WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:39 am GMT

PDB ID	:	1DOF
Title	:	THE CRYSTAL STRUCTURE OF ADENYLOSUCCINATE LYASE FROM PYROBACULUM AEROPHILUM: INSIGHTS INTO THERMAL STABILITY AND HUMAN PATHOLOGY
Authors	:	Toth, E.A.; Yeates, T.O.; Goedken, E.; Dixon, J.E.; Marqusee, S.
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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.
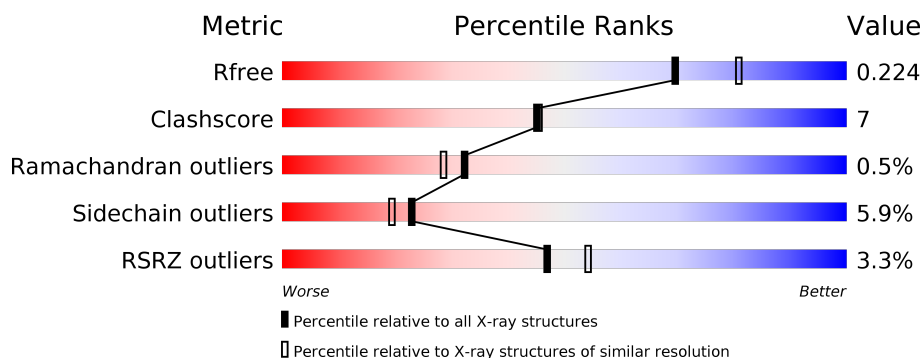
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% / 77% / 14% • •
1	B	403	3% / 70% / 19% / 5% •
1	C	403	5% / 72% / 20% • • •
1	D	403	2% / 73% / 18% • • •

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 ⓘ

These plots are drawn for all protein, RNA and DNA 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
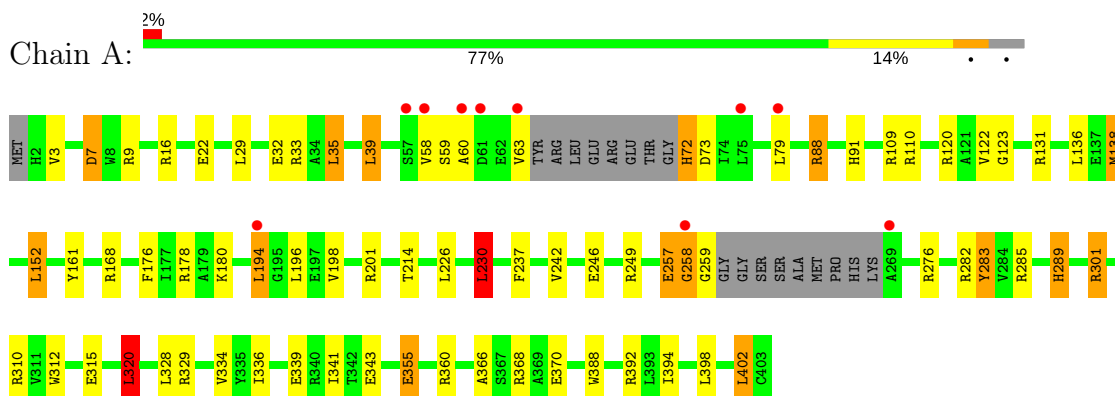
• Molecule 1: ADENYLOSUCCINATE LYASE

• Molecule 1: ADENYLOSUCCINATE LYASE

• Molecule 1: ADENYLOSUCCINATE LYASE

Chain D:
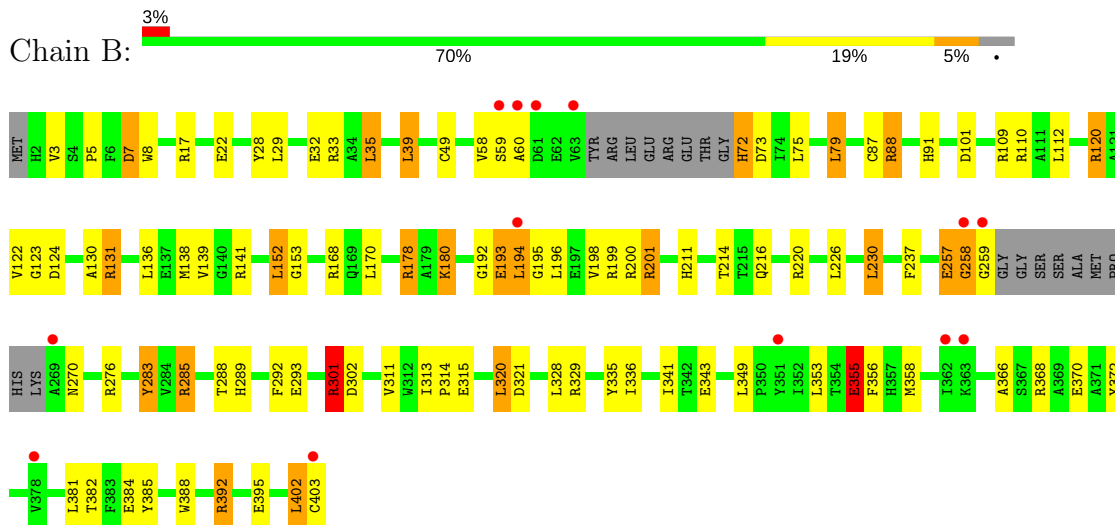
4 Data and refinement statistics (i)

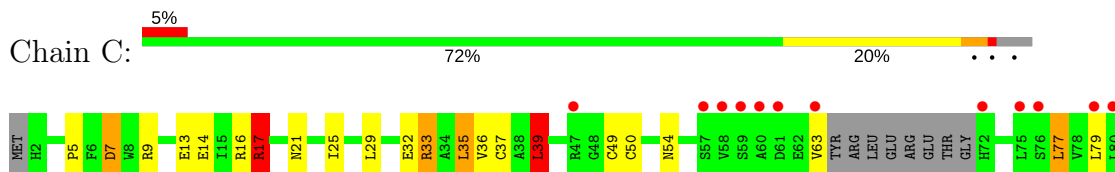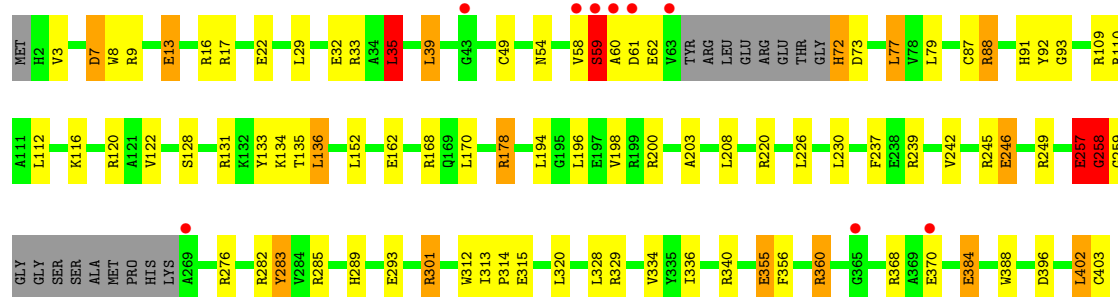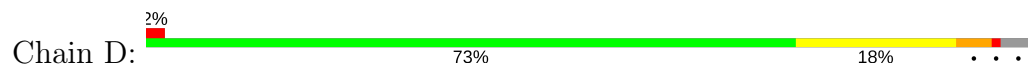| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.62Å 150.31Å 173.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 48.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 99.5 (48.13-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	5014 reflections (5.26%)	DCC
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 , 63.3	EDS
L-test for twinning[2]	$< |L| > = 0.59, < L^2 > = 0.45$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.78	6/3028 (0.2%)	1.61	46/4109 (1.1%)
1	B	0.94	6/3012 (0.2%)	1.69	58/4090 (1.4%)
1	C	0.90	5/3014 (0.2%)	1.69	51/4093 (1.2%)
1	D	0.84	6/3022 (0.2%)	1.93	54/4102 (1.3%)
All	All	0.87	23/12076 (0.2%)	1.74	209/16394 (1.3%)

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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	GLY	N-CA	-24.07	1.09	1.46
1	C	259	GLY	N-CA	-18.49	1.18	1.46
1	C	344	ASN	N-CA	16.08	1.78	1.46
1	C	258	GLY	CA-C	-14.79	1.28	1.51
1	B	258	GLY	CA-C	-14.41	1.28	1.51
1	D	59	SER	C-N	12.36	1.62	1.34
1	A	259	GLY	N-CA	-10.71	1.29	1.46
1	D	257	GLU	C-N	9.91	1.50	1.33
1	B	258	GLY	C-N	-9.79	1.15	1.33
1	B	73	ASP	N-CA	-9.58	1.27	1.46
1	D	259	GLY	N-CA	-8.21	1.33	1.46
1	A	73	ASP	N-CA	-7.31	1.31	1.46
1	D	315	GLU	CD-OE2	7.21	1.33	1.25
1	A	315	GLU	CD-OE2	7.15	1.33	1.25
1	B	72	HIS	CA-C	-6.95	1.34	1.52
1	A	258	GLY	C-N	-6.93	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	GLU	CD-OE2	6.52	1.32	1.25
1	C	258	GLY	C-N	-6.40	1.21	1.33
1	D	258	GLY	CA-C	-6.34	1.41	1.51
1	A	194	LEU	N-CA	6.20	1.58	1.46
1	B	315	GLU	CD-OE2	5.79	1.32	1.25
1	D	59	SER	N-CA	5.47	1.57	1.46
1	A	72	HIS	CA-C	-5.18	1.39	1.52

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	178	ARG	CD-NE-CZ	38.88	178.03	123.60
1	D	109	ARG	CD-NE-CZ	28.63	163.68	123.60
1	D	59	SER	O-C-N	25.31	163.20	122.70
1	B	258	GLY	O-C-N	23.65	163.40	123.20
1	D	257	GLU	C-N-CA	-23.41	73.14	122.30
1	D	59	SER	CA-C-N	-22.26	68.23	117.20
1	A	178	ARG	CD-NE-CZ	22.25	154.75	123.60
1	B	178	ARG	CD-NE-CZ	22.19	154.67	123.60
1	B	258	GLY	CA-C-N	-21.71	72.77	116.20
1	A	109	ARG	NE-CZ-NH2	-19.82	110.39	120.30
1	C	329	ARG	NE-CZ-NH2	-18.98	110.81	120.30
1	D	33	ARG	NE-CZ-NH2	18.80	129.70	120.30
1	C	17	ARG	NE-CZ-NH1	18.48	129.54	120.30
1	C	258	GLY	O-C-N	17.02	152.13	123.20
1	A	168	ARG	NE-CZ-NH1	16.73	128.67	120.30
1	D	59	SER	C-N-CA	-16.71	79.94	121.70
1	B	329	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	D	258	GLY	O-C-N	15.60	149.72	123.20
1	A	33	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	C	258	GLY	CA-C-N	-14.64	86.93	116.20
1	B	109	ARG	NE-CZ-NH2	-14.13	113.23	120.30
1	B	110	ARG	NE-CZ-NH1	13.97	127.28	120.30
1	A	283	TYR	CB-CG-CD1	-13.57	112.86	121.00
1	C	392	ARG	CD-NE-CZ	13.35	142.29	123.60
1	D	258	GLY	CA-C-N	-13.35	89.51	116.20
1	C	329	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	A	33	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	C	88	ARG	NE-CZ-NH2	12.76	126.68	120.30
1	B	276	ARG	NE-CZ-NH1	12.75	126.68	120.30
1	C	283	TYR	CB-CG-CD1	-12.41	113.55	121.00
1	C	329	ARG	CD-NE-CZ	12.29	140.81	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	392	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	B	109	ARG	NE-CZ-NH1	12.19	126.39	120.30
1	B	283	TYR	CB-CG-CD1	-12.01	113.79	121.00
1	D	168	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	D	72	HIS	C-N-CA	11.94	151.56	121.70
1	C	110	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	C	110	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	C	131	ARG	NE-CZ-NH1	-11.16	114.72	120.30
1	A	258	GLY	O-C-N	11.06	142.01	123.20
1	B	194	LEU	N-CA-CB	-10.98	88.44	110.40
1	B	168	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	D	131	ARG	NE-CZ-NH2	10.83	125.71	120.30
1	D	283	TYR	CB-CG-CD1	-10.79	114.52	121.00
1	C	178	ARG	CD-NE-CZ	10.65	138.50	123.60
1	D	355	GLU	OE1-CD-OE2	10.61	136.03	123.30
1	B	109	ARG	CD-NE-CZ	10.57	138.41	123.60
1	A	329	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	D	73	ASP	N-CA-CB	10.21	128.98	110.60
1	B	72	HIS	O-C-N	10.20	139.01	122.70
1	B	368	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	A	355	GLU	OE1-CD-OE2	10.05	135.35	123.30
1	B	110	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	283	TYR	CB-CG-CD2	9.98	126.99	121.00
1	C	200	ARG	CD-NE-CZ	9.93	137.50	123.60
1	D	370	GLU	CA-CB-CG	9.84	135.04	113.40
1	C	343	GLU	C-N-CA	-9.77	97.27	121.70
1	A	88	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	A	249	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	A	109	ARG	CD-NE-CZ	9.36	136.71	123.60
1	C	120	ARG	NE-CZ-NH2	9.35	124.98	120.30
1	A	368	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	B	392	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	B	220	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	9	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	258	GLY	CA-C-N	-8.89	98.42	116.20
1	A	282	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	D	258	GLY	N-CA-C	-8.88	90.89	113.10
1	B	355	GLU	OE1-CD-OE2	8.78	133.83	123.30
1	C	276	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	D	340	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	D	282	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	D	249	ARG	NE-CZ-NH1	8.50	124.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	17	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	D	329	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	109	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	D	245	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	A	9	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	72	HIS	O-C-N	8.10	135.66	122.70
1	B	193	GLU	N-CA-C	8.08	132.82	111.00
1	C	33	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	C	283	TYR	CB-CG-CD2	8.02	125.81	121.00
1	A	178	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	C	293	GLU	OE1-CD-OE2	-7.98	113.72	123.30
1	A	178	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	C	88	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	D	276	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	283	TYR	CB-CG-CD2	7.82	125.69	121.00
1	B	329	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	C	249	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	D	384	GLU	OE1-CD-OE2	7.68	132.51	123.30
1	A	201	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	D	220	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	72	HIS	CA-C-N	-7.41	100.90	117.20
1	A	168	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	D	402	LEU	CB-CA-C	-7.30	96.33	110.20
1	C	368	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	C	199	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	178	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	33	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	C	7	ASP	CB-CG-OD1	7.16	124.74	118.30
1	C	200	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	D	9	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	168	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	D	110	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	199	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	D	360	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	141	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	C	7	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	C	395	GLU	OE1-CD-OE2	6.85	131.52	123.30
1	C	199	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	259	GLY	N-CA-C	-6.60	96.59	113.10
1	B	368	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	310	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	124	ASP	CB-CG-OD2	-6.51	112.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	201	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	7	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	B	180	LYS	CD-CE-NZ	6.43	126.49	111.70
1	D	33	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	B	285	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	258	GLY	C-N-CA	6.35	135.64	122.30
1	A	72	HIS	CA-C-N	-6.35	103.23	117.20
1	C	285	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	340	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	88	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	B	200	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	370	GLU	CA-CB-CG	6.26	127.18	113.40
1	A	110	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	199	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	D	7	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	C	344	ASN	N-CA-CB	-6.15	99.53	110.60
1	C	109	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	101	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	120	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	276	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	168	ARG	CD-NE-CZ	6.03	132.03	123.60
1	B	293	GLU	OE1-CD-OE2	-6.02	116.07	123.30
1	C	141	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	B	402	LEU	CB-CA-C	-6.00	98.80	110.20
1	B	131	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	D	276	ARG	CD-NE-CZ	5.97	131.96	123.60
1	D	246	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	D	293	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	D	396	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	C	344	ASN	N-CA-C	5.91	126.96	111.00
1	B	120	ARG	CD-NE-CZ	5.91	131.87	123.60
1	D	54	ASN	O-C-N	-5.89	113.27	122.70
1	B	7	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	276	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	257	GLU	CB-CA-C	-5.87	98.66	110.40
1	D	9	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	257	GLU	CB-CA-C	-5.84	98.71	110.40
1	C	196	LEU	CA-CB-CG	5.83	128.71	115.30
1	C	239	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	355	GLU	CG-CD-OE2	-5.81	106.69	118.30
1	C	282	ARG	CD-NE-CZ	5.79	131.71	123.60
1	B	17	ARG	NE-CZ-NH1	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	33	ARG	NH1-CZ-NH2	-5.74	113.08	119.40
1	D	178	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	17	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	368	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	120	ARG	CD-NE-CZ	5.67	131.54	123.60
1	A	161	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	D	128	SER	N-CA-CB	-5.65	102.03	110.50
1	A	9	ARG	CD-NE-CZ	5.62	131.47	123.60
1	B	321	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	200	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	B	28	TYR	CB-CG-CD2	5.58	124.35	121.00
1	B	302	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	249	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	168	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	A	138	MET	CA-CB-CG	5.51	122.67	113.30
1	D	35	LEU	CB-CG-CD2	5.45	120.26	111.00
1	B	335	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	C	334	VAL	CB-CA-C	-5.43	101.08	111.40
1	B	392	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	B	192	GLY	C-N-CA	-5.41	108.17	121.70
1	B	79	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	392	ARG	CD-NE-CZ	-5.36	116.10	123.60
1	B	139	VAL	CG1-CB-CG2	-5.33	102.36	110.90
1	D	283	TYR	CB-CG-CD2	5.31	124.19	121.00
1	A	320	LEU	CB-CG-CD2	5.30	120.00	111.00
1	C	98	ASP	CB-CG-OD1	5.29	123.07	118.30
1	B	270	ASN	N-CA-CB	5.29	120.12	110.60
1	D	239	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	301	ARG	N-CA-CB	5.25	120.05	110.60
1	C	204	GLU	OE1-CD-OE2	5.24	129.58	123.30
1	B	385	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	D	88	ARG	CD-NE-CZ	-5.22	116.30	123.60
1	A	258	GLY	C-N-CA	5.21	133.25	122.30
1	C	39	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	368	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	370	GLU	CA-CB-CG	5.21	124.87	113.40
1	A	109	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	B	276	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	110	ARG	CD-NE-CZ	5.15	130.81	123.60
1	B	258	GLY	C-N-CA	5.15	133.11	122.30
1	D	109	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	301	ARG	N-CA-CB	5.13	119.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	368	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	124	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	136	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	188	MET	CG-SD-CE	-5.08	92.08	100.20
1	A	194	LEU	CB-CA-C	5.07	119.83	110.20
1	A	131	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	257	GLU	CB-CA-C	-5.04	100.31	110.40
1	B	168	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	A	230	LEU	CB-CG-CD1	5.00	119.50	111.00
1	A	402	LEU	CB-CA-C	-5.00	100.69	110.20

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	33	3
1	B	2961	0	2932	45	0
1	C	2963	0	2926	59	0
1	D	2971	0	2940	51	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	11750	164	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 7.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	0.94
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	0.84
1:B:120:ARG:NH1	1:B:403:CYS:O	2.14	0.80
1:B:49:CYS:HG	1:B:87:CYS:HG	0.84	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:NH1	1:C:17:ARG:HG2	1.85	0.76
1:D:49:CYS:HG	1:D:87:CYS:HG	0.76	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: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: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	0.65
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:C:13:GLU:C	1:C:17:ARG:NH1	2.53	0.61
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:402:LEU:O	1:C:403:CYS:C	2.48	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:D:402:LEU:O	1:D:403:CYS:C	2.49	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:193:GLU:C	1:B:195:GLY:H	2.15	0.48
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:D:59:SER:OG	1:D:61:ASP:C	2.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:344:ASN:N	1:C:344:ASN:CG	2.73	0.41
1:D:242:VAL:O	1:D:246:GLU:HG2	2.19	0.41
1:C:313:ILE:HB	1:C:314:PRO:HD3	2.03	0.41
1:C:33:ARG:HD3	1:C:54:ASN:HA	2.02	0.41
1:D:116:LYS:O	1:D:120:ARG:HG3	2.21	0.41
1:D:61:ASP:O	1:D:62:GLU:C	2.58	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:C:358:MET:HE2	1:C:372:TYR:HA	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:B:358:MET:HE2	1:B:372:TYR:HA	2.02	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:D:360:ARG:NH1	2:D:512:HOH:O	2.52	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:A:394:ILE:O	1:A:398:LEU:HG	2.21	0.40
1:B:193:GLU:C	1:B:195:GLY:N	2.74	0.40
1:B:356:PHE:CD2	1:B:384:GLU:HG3	2.56	0.40
1:D:59:SER:C	1:D:61:ASP:N	2.59	0.40
1:C:319:ALA:O	1:C:323:ILE:HG13	2.20	0.40
1:B:112:LEU:HD22	1:B:170:LEU:HD11	2.02	0.40
1:B:58:VAL:HG12	1:B:59:SER:N	2.37	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 sym-

metry 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%)	44	44
1	B	379/403 (94%)	368 (97%)	9 (2%)	2 (0%)	32	28
1	C	379/403 (94%)	366 (97%)	12 (3%)	1 (0%)	44	44
1	D	379/403 (94%)	363 (96%)	13 (3%)	3 (1%)	22	17
All	All	1516/1612 (94%)	1465 (97%)	44 (3%)	7 (0%)	32	28

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%)	278 (95%)	16 (5%)	26	23
1	B	292/329 (89%)	275 (94%)	17 (6%)	23	20
1	C	291/329 (88%)	274 (94%)	17 (6%)	23	20
1	D	293/329 (89%)	274 (94%)	19 (6%)	20	16
All	All	1170/1316 (89%)	1101 (94%)	69 (6%)	23	19

All (69) 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	301	ARG
1	A	312	TRP
1	A	320	LEU
1	A	328	LEU
1	A	334	VAL
1	A	388	TRP
1	B	35	LEU
1	B	39	LEU
1	B	79	LEU
1	B	136	LEU
1	B	152	LEU
1	B	196	LEU
1	B	226	LEU
1	B	230	LEU

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Mol	Chain	Res	Type
1	B	301	ARG
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	B	388	TRP
1	B	392	ARG
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	301	ARG
1	C	320	LEU
1	C	328	LEU
1	C	334	VAL
1	C	343	GLU
1	C	382	THR
1	C	388	TRP
1	D	13	GLU
1	D	35	LEU
1	D	39	LEU
1	D	58	VAL
1	D	59	SER
1	D	77	LEU
1	D	79	LEU
1	D	136	LEU
1	D	152	LEU
1	D	178	ARG
1	D	196	LEU
1	D	226	LEU
1	D	230	LEU
1	D	301	ARG
1	D	312	TRP
1	D	320	LEU

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Mol	Chain	Res	Type
1	D	328	LEU
1	D	334	VAL
1	D	388	TRP

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

Mol	Chain	Res	Type
1	A	91	HIS
1	A	125	GLN
1	A	145	GLN
1	A	359	ASN
1	B	91	HIS
1	B	125	GLN
1	B	145	GLN
1	B	289	HIS
1	B	359	ASN
1	C	91	HIS
1	C	125	GLN
1	C	145	GLN
1	C	210	HIS
1	C	359	ASN
1	D	91	HIS
1	D	145	GLN
1	D	289	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	385/403 (95%)	-0.24	10 (2%)	56	62	10, 19, 47, 84	0
1	B	385/403 (95%)	-0.18	13 (3%)	46	53	9, 19, 48, 84	0
1	C	385/403 (95%)	-0.20	19 (4%)	30	37	10, 18, 50, 78	0
1	D	385/403 (95%)	-0.27	9 (2%)	61	66	10, 19, 42, 87	0
All	All	1540/1612 (95%)	-0.22	51 (3%)	47	54	9, 19, 47, 87	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	ASP	6.5
1	C	259	GLY	5.3
1	B	60	ALA	4.2
1	C	79	LEU	4.1
1	B	59	SER	4.0
1	C	58	VAL	3.5
1	A	258	GLY	3.5
1	B	63	VAL	3.4
1	C	80	LEU	3.3
1	D	269	ALA	3.3
1	A	61	ASP	3.3
1	C	61	ASP	3.2
1	C	59	SER	3.2
1	D	60	ALA	3.1
1	A	60	ALA	3.1
1	C	269	ALA	3.0
1	C	63	VAL	3.0
1	C	72	HIS	2.9
1	D	63	VAL	2.9
1	A	58	VAL	2.9
1	C	57	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	75	LEU	2.8
1	D	43	GLY	2.7
1	C	60	ALA	2.6
1	A	79	LEU	2.6
1	B	269	ALA	2.5
1	B	378	VAL	2.5
1	B	351	TYR	2.5
1	B	362	ILE	2.5
1	C	378	VAL	2.5
1	B	61	ASP	2.4
1	D	365	GLY	2.4
1	A	63	VAL	2.4
1	A	269	ALA	2.4
1	A	75	LEU	2.4
1	A	194	LEU	2.4
1	C	76	SER	2.3
1	D	58	VAL	2.3
1	D	59	SER	2.3
1	D	370	GLU	2.3
1	B	259	GLY	2.2
1	C	83	GLN	2.2
1	C	377	GLU	2.2
1	C	363	LYS	2.2
1	C	86	GLY	2.2
1	B	258	GLY	2.2
1	B	363	LYS	2.1
1	B	403	CYS	2.1
1	A	57	SER	2.1
1	B	194	LEU	2.0
1	C	47	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.