0
			2963	1892	518	541	12			
1	D	385	Total	C	N	O	S	0	0	0
			2971	1896	520	543	12			

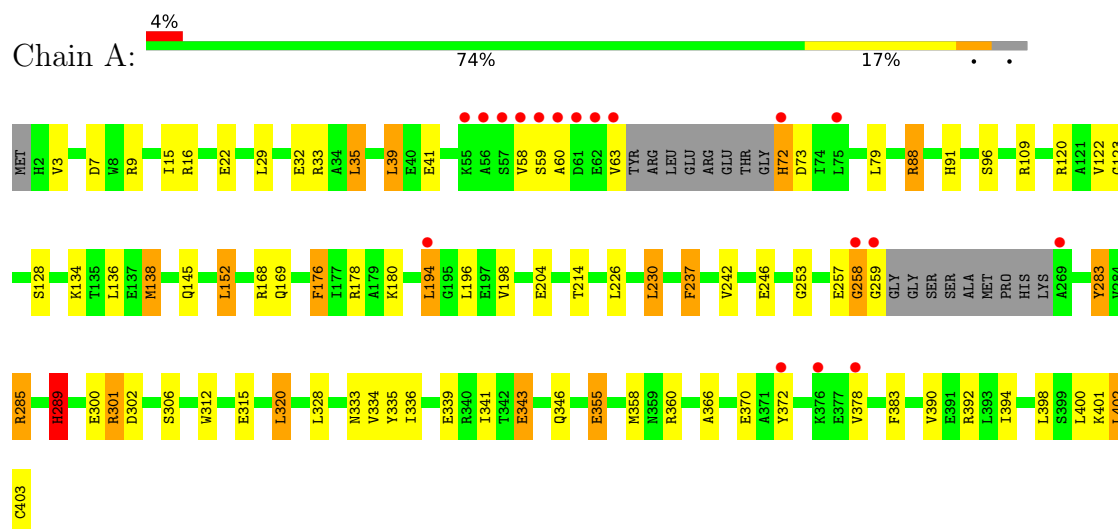
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	197	Total	O	0	0
			197	197		
2	B	198	Total	O	0	0
			198	198		
2	C	202	Total	O	0	0
			202	202		
2	D	195	Total	O	0	0
			195	195		

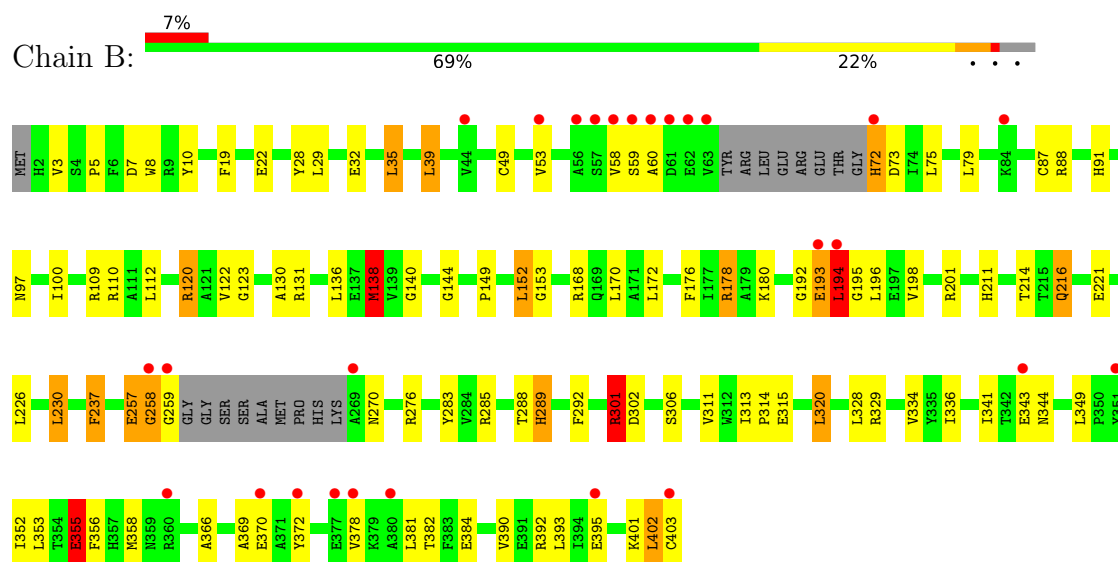
3 Residue-property plots [i](#)

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: ADENYLOSUCCINATE LYASE

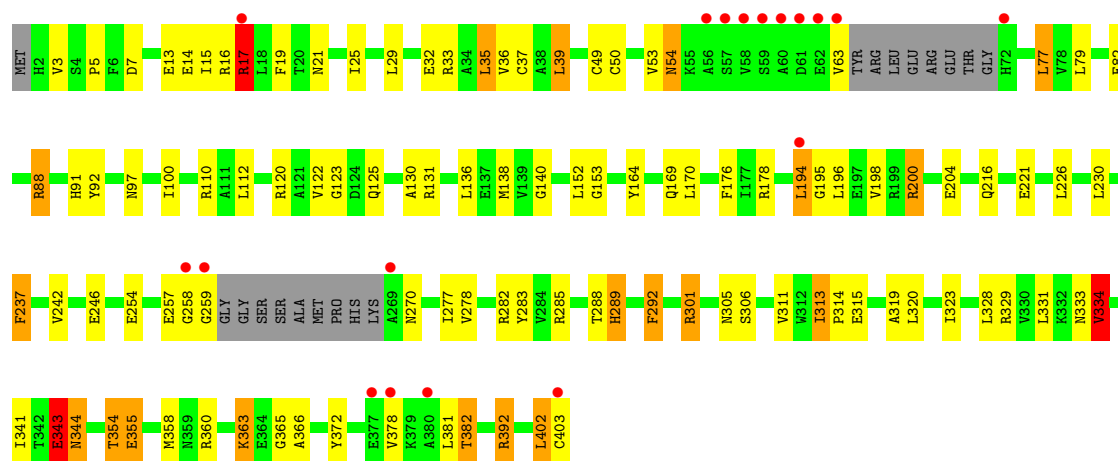


• Molecule 1: ADENYLOSUCCINATE LYASE

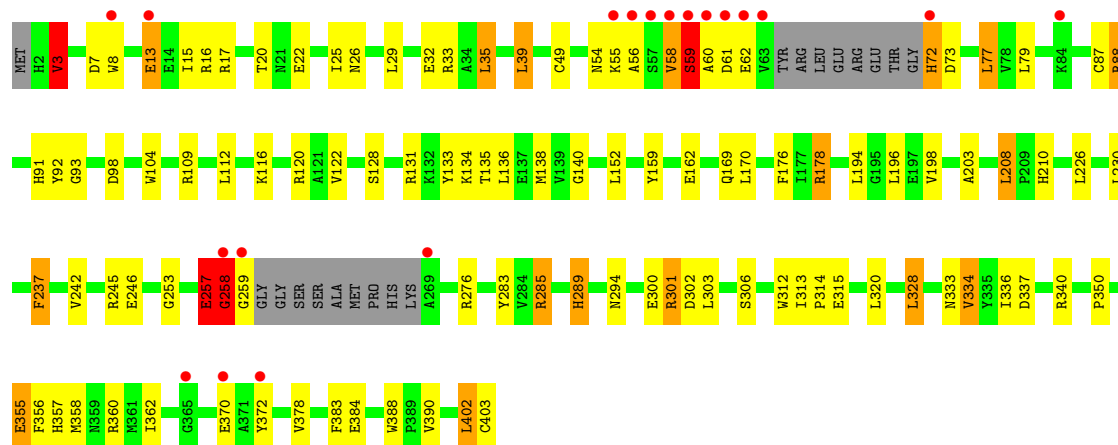


• Molecule 1: ADENYLOSUCCINATE LYASE





• Molecule 1: ADENYLOSUCCINATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.62Å 150.31Å 173.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 99.8 (50.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.41 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.245 0.187 , 0.224	Depositor DCC
R_{free} test set	5017 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.45$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12664	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 46.91 % 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 1.0701e-04. 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	0.98	7/3028 (0.2%)	1.77	54/4109 (1.3%)
1	B	1.12	10/3012 (0.3%)	1.86	53/4090 (1.3%)
1	C	1.12	5/3014 (0.2%)	1.89	59/4093 (1.4%)
1	D	1.11	13/3022 (0.4%)	2.30	76/4102 (1.9%)
All	All	1.09	35/12076 (0.3%)	1.96	242/16394 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	344	ASN	N-CA	26.56	1.78	1.46
1	B	259	GLY	N-CA	-22.25	1.09	1.45
1	D	59	SER	C-N	21.95	1.62	1.33
1	C	259	GLY	N-CA	-17.02	1.18	1.45
1	C	258	GLY	CA-C	-16.81	1.28	1.51
1	B	258	GLY	CA-C	-16.38	1.28	1.51
1	B	73	ASP	N-CA	-15.98	1.27	1.46
1	B	258	GLY	C-N	-12.81	1.15	1.33
1	D	257	GLU	C-N	11.90	1.50	1.33
1	A	73	ASP	N-CA	-11.89	1.31	1.46
1	A	259	GLY	N-CA	-9.72	1.29	1.45
1	A	258	GLY	C-N	-9.13	1.20	1.33
1	D	59	SER	N-CA	9.09	1.57	1.46
1	A	194	LEU	N-CA	9.02	1.58	1.46
1	B	72	HIS	CA-C	-8.61	1.34	1.52
1	C	258	GLY	C-N	-8.44	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	ASN	CA-C	8.03	1.63	1.52
1	D	55	LYS	N-CA	7.68	1.55	1.46
1	B	72	HIS	C-N	-7.60	1.23	1.33
1	D	259	GLY	N-CA	-7.39	1.33	1.45
1	B	393	LEU	N-CA	7.35	1.55	1.46
1	D	258	GLY	CA-C	-7.22	1.41	1.51
1	B	193	GLU	C-N	-6.64	1.22	1.33
1	A	72	HIS	CA-C	-6.42	1.39	1.52
1	D	54	ASN	C-N	6.33	1.42	1.33
1	A	72	HIS	C-N	-6.31	1.25	1.33
1	C	194	LEU	N-CA	6.30	1.53	1.46
1	D	58	VAL	C-N	5.75	1.41	1.33
1	D	72	HIS	C-N	-5.73	1.27	1.33
1	A	178	ARG	CD-NE	-5.50	1.38	1.46
1	D	73	ASP	N-CA	-5.39	1.39	1.46
1	D	58	VAL	CA-C	5.31	1.59	1.52
1	D	109	ARG	NE-CZ	-5.24	1.27	1.33
1	B	344	ASN	N-CA	5.07	1.52	1.46
1	B	178	ARG	CD-NE	-5.06	1.39	1.46

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	ARG	CD-NE-CZ	38.31	178.03	124.40
1	D	59	SER	O-C-N	35.34	163.20	123.27
1	B	258	GLY	O-C-N	31.31	163.40	122.70
1	D	59	SER	CA-C-N	-29.52	79.94	120.38
1	D	59	SER	C-N-CA	-29.52	79.94	120.38
1	D	109	ARG	CD-NE-CZ	28.06	163.68	124.40
1	D	257	GLU	CA-C-N	-24.63	73.14	121.41
1	D	257	GLU	C-N-CA	-24.63	73.14	121.41
1	C	258	GLY	O-C-N	22.64	152.13	122.70
1	A	178	ARG	CD-NE-CZ	21.68	154.75	124.40
1	B	178	ARG	CD-NE-CZ	21.62	154.67	124.40
1	D	258	GLY	O-C-N	20.78	149.72	122.70
1	D	72	HIS	CA-C-N	19.10	151.56	121.19
1	D	72	HIS	C-N-CA	19.10	151.56	121.19
1	B	193	GLU	N-CA-C	17.76	132.82	111.33
1	C	343	GLU	CA-C-N	-17.17	97.27	120.28
1	C	343	GLU	C-N-CA	-17.17	97.27	120.28
1	A	258	GLY	O-C-N	14.85	142.01	122.70
1	C	344	ASN	N-CA-C	14.39	126.96	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	LEU	N-CA-CB	-14.30	88.44	110.46
1	C	392	ARG	CD-NE-CZ	12.78	142.29	124.40
1	C	329	ARG	CD-NE-CZ	11.72	140.81	124.40
1	D	33	ARG	NE-CZ-NH2	11.66	129.70	119.20
1	D	73	ASP	N-CA-CB	11.33	128.98	109.72
1	C	237	PHE	CA-CB-CG	-10.70	103.10	113.80
1	D	370	GLU	CA-CB-CG	10.47	135.04	114.10
1	C	178	ARG	CD-NE-CZ	10.07	138.50	124.40
1	B	72	HIS	O-C-N	10.01	139.01	123.00
1	B	109	ARG	CD-NE-CZ	10.00	138.41	124.40
1	A	237	PHE	CA-CB-CG	-9.87	103.93	113.80
1	A	109	ARG	NE-CZ-NH2	-9.79	110.39	119.20
1	C	194	LEU	N-CA-C	-9.68	100.39	112.88
1	A	176	PHE	CA-CB-CG	-9.52	104.28	113.80
1	D	258	GLY	N-CA-C	-9.41	90.89	113.18
1	C	200	ARG	CD-NE-CZ	9.36	137.50	124.40
1	A	169	GLN	OE1-CD-NE2	-9.34	113.26	122.60
1	C	329	ARG	NE-CZ-NH2	-9.32	110.81	119.20
1	B	194	LEU	N-CA-C	-9.11	102.31	113.15
1	D	176	PHE	CA-CB-CG	-9.11	104.69	113.80
1	D	237	PHE	CA-CB-CG	-8.99	104.81	113.80
1	B	192	GLY	CA-C-N	-8.91	108.17	120.38
1	B	192	GLY	C-N-CA	-8.91	108.17	120.38
1	A	109	ARG	CD-NE-CZ	8.79	136.71	124.40
1	B	237	PHE	CA-CB-CG	-8.75	105.05	113.80
1	D	306	SER	N-CA-C	8.62	120.59	111.03
1	C	216	GLN	OE1-CD-NE2	-8.61	113.99	122.60
1	C	289	HIS	CA-CB-CG	-8.51	105.29	113.80
1	D	54	ASN	O-C-N	-8.35	113.27	122.12
1	C	88	ARG	NE-CZ-NH2	8.31	126.68	119.20
1	B	289	HIS	CA-CB-CG	-8.12	105.68	113.80
1	C	17	ARG	NE-CZ-NH1	8.04	129.54	121.50
1	C	402	LEU	N-CA-C	8.02	122.50	109.59
1	D	289	HIS	CA-CB-CG	-8.01	105.79	113.80
1	A	72	HIS	O-C-N	7.91	135.66	123.00
1	B	329	ARG	NE-CZ-NH2	-7.79	112.19	119.20
1	D	258	GLY	CA-C-N	7.75	135.64	121.70
1	D	258	GLY	C-N-CA	7.75	135.64	121.70
1	D	362	ILE	CA-C-O	-7.74	112.96	121.17
1	D	169	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	D	378	VAL	N-CA-C	7.70	119.05	108.89
1	C	306	SER	N-CA-C	7.66	119.32	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	GLY	N-CA-C	-7.56	102.39	112.82
1	C	176	PHE	CA-CB-CG	-7.49	106.31	113.80
1	A	390	VAL	CA-C-O	-7.48	112.56	120.57
1	A	333	ASN	CA-CB-CG	-7.43	105.17	112.60
1	A	402	LEU	N-CA-C	7.40	121.90	109.76
1	B	193	GLU	CA-C-O	-7.32	112.73	120.63
1	A	306	SER	N-CA-C	7.31	119.15	111.03
1	D	131	ARG	NE-CZ-NH2	7.24	125.71	119.20
1	C	313	ILE	CA-C-O	7.22	123.53	118.69
1	C	344	ASN	N-CA-CB	-7.21	99.53	110.12
1	B	138	MET	CA-C-O	-7.19	113.76	121.45
1	A	168	ARG	NE-CZ-NH1	7.17	128.67	121.50
1	D	402	LEU	CB-CA-C	-7.12	96.33	109.37
1	C	292	PHE	CA-CB-CG	-7.11	106.69	113.80
1	B	392	ARG	CA-C-N	-7.09	110.97	120.54
1	B	392	ARG	C-N-CA	-7.09	110.97	120.54
1	A	33	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	D	357	HIS	CA-C-O	6.91	127.74	120.42
1	A	96	SER	CA-C-O	-6.83	113.25	120.63
1	C	305	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	C	313	ILE	O-C-N	-6.81	116.06	120.42
1	C	334	VAL	CB-CA-C	-6.80	101.08	111.08
1	A	315	GLU	CB-CG-CD	6.79	124.14	112.60
1	C	131	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	D	315	GLU	CB-CG-CD	6.73	124.05	112.60
1	B	176	PHE	CA-CB-CG	-6.71	107.08	113.80
1	C	97	ASN	CA-CB-CG	-6.70	105.90	112.60
1	C	100	ILE	CA-C-O	-6.68	114.09	121.17
1	B	270	ASN	N-CA-CB	6.64	120.12	109.90
1	B	109	ARG	NE-CZ-NH2	-6.63	113.23	119.20
1	A	289	HIS	CA-CB-CG	-6.61	107.19	113.80
1	C	378	VAL	N-CA-C	6.60	117.60	108.89
1	B	140	GLY	N-CA-C	-6.56	103.77	112.82
1	A	370	GLU	CA-CB-CG	6.54	127.18	114.10
1	D	26	ASN	CA-CB-CG	-6.54	106.06	112.60
1	D	328	LEU	CA-C-N	6.53	128.93	120.44
1	D	328	LEU	C-N-CA	6.53	128.93	120.44
1	B	390	VAL	N-CA-CB	6.44	119.29	110.54
1	A	258	GLY	CA-C-N	6.42	133.25	121.70
1	A	258	GLY	C-N-CA	6.42	133.25	121.70
1	C	120	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	C	315	GLU	CB-CG-CD	6.42	123.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLU	O-C-N	-6.38	115.36	122.12
1	B	258	GLY	CA-C-N	6.34	133.11	121.70
1	B	258	GLY	C-N-CA	6.34	133.11	121.70
1	D	104	TRP	CA-C-O	-6.33	113.84	120.55
1	C	382	THR	CA-C-O	-6.33	113.90	120.99
1	C	360	ARG	CA-C-N	6.28	128.69	120.28
1	C	360	ARG	C-N-CA	6.28	128.69	120.28
1	A	15	ILE	CB-CG1-CD1	6.26	126.94	113.80
1	B	315	GLU	CB-CG-CD	6.22	123.17	112.60
1	B	306	SER	N-CA-C	6.20	124.01	110.80
1	D	55	LYS	O-C-N	6.20	129.22	122.15
1	D	300	GLU	CA-C-N	6.17	133.33	121.54
1	D	300	GLU	C-N-CA	6.17	133.33	121.54
1	A	134	LYS	CA-C-O	-6.13	113.34	120.20
1	A	88	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	383	PHE	CA-CB-CG	-6.01	107.79	113.80
1	C	270	ASN	N-CA-CB	5.99	119.19	110.32
1	D	378	VAL	CA-C-O	5.95	127.63	120.85
1	B	97	ASN	CA-CB-CG	-5.93	106.67	112.60
1	A	392	ARG	CD-NE-CZ	-5.93	116.10	124.40
1	B	352	ILE	N-CA-CB	-5.90	103.48	112.15
1	C	257	GLU	CB-CA-C	-5.87	98.66	109.46
1	D	128	SER	O-C-N	-5.87	115.90	122.12
1	B	257	GLU	CB-CA-C	-5.84	98.71	109.46
1	A	285	ARG	CA-C-O	-5.84	113.26	119.97
1	B	392	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	D	253	GLY	N-CA-C	5.81	121.96	113.48
1	D	88	ARG	CD-NE-CZ	-5.79	116.30	124.40
1	B	110	ARG	NE-CZ-NH1	5.79	127.28	121.50
1	C	365	GLY	N-CA-C	5.79	122.73	115.21
1	D	58	VAL	CB-CA-C	5.78	119.40	110.50
1	B	402	LEU	CB-CA-C	-5.78	98.80	109.37
1	B	378	VAL	N-CA-C	5.77	117.06	108.23
1	A	259	GLY	N-CA-C	-5.76	96.59	113.30
1	D	55	LYS	CA-C-N	5.75	128.87	120.71
1	D	55	LYS	C-N-CA	5.75	128.87	120.71
1	B	393	LEU	N-CA-C	5.74	118.00	111.11
1	D	178	ARG	N-CA-C	5.73	118.40	109.52
1	C	343	GLU	N-CA-CB	5.72	118.37	110.07
1	D	383	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	401	LYS	CA-C-O	-5.70	114.48	120.80
1	B	401	LYS	CA-C-O	-5.69	114.49	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	GLY	N-CA-C	-5.69	104.97	112.82
1	B	100	ILE	CA-C-O	-5.67	115.16	121.17
1	D	390	VAL	CA-C-O	-5.66	114.51	120.57
1	C	301	ARG	N-CA-CB	5.66	120.05	110.49
1	C	54	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	B	53	VAL	CA-C-O	-5.62	114.89	120.85
1	B	221	GLU	N-CA-C	-5.62	105.15	111.28
1	D	334	VAL	CB-CA-C	-5.62	102.82	111.08
1	A	378	VAL	N-CA-C	5.62	116.30	108.89
1	B	10	TYR	CA-C-O	-5.60	114.27	120.38
1	D	159	TYR	O-C-N	-5.58	116.21	122.12
1	C	278	VAL	CA-C-O	-5.54	115.29	121.17
1	C	354	THR	CB-CA-C	-5.54	101.55	110.74
1	C	195	GLY	CA-C-O	5.53	126.97	121.00
1	B	301	ARG	N-CA-CB	5.53	119.83	110.49
1	A	390	VAL	N-CA-CB	5.51	120.07	110.65
1	C	164	TYR	CA-C-O	-5.51	114.71	120.55
1	D	20	THR	N-CA-C	-5.51	103.64	110.41
1	D	128	SER	N-CA-CB	-5.50	102.03	110.12
1	D	58	VAL	O-C-N	-5.50	117.21	123.10
1	D	210	HIS	CA-C-O	-5.50	114.67	121.11
1	D	402	LEU	N-CA-C	5.49	118.68	109.95
1	C	19	PHE	CA-CB-CG	-5.49	108.31	113.80
1	D	56	ALA	N-CA-C	5.48	118.17	110.23
1	D	355	GLU	OE1-CD-OE2	5.47	136.03	122.90
1	D	128	SER	CA-C-O	5.46	126.34	120.55
1	B	168	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	28	TYR	CA-C-O	-5.45	114.77	120.55
1	A	128	SER	O-C-N	-5.44	116.36	122.12
1	D	302	ASP	CA-C-O	-5.42	115.29	121.58
1	C	329	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	D	245	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	D	276	ARG	CD-NE-CZ	5.40	131.96	124.40
1	C	15	ILE	N-CA-C	-5.40	106.43	111.45
1	A	346	GLN	OE1-CD-NE2	-5.39	117.20	122.60
1	A	400	LEU	CA-C-O	-5.39	115.68	121.56
1	A	128	SER	CA-CB-OG	-5.39	100.32	111.10
1	D	333	ASN	CA-CB-CG	-5.39	107.21	112.60
1	B	370	GLU	CA-CB-CG	5.38	124.87	114.10
1	C	254	GLU	N-CA-C	5.38	117.96	111.40
1	C	125	GLN	OE1-CD-NE2	5.37	127.97	122.60
1	B	334	VAL	CB-CA-C	-5.36	103.21	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	GLU	N-CA-C	5.35	117.11	111.28
1	C	169	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	343	GLU	CB-CA-C	-5.34	102.27	110.81
1	B	120	ARG	CD-NE-CZ	5.34	131.87	124.40
1	D	178	ARG	N-CA-CB	-5.34	102.26	111.55
1	A	301	ARG	N-CA-CB	5.33	119.50	110.49
1	B	19	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	283	TYR	CB-CG-CD1	-5.29	112.86	120.80
1	B	144	GLY	N-CA-C	-5.29	108.33	115.36
1	D	131	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	D	15	ILE	CA-C-O	5.25	126.29	120.46
1	C	110	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	A	145	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	392	ARG	CA-CB-CG	-5.24	103.62	114.10
1	A	300	GLU	CA-C-N	5.23	131.54	121.54
1	A	300	GLU	C-N-CA	5.23	131.54	121.54
1	A	402	LEU	CB-CA-C	-5.23	100.69	109.48
1	C	282	ARG	CD-NE-CZ	5.22	131.71	124.40
1	D	294	ASN	CA-C-O	-5.21	112.28	119.05
1	C	200	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	D	98	ASP	N-CA-C	-5.19	105.70	111.36
1	A	355	GLU	OE1-CD-OE2	5.19	135.35	122.90
1	C	53	VAL	CA-C-O	-5.19	115.35	120.85
1	D	370	GLU	N-CA-CB	5.19	117.81	110.13
1	A	33	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	B	216	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	276	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	B	28	TYR	CB-CA-C	-5.17	102.20	110.79
1	A	253	GLY	O-C-N	-5.17	118.32	122.51
1	C	17	ARG	CD-NE-CZ	5.15	131.61	124.40
1	B	302	ASP	N-CA-C	-5.14	101.56	109.52
1	D	104	TRP	O-C-N	5.13	127.56	122.12
1	C	88	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	194	LEU	CB-CA-C	5.12	119.83	110.36
1	A	335	TYR	O-C-N	-5.11	117.40	123.22
1	A	120	ARG	CD-NE-CZ	5.10	131.54	124.40
1	D	3	VAL	CB-CA-C	5.10	116.19	111.30
1	C	242	VAL	CB-CA-C	-5.09	105.26	112.14
1	C	355	GLU	CA-CB-CG	-5.09	103.92	114.10
1	D	355	GLU	CG-CD-OE2	-5.09	106.69	118.40
1	A	285	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	D	285	ARG	CA-C-O	-5.09	114.12	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	VAL	N-CA-CB	5.09	119.35	110.65
1	B	369	ALA	CA-C-O	-5.08	114.36	120.10
1	D	350	PRO	CB-CA-C	-5.07	103.79	112.26
1	A	41	GLU	N-CA-CB	5.07	117.57	110.12
1	B	172	LEU	O-C-N	-5.07	116.75	122.12
1	C	333	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	9	ARG	CD-NE-CZ	5.05	131.47	124.40
1	A	138	MET	CA-C-O	-5.04	115.88	121.33
1	A	302	ASP	N-CA-C	-5.04	101.75	109.41
1	D	72	HIS	O-C-N	-5.03	114.95	123.00
1	D	208	LEU	N-CA-C	5.03	117.79	110.10
1	D	303	LEU	N-CA-CB	-5.01	103.24	110.56
1	D	73	ASP	N-CA-C	-5.00	103.16	111.37

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	257	GLU	Mainchain
1	D	72	HIS	Mainchain

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	2977	0	2952	35	3
1	B	2961	0	2932	45	0
1	C	2963	0	2926	59	0
1	D	2971	0	2941	54	3
2	A	197	0	0	1	0
2	B	198	0	0	3	3
2	C	202	0	0	2	3
2	D	195	0	0	4	0
All	All	12664	0	11751	169	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 8.

All (169) 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:C:344:ASN:N	1:C:344:ASN:CA	1.78	1.42
1:D:13:GLU:HG2	2:D:549:HOH:O	1.13	1.26
1:C:17:ARG:HH11	1:C:17:ARG:HG2	1.21	1.06
1:C:343:GLU:C	1:C:344:ASN:CA	2.35	0.98
1:C:14:GLU:HA	1:C:17:ARG:NH1	1.84	0.92
1:D:59:SER:OG	1:D:62:GLU:N	2.04	0.90
1:A:355:GLU:HG3	2:B:411:HOH:O	1.73	0.88
1:D:59:SER:OG	1:D:61:ASP:N	2.06	0.88
1:A:257:GLU:HG2	1:A:258:GLY:N	1.91	0.83
1:B:49:CYS:HG	1:B:87:CYS:HG	0.84	0.80
1:B:120:ARG:NH1	1:B:403:CYS:O	2.14	0.80
1:D:59:SER:OG	1:D:61:ASP:CA	2.30	0.79
1:A:7:ASP:OD2	1:D:7:ASP:OD2	2.02	0.77
1:C:17:ARG:HG2	1:C:17:ARG:NH1	1.85	0.76
1:D:49:CYS:HG	1:D:87:CYS:HG	0.76	0.76
1:B:358:MET:HE2	1:B:372:TYR:HA	1.66	0.76
1:A:194:LEU:O	1:A:198:VAL:HG23	1.87	0.74
1:C:344:ASN:N	1:C:344:ASN:CB	2.52	0.72
1:C:289:HIS:CE1	1:D:285:ARG:HD2	2.23	0.72
1:D:35:LEU:HD22	1:D:39:LEU:HD22	1.72	0.71
1:D:59:SER:OG	1:D:61:ASP:CB	2.38	0.71
1:A:358:MET:HE2	1:A:372:TYR:HA	1.72	0.71
1:B:131:ARG:NH1	1:B:395:GLU:OE1	2.23	0.71
1:B:7:ASP:OD2	1:C:7:ASP:OD2	2.09	0.70
1:A:257:GLU:CG	1:A:258:GLY:N	2.53	0.70
1:C:343:GLU:O	1:C:344:ASN:CA	2.40	0.70
1:C:358:MET:HE2	1:C:372:TYR:HA	1.74	0.68
1:A:35:LEU:HD22	1:A:39:LEU:HD22	1.76	0.67
1:C:14:GLU:CA	1:C:17:ARG:NH1	2.57	0.67
1:B:283:TYR:HH	1:C:283:TYR:HH	1.43	0.67
1:C:13:GLU:C	1:C:17:ARG:NH1	2.53	0.66
1:B:285:ARG:HB3	2:B:494:HOH:O	1.97	0.65
1:A:283:TYR:HH	1:D:283:TYR:HH	1.46	0.64
1:A:285:ARG:HD2	1:B:289:HIS:CE1	2.34	0.62
1:B:138:MET:HB2	1:B:341:ILE:HG23	1.81	0.62
1:D:59:SER:HG	1:D:62:GLU:H	1.43	0.62
1:C:285:ARG:HB3	2:C:492:HOH:O	1.99	0.62
1:D:13:GLU:OE1	1:D:17:ARG:HB3	2.00	0.62
1:A:88:ARG:HD2	1:B:366:ALA:O	2.01	0.61
1:C:13:GLU:O	1:C:17:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ALA:O	1:B:88:ARG:HD2	2.01	0.60
1:D:355:GLU:HG3	2:D:567:HOH:O	2.02	0.59
1:B:257:GLU:HG2	1:B:258:GLY:N	2.17	0.59
1:D:59:SER:HG	1:D:61:ASP:CB	2.14	0.58
1:A:152:LEU:HD11	1:A:336:ILE:HD12	1.85	0.58
1:A:257:GLU:CG	1:A:258:GLY:H	2.16	0.57
1:C:200:ARG:NH2	1:C:204:GLU:OE2	2.36	0.57
1:C:343:GLU:O	1:C:344:ASN:HA	2.04	0.56
1:B:35:LEU:HD22	1:B:39:LEU:HD22	1.88	0.55
1:C:355:GLU:HG3	2:C:566:HOH:O	2.06	0.55
1:B:152:LEU:HD11	1:B:336:ILE:HD12	1.89	0.54
1:D:402:LEU:O	1:D:403:CYS:C	2.49	0.54
1:C:402:LEU:O	1:C:403:CYS:C	2.48	0.54
1:C:32:GLU:OE2	1:C:91:HIS:HD2	1.91	0.54
1:C:366:ALA:O	1:D:88:ARG:HD2	2.07	0.53
1:B:193:GLU:C	1:B:195:GLY:H	2.15	0.53
1:D:59:SER:OG	1:D:61:ASP:C	2.51	0.53
1:A:289:HIS:CE1	1:B:285:ARG:HD2	2.43	0.52
1:B:311:VAL:HG22	1:C:5:PRO:HG2	1.91	0.52
1:A:122:VAL:HG11	1:A:237:PHE:CE2	2.44	0.52
1:A:230:LEU:HD12	1:A:320:LEU:HD12	1.91	0.52
1:C:331:LEU:O	1:C:334:VAL:HG22	2.11	0.51
1:B:5:PRO:HG2	1:C:311:VAL:HG22	1.92	0.51
1:D:32:GLU:OE2	1:D:91:HIS:HD2	1.94	0.50
1:A:176:PHE:HB2	2:A:500:HOH:O	2.11	0.50
1:A:123:GLY:HA3	1:A:402:LEU:HD12	1.93	0.50
1:C:13:GLU:O	1:C:17:ARG:HG2	2.12	0.49
1:D:285:ARG:HB3	2:D:497:HOH:O	2.12	0.49
1:D:22:GLU:HA	1:D:60:ALA:HB2	1.93	0.49
1:B:123:GLY:HA3	1:B:402:LEU:HD12	1.94	0.49
1:C:35:LEU:HD22	1:C:39:LEU:HD22	1.95	0.49
1:D:122:VAL:HG11	1:D:237:PHE:HE2	1.77	0.49
1:A:29:LEU:HD11	1:A:58:VAL:HB	1.95	0.49
1:D:59:SER:CB	1:D:61:ASP:N	2.76	0.49
1:A:32:GLU:OE2	1:A:91:HIS:HD2	1.96	0.49
1:B:313:ILE:HB	1:B:314:PRO:HD3	1.95	0.48
1:D:133:TYR:CE1	1:D:336:ILE:HD13	2.47	0.48
1:C:130:ALA:HA	1:C:153:GLY:HA2	1.96	0.48
1:B:122:VAL:HG11	1:B:237:PHE:CE2	2.48	0.48
1:B:29:LEU:HD11	1:B:58:VAL:HB	1.95	0.48
1:D:116:LYS:HB3	1:D:403:CYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLU:N	1:C:17:ARG:NH1	2.62	0.48
1:B:22:GLU:HA	1:B:60:ALA:HB2	1.96	0.47
1:C:138:MET:HB2	1:C:341:ILE:HG23	1.97	0.47
1:C:363:LYS:HE3	1:D:92:TYR:OH	2.14	0.47
1:B:178:ARG:HB2	1:B:211:HIS:CD2	2.49	0.47
1:C:285:ARG:HD2	1:D:289:HIS:CE1	2.49	0.47
1:D:59:SER:CB	1:D:61:ASP:H	2.28	0.47
1:B:349:LEU:HD22	1:B:353:LEU:HD11	1.95	0.47
1:A:339:GLU:O	1:A:343:GLU:HG3	2.14	0.46
1:C:123:GLY:HA3	1:C:402:LEU:CD1	2.44	0.46
1:C:344:ASN:N	1:C:344:ASN:CG	2.73	0.46
1:A:180:LYS:HG2	1:A:214:THR:HG21	1.97	0.46
1:D:29:LEU:HD21	1:D:77:LEU:HD21	1.97	0.46
1:D:257:GLU:HG2	1:D:258:GLY:HA2	1.97	0.46
1:D:358:MET:HE2	1:D:372:TYR:HA	1.98	0.46
1:C:29:LEU:HD21	1:C:77:LEU:HD21	1.98	0.46
1:B:289:HIS:ND1	1:D:289:HIS:CE1	2.84	0.46
1:B:123:GLY:HA3	1:B:402:LEU:CD1	2.46	0.46
1:A:16:ARG:HG3	1:D:3:VAL:HG21	1.97	0.46
1:B:130:ALA:HA	1:B:153:GLY:HA2	1.98	0.46
1:D:61:ASP:O	1:D:62:GLU:C	2.58	0.46
1:D:134:LYS:HG3	1:D:135:THR:HG23	1.97	0.46
1:B:257:GLU:CG	1:B:258:GLY:N	2.79	0.45
1:C:35:LEU:O	1:C:39:LEU:HB2	2.16	0.45
1:A:123:GLY:HA3	1:A:402:LEU:CD1	2.45	0.45
1:B:32:GLU:OE2	1:B:91:HIS:HD2	1.99	0.45
1:B:193:GLU:C	1:B:195:GLY:N	2.74	0.45
1:D:59:SER:C	1:D:61:ASP:N	2.59	0.45
1:A:289:HIS:CE1	1:C:289:HIS:ND1	2.85	0.45
1:C:39:LEU:HD21	1:C:92:TYR:HB3	1.98	0.44
1:D:112:LEU:HD22	1:D:170:LEU:HD11	1.98	0.44
1:A:3:VAL:HG21	1:D:16:ARG:HG3	1.99	0.44
1:D:122:VAL:HG11	1:D:237:PHE:CE2	2.51	0.44
1:A:289:HIS:ND1	1:C:289:HIS:CE1	2.85	0.44
1:C:37:CYS:CB	1:C:50:CYS:HG	2.28	0.44
1:C:277:ILE:HG23	1:C:323:ILE:HG23	2.00	0.44
1:B:289:HIS:CE1	1:D:289:HIS:ND1	2.86	0.44
1:A:32:GLU:OE2	1:A:91:HIS:CD2	2.70	0.44
1:D:29:LEU:CD2	1:D:77:LEU:HD21	2.48	0.43
1:B:194:LEU:O	1:B:198:VAL:HG23	2.18	0.43
1:A:242:VAL:O	1:A:246:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLU:HG3	2:B:564:HOH:O	2.17	0.43
1:C:288:THR:O	1:C:292:PHE:HD1	2.01	0.43
1:C:343:GLU:HG2	1:C:344:ASN:N	2.33	0.43
1:D:301:ARG:C	1:D:301:ARG:HD3	2.43	0.43
1:C:21:ASN:O	1:C:25:ILE:HG12	2.19	0.43
1:A:22:GLU:HA	1:A:60:ALA:HB2	2.00	0.43
1:B:180:LYS:HG2	1:B:214:THR:HG21	2.01	0.43
1:C:122:VAL:HG11	1:C:237:PHE:CE2	2.54	0.43
1:A:246:GLU:OE2	1:C:246:GLU:OE2	2.37	0.43
1:D:356:PHE:HB3	1:D:384:GLU:OE1	2.19	0.43
1:A:59:SER:O	1:A:63:VAL:HG23	2.19	0.42
1:B:230:LEU:HD12	1:B:320:LEU:HD12	2.01	0.42
1:B:288:THR:O	1:B:292:PHE:HD1	2.02	0.42
1:D:313:ILE:HB	1:D:314:PRO:HD3	2.02	0.42
1:C:82:GLU:OE2	1:C:88:ARG:HA	2.20	0.42
1:A:138:MET:HB2	1:A:341:ILE:HG23	2.01	0.42
1:C:194:LEU:O	1:C:198:VAL:HG23	2.19	0.42
1:C:221:GLU:OE1	1:D:162:GLU:OE1	2.37	0.42
1:D:194:LEU:O	1:D:198:VAL:HG23	2.19	0.42
1:B:32:GLU:OE2	1:B:91:HIS:CD2	2.72	0.42
1:D:203:ALA:HB1	1:D:208:LEU:O	2.20	0.42
1:C:32:GLU:OE2	1:C:91:HIS:CD2	2.72	0.42
1:B:201:ARG:HH11	1:B:201:ARG:HD3	1.70	0.42
1:D:32:GLU:OE2	1:D:91:HIS:CD2	2.73	0.42
1:C:355:GLU:OE2	1:D:93:GLY:HA2	2.19	0.42
1:D:242:VAL:O	1:D:246:GLU:HG2	2.19	0.41
1:C:33:ARG:HD3	1:C:54:ASN:HA	2.02	0.41
1:C:313:ILE:HB	1:C:314:PRO:HD3	2.03	0.41
1:D:116:LYS:O	1:D:120:ARG:HG3	2.21	0.41
1:C:14:GLU:N	1:C:17:ARG:HH12	2.18	0.41
1:C:123:GLY:HA3	1:C:402:LEU:HD12	2.02	0.41
1:B:216:GLN:HB3	1:B:301:ARG:HG2	2.02	0.41
1:C:112:LEU:HD22	1:C:170:LEU:HD11	2.03	0.41
1:A:402:LEU:O	1:A:403:CYS:C	2.63	0.41
1:B:72:HIS:HB3	1:B:75:LEU:HB3	2.03	0.41
1:C:36:VAL:HG13	1:C:49:CYS:HB3	2.03	0.41
1:B:3:VAL:HG21	1:C:16:ARG:HG3	2.02	0.41
1:D:356:PHE:CD2	1:D:384:GLU:HG3	2.55	0.41
1:D:360:ARG:NH1	2:D:512:HOH:O	2.52	0.41
1:A:394:ILE:O	1:A:398:LEU:HG	2.21	0.40
1:B:356:PHE:CD2	1:B:384:GLU:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:ASP:CG	1:D:340:ARG:HG3	2.47	0.40
1:C:319:ALA:O	1:C:323:ILE:HG13	2.20	0.40
1:B:58:VAL:HG12	1:B:59:SER:N	2.37	0.40
1:B:112:LEU:HD22	1:B:170:LEU:HD11	2.02	0.40
1:D:13:GLU:OE1	1:D:13:GLU:O	2.39	0.40
1:C:63:VAL:HG21	1:C:77:LEU:HD23	2.04	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:A:360:ARG:NH1	2:B:563:HOH:O[2_454]	0.60	1.60
1:A:360:ARG:CZ	2:B:563:HOH:O[2_454]	1.01	1.19
1:D:360:ARG:CZ	2:C:565:HOH:O[2_555]	1.14	1.06
1:D:360:ARG:NH1	2:C:565:HOH:O[2_555]	1.19	1.01
1:A:360:ARG:NH2	2:B:563:HOH:O[2_454]	1.73	0.47
1:D:360:ARG:NH2	2:C:565:HOH:O[2_555]	1.73	0.47

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	379/403 (94%)	368 (97%)	10 (3%)	1 (0%)	36	36
1	B	379/403 (94%)	368 (97%)	9 (2%)	2 (0%)	24	22
1	C	379/403 (94%)	366 (97%)	12 (3%)	1 (0%)	36	36
1	D	379/403 (94%)	363 (96%)	13 (3%)	3 (1%)	16	12
All	All	1516/1612 (94%)	1465 (97%)	44 (3%)	7 (0%)	24	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	ARG
1	B	301	ARG
1	C	301	ARG
1	D	301	ARG
1	B	8	TRP
1	D	8	TRP
1	D	258	GLY

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	294/329 (89%)	280 (95%)	14 (5%)	23	23
1	B	292/329 (89%)	275 (94%)	17 (6%)	18	16
1	C	291/329 (88%)	271 (93%)	20 (7%)	14	12
1	D	293/329 (89%)	272 (93%)	21 (7%)	13	11
All	All	1170/1316 (89%)	1098 (94%)	72 (6%)	16	14

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	39	LEU
1	A	72	HIS
1	A	79	LEU
1	A	136	LEU
1	A	152	LEU
1	A	196	LEU
1	A	226	LEU
1	A	230	LEU
1	A	289	HIS
1	A	312	TRP
1	A	320	LEU
1	A	328	LEU
1	A	334	VAL
1	B	35	LEU

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	79	LEU
1	B	136	LEU
1	B	138	MET
1	B	149	PRO
1	B	152	LEU
1	B	194	LEU
1	B	196	LEU
1	B	226	LEU
1	B	230	LEU
1	B	320	LEU
1	B	328	LEU
1	B	343	GLU
1	B	355	GLU
1	B	381	LEU
1	B	382	THR
1	C	3	VAL
1	C	17	ARG
1	C	35	LEU
1	C	39	LEU
1	C	77	LEU
1	C	79	LEU
1	C	136	LEU
1	C	152	LEU
1	C	196	LEU
1	C	226	LEU
1	C	230	LEU
1	C	320	LEU
1	C	328	LEU
1	C	334	VAL
1	C	343	GLU
1	C	354	THR
1	C	363	LYS
1	C	381	LEU
1	C	382	THR
1	C	392	ARG
1	D	3	VAL
1	D	13	GLU
1	D	25	ILE
1	D	35	LEU
1	D	39	LEU
1	D	58	VAL

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Mol	Chain	Res	Type
1	D	59	SER
1	D	77	LEU
1	D	79	LEU
1	D	136	LEU
1	D	138	MET
1	D	152	LEU
1	D	178	ARG
1	D	196	LEU
1	D	226	LEU
1	D	230	LEU
1	D	312	TRP
1	D	320	LEU
1	D	328	LEU
1	D	334	VAL
1	D	388	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	91	HIS
1	A	125	GLN
1	A	169	GLN
1	A	346	GLN
1	B	91	HIS
1	B	125	GLN
1	B	145	GLN
1	B	169	GLN
1	B	289	HIS
1	B	346	GLN
1	B	359	ASN
1	C	91	HIS
1	C	125	GLN
1	C	145	GLN
1	C	169	GLN
1	C	333	ASN
1	D	91	HIS
1	D	169	GLN
1	D	289	HIS
1	D	346	GLN
1	D	359	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	D	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	59:SER	C	60:ALA	N	1.62
1	B	258:GLY	C	259:GLY	N	1.15

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	385/403 (95%)	-0.12	18 (4%) 36 38	10, 19, 47, 84	0
1	B	385/403 (95%)	-0.01	27 (7%) 22 24	9, 19, 48, 84	0
1	C	385/403 (95%)	-0.18	18 (4%) 36 38	10, 18, 50, 78	0
1	D	385/403 (95%)	-0.15	19 (4%) 35 37	10, 19, 42, 87	0
All	All	1540/1612 (95%)	-0.11	82 (5%) 32 34	9, 19, 47, 87	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	VAL	7.3
1	B	56	ALA	6.3
1	B	60	ALA	6.3
1	D	63	VAL	6.2
1	A	258	GLY	6.0
1	A	63	VAL	6.0
1	D	259	GLY	5.9
1	D	60	ALA	5.8
1	B	61	ASP	5.4
1	B	59	SER	5.4
1	B	58	VAL	5.3
1	D	56	ALA	5.3
1	D	269	ALA	5.2
1	A	269	ALA	5.2
1	D	58	VAL	5.1
1	A	56	ALA	4.8
1	A	58	VAL	4.8
1	D	61	ASP	4.6
1	B	72	HIS	4.5
1	B	57	SER	4.4
1	D	55	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	259	GLY	4.1
1	C	63	VAL	4.1
1	A	259	GLY	4.1
1	A	60	ALA	4.0
1	C	60	ALA	3.9
1	D	59	SER	3.9
1	D	72	HIS	3.8
1	D	57	SER	3.7
1	A	72	HIS	3.7
1	C	72	HIS	3.7
1	B	377	GLU	3.6
1	C	269	ALA	3.6
1	D	62	GLU	3.6
1	B	258	GLY	3.5
1	D	372	TYR	3.5
1	A	194	LEU	3.5
1	B	269	ALA	3.4
1	A	57	SER	3.3
1	C	58	VAL	3.2
1	B	259	GLY	3.1
1	B	62	GLU	3.1
1	D	13	GLU	3.0
1	B	380	ALA	2.9
1	B	403	CYS	2.9
1	C	59	SER	2.9
1	C	61	ASP	2.8
1	B	395	GLU	2.7
1	B	351	TYR	2.7
1	A	59	SER	2.7
1	C	378	VAL	2.6
1	A	372	TYR	2.6
1	B	343	GLU	2.6
1	C	258	GLY	2.6
1	D	258	GLY	2.6
1	C	56	ALA	2.6
1	B	194	LEU	2.6
1	B	360	ARG	2.5
1	D	365	GLY	2.5
1	A	61	ASP	2.5
1	D	370	GLU	2.4
1	A	75	LEU	2.4
1	C	380	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	84	LYS	2.3
1	C	57	SER	2.3
1	A	62	GLU	2.3
1	B	378	VAL	2.3
1	A	55	LYS	2.3
1	B	193	GLU	2.2
1	B	44	VAL	2.2
1	B	53	VAL	2.2
1	C	194	LEU	2.2
1	B	372	TYR	2.2
1	B	370	GLU	2.1
1	C	62	GLU	2.1
1	C	377	GLU	2.1
1	C	17	ARG	2.1
1	A	378	VAL	2.1
1	A	376	LYS	2.1
1	C	403	CYS	2.1
1	D	84	LYS	2.0
1	D	8	TRP	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.