



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 09:26 PM JST

PDB ID : 6LD6
Title : Structure of Bifidobacterium dentium beta-glucuronidase
Authors : Lin, H.-Y.; Hsieh, T.-J.; Lin, C.-H.
Deposited on : 2019-11-20
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

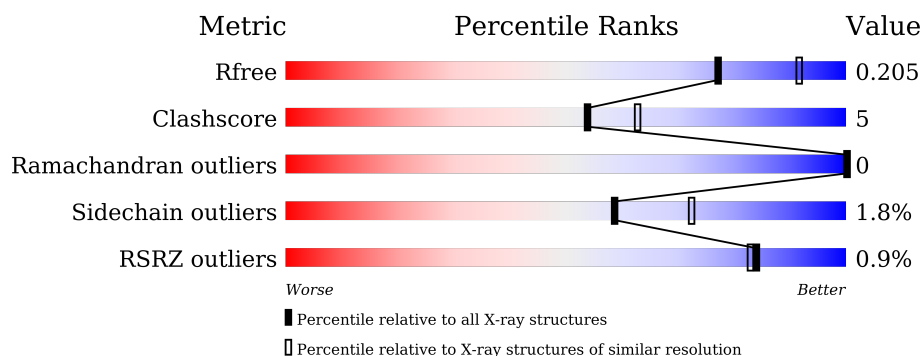
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	670	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 78% 12% • 7% </div> </div>
1	B	670	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 81%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 10% • 7% </div> </div>
1	C	670	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 81%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 10% • 7% </div> </div>
1	D	670	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 77%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 77% 14% • 7% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21571 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 LacZ1 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			
1	B	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			
1	C	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			
1	D	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP D2Q7B1
A	0	GLY	-	expression tag	UNP D2Q7B1
B	-1	ASN	-	expression tag	UNP D2Q7B1
B	0	GLY	-	expression tag	UNP D2Q7B1
C	-1	ASN	-	expression tag	UNP D2Q7B1
C	0	GLY	-	expression tag	UNP D2Q7B1
D	-1	ASN	-	expression tag	UNP D2Q7B1
D	0	GLY	-	expression tag	UNP D2Q7B1

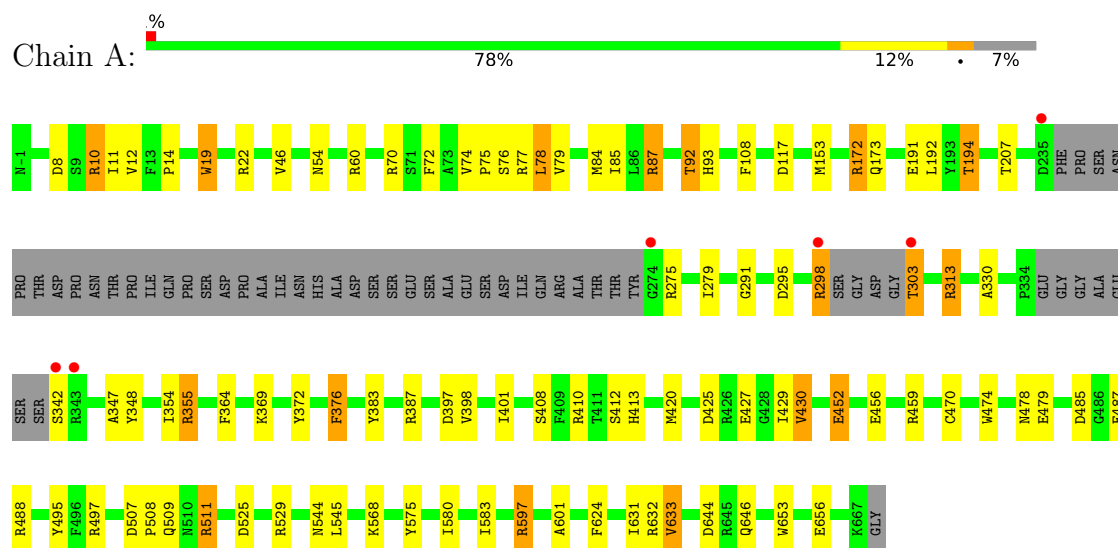
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	527	Total	O	0	0
			527	527		
2	B	455	Total	O	0	0
			455	455		
2	C	521	Total	O	0	0
			521	521		
2	D	432	Total	O	0	0
			432	432		

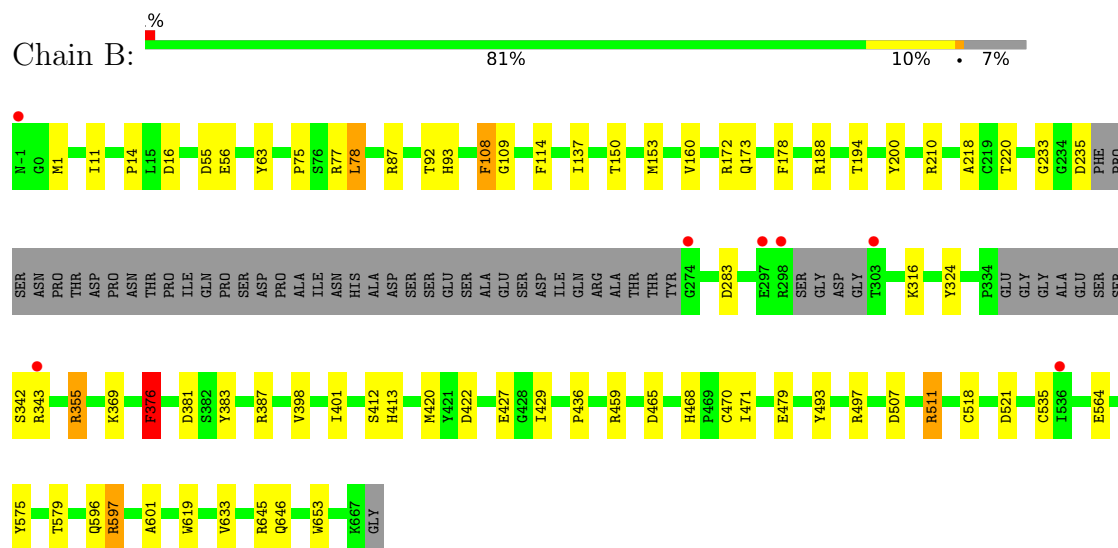
3 Residue-property plots

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.

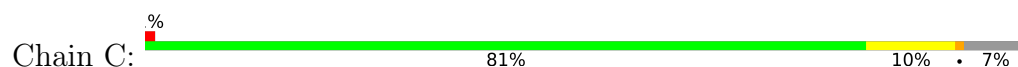
• Molecule 1: LacZ1 Beta-galactosidase

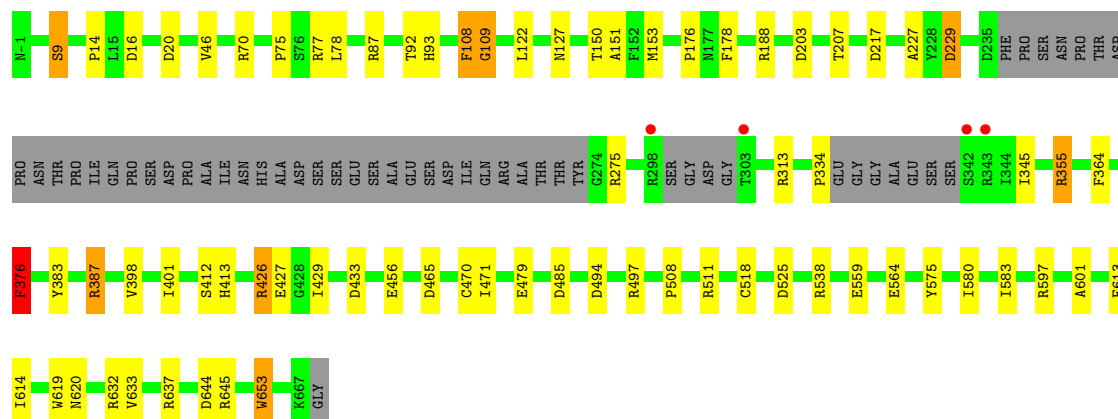


• Molecule 1: LacZ1 Beta-galactosidase

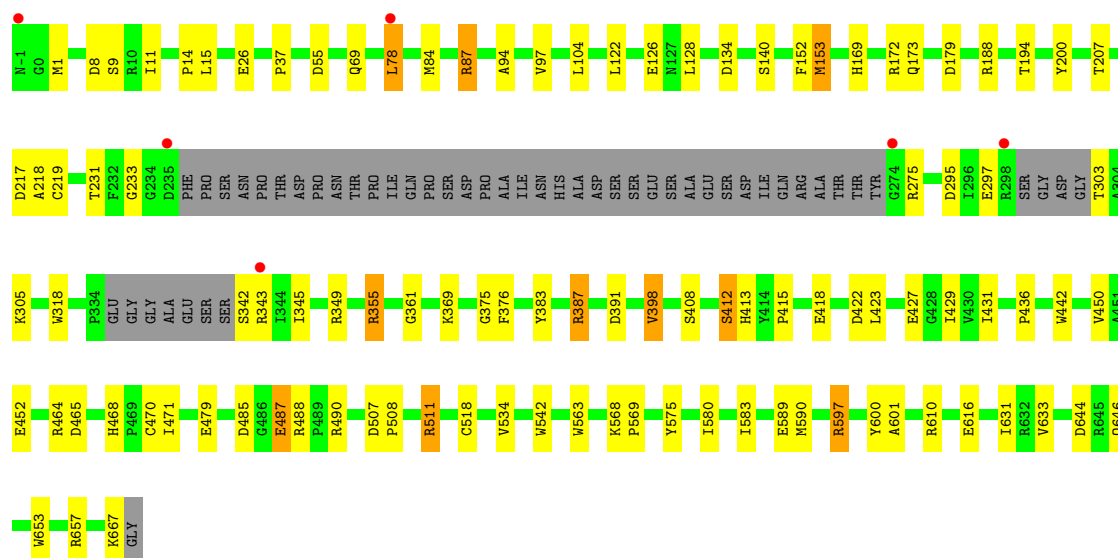
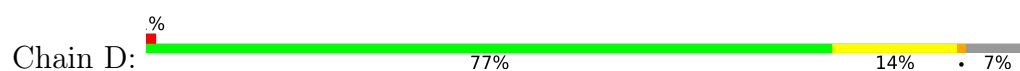


• Molecule 1: LacZ1 Beta-galactosidase





● Molecule 1: LacZ1 Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.58Å 104.90Å 160.62Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	29.60 – 2.20 29.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.60-2.20) 94.7 (29.60-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.41 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.151 , 0.205 0.151 , 0.205	Depositor DCC
R_{free} test set	2012 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21571	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	21/5040 (0.4%)	1.11	33/6857 (0.5%)
1	B	1.07	9/5040 (0.2%)	1.09	22/6857 (0.3%)
1	C	1.13	8/5040 (0.2%)	1.10	28/6857 (0.4%)
1	D	1.05	9/5040 (0.2%)	1.05	19/6857 (0.3%)
All	All	1.10	47/20160 (0.2%)	1.09	102/27428 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	398	VAL	CB-CG1	-7.62	1.36	1.52
1	B	78	LEU	CG-CD2	7.30	1.78	1.51
1	A	511	ARG	CD-NE	-7.07	1.34	1.46
1	A	430	VAL	CB-CG1	-7.06	1.38	1.52
1	D	452	GLU	CG-CD	7.05	1.62	1.51
1	D	487	GLU	CG-CD	7.04	1.62	1.51
1	A	656	GLU	CG-CD	6.81	1.62	1.51
1	C	109	GLY	N-CA	6.76	1.56	1.46
1	D	297	GLU	CG-CD	6.54	1.61	1.51
1	A	633	VAL	CB-CG2	-6.48	1.39	1.52
1	A	369	LYS	CD-CE	6.27	1.67	1.51
1	B	383	TYR	CD2-CE2	6.18	1.48	1.39
1	A	72	PHE	CE1-CZ	6.15	1.49	1.37
1	B	160	VAL	CB-CG2	6.09	1.65	1.52
1	C	229	ASP	CB-CG	-6.07	1.39	1.51
1	A	487	GLU	CG-CD	5.99	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	456	GLU	CG-CD	5.86	1.60	1.51
1	B	535	CYS	CB-SG	5.75	1.92	1.82
1	A	474	TRP	CB-CG	-5.73	1.40	1.50
1	C	653	TRP	CE3-CZ3	5.71	1.48	1.38
1	A	348	TYR	CD2-CE2	-5.67	1.30	1.39
1	B	178	PHE	CE2-CZ	5.67	1.48	1.37
1	A	60	ARG	CZ-NH1	5.65	1.40	1.33
1	C	511	ARG	CD-NE	-5.64	1.36	1.46
1	A	364	PHE	CE1-CZ	5.63	1.48	1.37
1	D	563	TRP	CE3-CZ3	5.62	1.48	1.38
1	C	613	PHE	CE1-CZ	5.58	1.48	1.37
1	B	564	GLU	CD-OE2	5.54	1.31	1.25
1	B	114	PHE	CG-CD1	5.50	1.47	1.38
1	C	632	ARG	CZ-NH1	5.44	1.40	1.33
1	D	219	CYS	CB-SG	5.44	1.91	1.82
1	A	369	LYS	CE-NZ	5.39	1.62	1.49
1	A	495	TYR	CD2-CE2	5.38	1.47	1.39
1	C	564	GLU	CD-OE2	5.31	1.31	1.25
1	D	534	VAL	CB-CG1	5.30	1.64	1.52
1	A	72	PHE	CD2-CE2	5.28	1.49	1.39
1	D	616	GLU	CD-OE2	5.26	1.31	1.25
1	D	600	TYR	CB-CG	5.25	1.59	1.51
1	A	19	TRP	CE3-CZ3	5.22	1.47	1.38
1	A	108	PHE	CE2-CZ	5.20	1.47	1.37
1	A	372	TYR	CD2-CE2	5.19	1.47	1.39
1	A	191	GLU	CG-CD	5.18	1.59	1.51
1	B	114	PHE	CE2-CZ	5.16	1.47	1.37
1	A	624	PHE	CE1-CZ	5.15	1.47	1.37
1	A	92	THR	CB-CG2	5.14	1.69	1.52
1	A	452	GLU	CG-CD	5.10	1.59	1.51
1	B	619	TRP	CE3-CZ3	5.09	1.47	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	LEU	CB-CG-CD1	-20.43	76.26	111.00
1	D	78	LEU	CB-CG-CD1	-20.21	76.65	111.00
1	A	511	ARG	NE-CZ-NH2	-18.73	110.94	120.30
1	C	87	ARG	NE-CZ-NH2	-16.25	112.18	120.30
1	C	511	ARG	NE-CZ-NH2	-16.11	112.24	120.30
1	B	87	ARG	NE-CZ-NH2	-14.91	112.85	120.30
1	D	87	ARG	NE-CZ-NH2	-14.05	113.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	ARG	NE-CZ-NH1	13.10	126.85	120.30
1	A	87	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	C	511	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	A	376	PHE	CB-CG-CD2	-10.77	113.26	120.80
1	B	376	PHE	CB-CG-CD2	-10.37	113.54	120.80
1	B	188	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	D	87	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	B	376	PHE	CB-CG-CD1	10.01	127.81	120.80
1	C	108	PHE	C-N-CA	-9.75	101.83	122.30
1	C	376	PHE	CB-CG-CD2	-9.50	114.15	120.80
1	D	657	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	A	87	ARG	CG-CD-NE	-9.20	92.49	111.80
1	B	387	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	188	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	B	283	ASP	CB-CG-OD1	8.30	125.77	118.30
1	C	87	ARG	CG-CD-NE	-8.15	94.69	111.80
1	B	78	LEU	CA-CB-CG	-8.00	96.91	115.30
1	A	387	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	C	313	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	D	511	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	C	376	PHE	CB-CG-CD1	7.40	125.98	120.80
1	B	16	ASP	CB-CG-OD2	7.37	124.93	118.30
1	D	511	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	70	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	488	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	C	355	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	C	383	TYR	C-N-CA	-6.91	104.43	121.70
1	A	22	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	C	387	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	D	657	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	87	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	78	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	C	108	PHE	O-C-N	-6.46	112.21	123.20
1	A	153	MET	CB-CG-SD	-6.45	93.05	112.40
1	A	644	ASP	CB-CG-OD2	6.42	124.08	118.30
1	C	203	ASP	CB-CG-OD1	6.40	124.06	118.30
1	C	494	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	117	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	A	376	PHE	CB-CG-CD1	6.17	125.12	120.80
1	D	597	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	87	ARG	CG-CD-NE	-6.07	99.05	111.80
1	B	511	ARG	CB-CG-CD	-5.99	96.02	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	TYR	C-N-CA	-5.93	106.89	121.70
1	D	383	TYR	C-N-CA	-5.91	106.93	121.70
1	C	20	ASP	CB-CG-OD1	5.91	123.61	118.30
1	A	295	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	C	229	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	295	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	117	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	188	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	108	PHE	CA-C-N	5.67	127.55	116.20
1	C	87	ARG	NH1-CZ-NH2	5.63	125.60	119.40
1	D	349	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	55	ASP	CB-CG-OD1	5.58	123.33	118.30
1	B	235	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	298	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	70	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	172	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C	153	MET	CB-CG-SD	-5.53	95.80	112.40
1	D	511	ARG	CB-CG-CD	-5.52	97.24	111.60
1	C	217	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	529	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	87	ARG	CD-NE-CZ	5.51	131.31	123.60
1	A	529	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	425	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	275	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	313	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	C	525	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	A	525	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	87	ARG	CD-NE-CZ	5.34	131.08	123.60
1	C	426	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	D	610	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	10	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	387	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	87	ARG	CD-NE-CZ	5.26	130.97	123.60
1	B	108	PHE	O-C-N	-5.26	114.26	123.20
1	A	355	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	511	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	78	LEU	CB-CG-CD1	5.21	119.85	111.00
1	B	108	PHE	CA-C-N	5.19	126.58	116.20
1	D	55	ASP	CB-CG-OD1	5.18	122.97	118.30
1	C	525	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	217	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	188	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MET	CG-SD-CE	-5.12	92.02	100.20
1	A	410	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	426	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	597	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	485	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	376	PHE	CG-CD1-CE1	-5.04	115.26	120.80
1	C	109	GLY	N-CA-C	5.02	125.66	113.10
1	D	1	MET	CG-SD-CE	-5.02	92.17	100.20
1	D	391	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	459	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	C	637	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	THR	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	4909	0	4659	49	0
1	B	4909	0	4659	63	0
1	C	4909	0	4659	39	0
1	D	4909	0	4659	68	0
2	A	527	0	0	11	1
2	B	455	0	0	15	0
2	C	521	0	0	7	1
2	D	432	0	0	15	0
All	All	21571	0	18636	202	1

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 5.

All (202) 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:B:78:LEU:CD2	1:B:78:LEU:CG	1.78	1.58
1:B:78:LEU:HA	1:B:78:LEU:HD23	1.33	1.10
1:B:172:ARG:NH2	2:B:701:HOH:O	1.86	1.08
1:B:78:LEU:CD2	1:B:78:LEU:HA	1.97	0.95
1:B:78:LEU:CD2	1:B:78:LEU:CA	2.47	0.93
1:B:78:LEU:CD2	1:B:78:LEU:CB	2.48	0.92
1:A:77:ARG:HD2	2:C:1109:HOH:O	1.76	0.86
1:A:646:GLN:OE1	2:A:701:HOH:O	1.94	0.85
1:A:459:ARG:NH1	2:A:702:HOH:O	2.03	0.82
1:B:78:LEU:HD23	1:B:78:LEU:CA	2.07	0.82
1:D:231:THR:OG1	1:D:305:LYS:NZ	2.14	0.79
1:A:497:ARG:NH1	2:A:703:HOH:O	2.07	0.76
1:D:172:ARG:NH2	2:D:701:HOH:O	2.10	0.75
1:C:497:ARG:NH1	2:C:701:HOH:O	2.09	0.74
1:B:172:ARG:NH1	2:B:708:HOH:O	2.21	0.73
1:B:342:SER:N	2:B:706:HOH:O	2.21	0.73
1:D:342:SER:N	2:D:707:HOH:O	2.22	0.72
1:B:14:PRO:HG2	1:D:14:PRO:HG2	1.71	0.71
1:D:218:ALA:HB2	1:D:369:LYS:HE2	1.72	0.71
1:B:355:ARG:NH2	1:B:511:ARG:HH21	1.88	0.71
1:B:343:ARG:NH2	2:B:706:HOH:O	2.24	0.70
1:D:152:PHE:CD2	1:D:153:MET:CE	2.75	0.70
1:B:56:GLU:OE1	2:B:702:HOH:O	2.09	0.69
1:A:298:ARG:NH2	1:A:303:THR:HB	2.09	0.67
1:B:646:GLN:OE1	2:B:703:HOH:O	2.14	0.65
1:A:580:ILE:HB	1:A:583:ILE:HD12	1.78	0.65
1:D:303:THR:N	2:D:714:HOH:O	2.30	0.65
1:D:152:PHE:CD2	1:D:153:MET:HE1	2.32	0.64
1:B:633:VAL:HG21	1:C:633:VAL:HG21	1.80	0.63
1:D:87:ARG:NH2	1:D:418:GLU:OE2	2.32	0.63
1:B:210:ARG:NH2	2:B:709:HOH:O	2.31	0.63
1:A:75:PRO:HD2	1:A:78:LEU:HD22	1.80	0.62
1:C:376:PHE:HZ	1:C:401:ILE:HG12	1.64	0.62
1:A:298:ARG:HH12	1:A:303:THR:N	1.98	0.61
1:D:490:ARG:NH1	2:D:713:HOH:O	2.29	0.61
1:B:398:VAL:HG11	1:B:427:GLU:HG3	1.83	0.61
1:B:93:HIS:O	1:B:108:PHE:O	2.19	0.61
1:A:452:GLU:OE2	2:A:704:HOH:O	2.16	0.61
1:D:169:HIS:ND1	2:D:716:HOH:O	2.31	0.61
1:B:343:ARG:NH1	2:B:706:HOH:O	2.33	0.60
1:D:152:PHE:CD2	1:D:153:MET:HE2	2.36	0.60
1:A:298:ARG:CZ	1:A:303:THR:HB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:GLU:HB3	1:B:518:CYS:HB3	1.84	0.59
1:B:78:LEU:HD22	1:D:78:LEU:CD2	2.33	0.58
1:C:580:ILE:HB	1:C:583:ILE:HD12	1.85	0.58
1:A:173:GLN:HB3	2:A:818:HOH:O	2.04	0.58
1:B:597:ARG:NH2	2:B:713:HOH:O	2.37	0.57
1:C:398:VAL:HG11	1:C:427:GLU:HG3	1.86	0.57
1:B:465:ASP:HB3	1:B:471:ILE:CD1	2.35	0.56
1:B:78:LEU:CD2	1:D:78:LEU:HD22	2.35	0.56
1:B:220:THR:HG22	1:B:316:LYS:HE2	1.87	0.56
1:B:78:LEU:CD2	1:B:78:LEU:CD1	2.76	0.56
1:B:78:LEU:HD22	1:D:78:LEU:HD22	1.88	0.56
1:A:78:LEU:HG	1:C:78:LEU:HD21	1.88	0.55
1:A:303:THR:N	2:A:717:HOH:O	2.39	0.55
1:D:84:MET:HG3	1:D:122:LEU:HD12	1.87	0.55
1:B:343:ARG:CZ	2:B:706:HOH:O	2.55	0.55
1:B:355:ARG:HH22	1:B:511:ARG:NH2	2.05	0.55
1:D:507:ASP:OD2	1:D:511:ARG:HD2	2.07	0.55
1:B:150:THR:HB	2:B:911:HOH:O	2.07	0.55
1:D:295:ASP:OD2	2:D:702:HOH:O	2.18	0.54
1:D:207:THR:HG21	1:D:508:PRO:HB2	1.90	0.54
1:B:376:PHE:HZ	1:B:401:ILE:HG12	1.73	0.53
1:A:77:ARG:HH22	1:C:9:SER:HA	1.72	0.53
1:A:14:PRO:HG2	1:C:14:PRO:HG2	1.90	0.53
1:A:194:THR:HG21	1:C:77:ARG:HH22	1.73	0.53
1:D:152:PHE:CG	1:D:153:MET:HE2	2.44	0.53
1:B:56:GLU:OE2	2:B:704:HOH:O	2.18	0.52
1:B:493:TYR:CZ	1:B:497:ARG:HG3	2.44	0.52
1:C:644:ASP:OD1	2:C:702:HOH:O	2.19	0.52
1:A:478:ASN:ND2	1:A:479:GLU:HG3	2.25	0.51
1:C:601:ALA:HA	1:C:653:TRP:CH2	2.46	0.51
1:D:303:THR:HG23	1:D:303:THR:O	2.11	0.51
1:A:78:LEU:HG	1:C:78:LEU:CD2	2.41	0.51
1:C:465:ASP:HB3	1:C:471:ILE:CD1	2.41	0.50
1:B:422:ASP:OD1	1:B:468:HIS:HE1	1.95	0.50
1:A:76:SER:HB2	2:A:1066:HOH:O	2.12	0.50
1:D:580:ILE:HB	1:D:583:ILE:HD12	1.94	0.50
1:B:601:ALA:HA	1:B:653:TRP:CH2	2.47	0.50
1:B:355:ARG:NH2	1:B:511:ARG:NH2	2.58	0.49
1:A:398:VAL:HG11	1:A:427:GLU:HG3	1.94	0.49
1:D:343:ARG:NH2	1:D:345:ILE:HD11	2.28	0.48
1:A:11:ILE:HD12	1:A:12:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:TYR:CZ	1:D:233:GLY:HA3	2.48	0.48
1:C:497:ARG:NH2	2:C:709:HOH:O	2.34	0.48
1:D:487:GLU:OE1	2:D:704:HOH:O	2.20	0.48
1:A:509:GLN:HB3	1:A:511:ARG:HD2	1.95	0.48
1:C:176:PRO:HB3	1:C:178:PHE:CZ	2.49	0.48
1:A:10:ARG:HA	1:A:194:THR:HG22	1.96	0.48
1:A:298:ARG:HH22	1:A:303:THR:HB	1.76	0.48
1:D:415:PRO:HD3	1:D:436:PRO:HD3	1.96	0.48
1:B:172:ARG:CZ	2:B:701:HOH:O	2.48	0.47
1:C:364:PHE:HB2	1:C:614:ILE:HD13	1.95	0.47
1:A:298:ARG:NH1	1:A:303:THR:HB	2.30	0.47
1:C:429:ILE:O	1:C:470:CYS:HB2	2.15	0.47
1:D:126:GLU:HG2	2:D:715:HOH:O	2.14	0.47
1:B:412:SER:HA	1:B:413:HIS:HA	1.75	0.47
1:B:633:VAL:HG21	1:C:633:VAL:CG2	2.45	0.47
1:A:429:ILE:O	1:A:470:CYS:HB2	2.15	0.46
1:D:361:GLY:O	1:D:569:PRO:HD3	2.15	0.46
1:A:408:SER:HA	1:A:430:VAL:O	2.15	0.46
1:D:153:MET:HE1	1:D:179:ASP:HB2	1.97	0.46
1:B:75:PRO:HA	1:D:8:ASP:HA	1.96	0.46
1:D:26:GLU:HG3	2:D:898:HOH:O	2.14	0.46
1:A:452:GLU:O	1:A:456:GLU:HG3	2.16	0.46
1:C:207:THR:OG1	1:C:227:ALA:HB3	2.15	0.46
1:A:354:ILE:HD13	1:A:354:ILE:HG21	1.65	0.46
1:A:633:VAL:HG21	1:D:633:VAL:HG21	1.98	0.46
1:B:77:ARG:HG3	1:B:78:LEU:HD21	1.98	0.46
1:B:479:GLU:CB	1:B:518:CYS:HB3	2.46	0.46
1:C:75:PRO:HB2	1:C:78:LEU:HD12	1.98	0.45
1:C:412:SER:HA	1:C:413:HIS:HA	1.76	0.45
1:C:92:THR:HA	1:C:93:HIS:HA	1.72	0.45
1:D:87:ARG:HH22	1:D:418:GLU:CD	2.19	0.45
1:D:398:VAL:HG11	1:D:427:GLU:HG3	1.99	0.45
1:D:631:ILE:HD13	1:D:631:ILE:HG21	1.76	0.45
1:D:542:TRP:CZ3	1:D:590:MET:HB3	2.51	0.45
1:B:92:THR:HA	1:B:93:HIS:HA	1.77	0.45
1:C:108:PHE:O	1:C:109:GLY:C	2.50	0.45
1:D:140:SER:HA	1:D:450:VAL:CG2	2.46	0.45
1:D:355:ARG:HH22	1:D:511:ARG:HH21	1.65	0.45
1:D:601:ALA:HA	1:D:653:TRP:CH2	2.52	0.45
1:B:63:TYR:CE1	1:B:172:ARG:HG2	2.52	0.45
1:D:429:ILE:O	1:D:470:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:HA	1:A:413:HIS:HA	1.71	0.45
1:C:497:ARG:NE	2:C:709:HOH:O	2.34	0.45
1:D:442:TRP:CE2	1:D:488:ARG:HG2	2.52	0.45
1:C:207:THR:HG21	1:C:508:PRO:HB2	1.99	0.44
1:B:108:PHE:O	1:B:109:GLY:C	2.53	0.44
1:D:465:ASP:HB3	1:D:471:ILE:CD1	2.47	0.44
1:B:355:ARG:HH22	1:B:511:ARG:HH21	1.58	0.44
1:C:538:ARG:NH2	1:C:559:GLU:OE2	2.42	0.44
1:A:79:VAL:HG12	1:A:84:MET:CE	2.48	0.44
1:D:667:LYS:O	2:D:705:HOH:O	2.21	0.44
1:B:200:TYR:CZ	1:B:233:GLY:HA3	2.53	0.44
1:B:521:ASP:OD2	2:B:705:HOH:O	2.20	0.44
1:D:94:ALA:HB3	1:D:134:ASP:HB3	2.00	0.44
1:B:218:ALA:HB2	1:B:369:LYS:HE2	2.00	0.44
1:C:75:PRO:HD2	1:C:78:LEU:HD13	2.00	0.44
1:D:153:MET:HE3	1:D:153:MET:HB2	1.75	0.44
1:B:78:LEU:HD22	1:D:78:LEU:HD21	1.99	0.43
1:C:16:ASP:HB3	1:C:46:VAL:O	2.18	0.43
1:A:631:ILE:HG22	1:D:631:ILE:HG22	2.01	0.43
1:A:54:ASN:C	2:A:706:HOH:O	2.57	0.43
1:A:19:TRP:CD1	1:A:46:VAL:HG13	2.54	0.43
1:A:544:ASN:O	1:A:545:LEU:C	2.55	0.43
1:B:77:ARG:O	1:B:78:LEU:HD23	2.18	0.43
1:B:413:HIS:O	1:B:436:PRO:HA	2.18	0.43
1:A:85:ILE:O	1:A:192:LEU:HD12	2.19	0.43
1:B:194:THR:HG21	2:D:744:HOH:O	2.17	0.43
1:C:93:HIS:O	1:C:108:PHE:O	2.37	0.43
1:B:173:GLN:HB3	2:B:776:HOH:O	2.18	0.43
1:C:122:LEU:HD23	1:C:127:ASN:OD1	2.19	0.43
1:B:579:THR:OG1	1:B:596:GLN:HB2	2.18	0.43
1:A:342:SER:N	2:A:750:HOH:O	2.51	0.43
1:B:77:ARG:HG3	1:B:78:LEU:CD2	2.48	0.43
1:A:8:ASP:HA	1:C:75:PRO:HA	2.01	0.43
1:B:429:ILE:O	1:B:470:CYS:HB2	2.19	0.43
1:D:644:ASP:HB2	1:D:646:GLN:OE1	2.18	0.43
1:D:37:PRO:HA	1:D:69:GLN:OE1	2.18	0.42
1:C:426:ARG:HD3	2:C:1169:HOH:O	2.19	0.42
1:B:507:ASP:OD2	1:B:511:ARG:HD2	2.20	0.42
1:D:173:GLN:HB3	2:D:813:HOH:O	2.19	0.42
1:A:330:ALA:O	1:A:347:ALA:HA	2.19	0.42
1:B:316:LYS:HB2	1:B:324:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:TRP:CH2	1:D:470:CYS:HA	2.55	0.42
1:D:418:GLU:CG	1:D:464:ARG:HD2	2.50	0.42
1:D:11:ILE:H	1:D:194:THR:HB	1.83	0.42
1:D:97:VAL:HG12	1:D:104:LEU:HD12	2.01	0.42
1:D:431:ILE:HD12	1:D:470:CYS:SG	2.59	0.42
1:D:490:ARG:HD2	2:D:713:HOH:O	2.19	0.42
1:B:75:PRO:HB3	1:D:8:ASP:O	2.19	0.42
1:C:275:ARG:NH2	1:C:345:ILE:CD1	2.83	0.42
1:A:92:THR:HA	1:A:93:HIS:HA	1.83	0.42
1:C:479:GLU:CG	1:C:518:CYS:HB3	2.50	0.42
1:D:15:LEU:HD23	1:D:15:LEU:HA	1.89	0.42
1:D:412:SER:HA	1:D:413:HIS:HA	1.79	0.42
1:D:422:ASP:OD1	1:D:468:HIS:HE1	2.01	0.42
1:A:397:ASP:O	1:A:401:ILE:HG13	2.19	0.42
1:B:137:ILE:HD13	1:B:137:ILE:HG21	1.89	0.42
1:D:275:ARG:HA	1:D:275:ARG:HD2	1.85	0.42
1:A:313:ARG:HB3	2:A:950:HOH:O	2.20	0.41
1:C:334:PRO:HA	1:C:345:ILE:HD11	2.03	0.41
1:A:172:ARG:NH2	2:A:710:HOH:O	2.30	0.41
1:A:279:ILE:O	1:A:291:GLY:HA2	2.21	0.41
1:B:11:ILE:H	1:B:194:THR:HB	1.85	0.41
1:C:150:THR:HG22	1:C:151:ALA:O	2.20	0.41
1:C:9:SER:OG	2:C:703:HOH:O	2.22	0.41
1:D:479:GLU:HB3	1:D:518:CYS:HB3	2.03	0.41
1:A:632:ARG:HA	1:A:632:ARG:HD3	1.83	0.41
1:C:433:ASP:OD2	1:C:465:ASP:OD2	2.39	0.41
1:A:601:ALA:HA	1:A:653:TRP:CH2	2.56	0.41
1:D:128:LEU:HD12	1:D:128:LEU:HA	1.83	0.41
1:D:303:THR:HG22	2:D:714:HOH:O	2.19	0.41
1:B:497:ARG:HD2	1:B:497:ARG:HA	1.92	0.40
1:C:619:TRP:HA	1:C:620:ASN:HA	1.89	0.40
1:D:398:VAL:HG21	1:D:423:LEU:HG	2.03	0.40
1:D:589:GLU:OE2	2:D:706:HOH:O	2.21	0.40
1:A:207:THR:CG2	1:A:508:PRO:HB2	2.51	0.40
1:A:507:ASP:OD2	1:A:511:ARG:CD	2.70	0.40
1:D:413:HIS:O	1:D:436:PRO:HA	2.21	0.40
1:D:375:GLY:HA3	1:D:408:SER:O	2.21	0.40

All (1) 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)
2:A:1166:HOH:O	2:C:1180:HOH:O[1_655]	2.16	0.04

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	612/670 (91%)	587 (96%)	25 (4%)	0	100	100
1	B	612/670 (91%)	587 (96%)	25 (4%)	0	100	100
1	C	612/670 (91%)	589 (96%)	23 (4%)	0	100	100
1	D	612/670 (91%)	591 (97%)	21 (3%)	0	100	100
All	All	2448/2680 (91%)	2354 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	503/543 (93%)	494 (98%)	9 (2%)	59	72
1	B	503/543 (93%)	495 (98%)	8 (2%)	62	76
1	C	503/543 (93%)	494 (98%)	9 (2%)	59	72
1	D	503/543 (93%)	493 (98%)	10 (2%)	55	69
All	All	2012/2172 (93%)	1976 (98%)	36 (2%)	59	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	87	ARG
1	A	194	THR
1	A	355	ARG
1	A	376	PHE
1	A	420	MET
1	A	568	LYS
1	A	575	TYR
1	A	597	ARG
1	B	153	MET
1	B	355	ARG
1	B	376	PHE
1	B	381	ASP
1	B	420	MET
1	B	575	TYR
1	B	597	ARG
1	B	645	ARG
1	C	9	SER
1	C	229	ASP
1	C	355	ARG
1	C	376	PHE
1	C	387	ARG
1	C	485	ASP
1	C	575	TYR
1	C	597	ARG
1	C	645	ARG
1	D	9	SER
1	D	153	MET
1	D	355	ARG
1	D	376	PHE
1	D	387	ARG
1	D	412	SER
1	D	485	ASP
1	D	568	LYS
1	D	575	TYR
1	D	597	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 monosaccharides 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	620/670 (92%)	-0.91	6 (0%) 82 81	7, 14, 30, 64	0
1	B	620/670 (92%)	-0.71	7 (1%) 80 79	9, 18, 36, 65	0
1	C	620/670 (92%)	-0.85	4 (0%) 89 88	7, 15, 31, 55	0
1	D	620/670 (92%)	-0.73	6 (0%) 82 81	7, 19, 37, 68	0
All	All	2480/2680 (92%)	-0.80	23 (0%) 84 83	7, 17, 34, 68	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	THR	4.3
1	C	342	SER	3.1
1	B	298	ARG	3.1
1	C	343	ARG	3.0
1	D	-1	ASN	2.9
1	B	303	THR	2.7
1	D	235	ASP	2.7
1	B	274	GLY	2.7
1	A	274	GLY	2.6
1	A	298	ARG	2.6
1	B	343	ARG	2.6
1	D	343	ARG	2.6
1	D	298	ARG	2.5
1	A	343	ARG	2.5
1	D	78	LEU	2.5
1	B	-1	ASN	2.5
1	C	298	ARG	2.4
1	A	235	ASP	2.4
1	B	536	ILE	2.2
1	D	274	GLY	2.1
1	B	297	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	303	THR	2.0
1	A	342	SER	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 monosaccharides 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.