



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 07:05 PM EDT

PDB ID : 3WL4
Title : N,N'-diacetylchitobiose deacetylase (Se-derivative) from *Pyrococcus furiosus*
Authors : Nakamura, T.; Niiyama, M.; Hashimoto, W.; Uegaki, K.
Deposited on : 2013-11-07
Resolution : 1.54 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

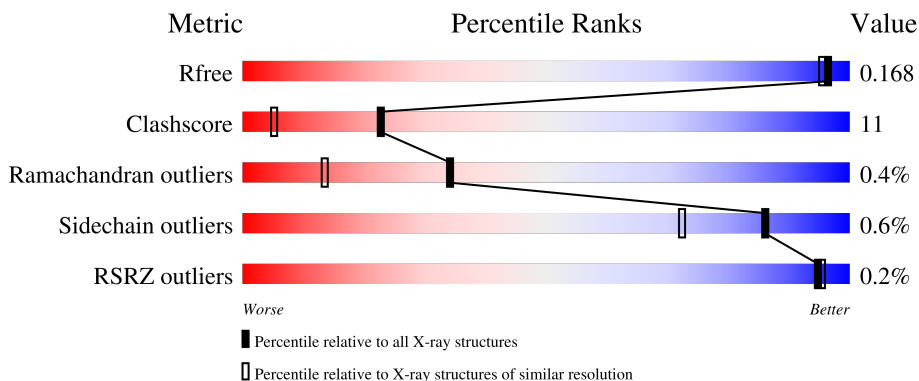
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	267	
1	B	267	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TAM	A	308	-	X	X	-
5	TAM	A	309	-	X	X	-
5	TAM	B	308	-	X	-	-
5	TAM	B	309	-	X	X	-
6	HEZ	A	316	-	-	X	-
6	HEZ	B	313	-	-	X	-
6	HEZ	B	320	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4941 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	267	2190	1416	360	404	3	7	0	0	0
1	B	267	2190	1416	360	404	3	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q8U3V1
B	1	MSE	-	EXPRESSION TAG	UNP Q8U3V1

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Cd 2	0	0
2	B	2	Total 2	Cd 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

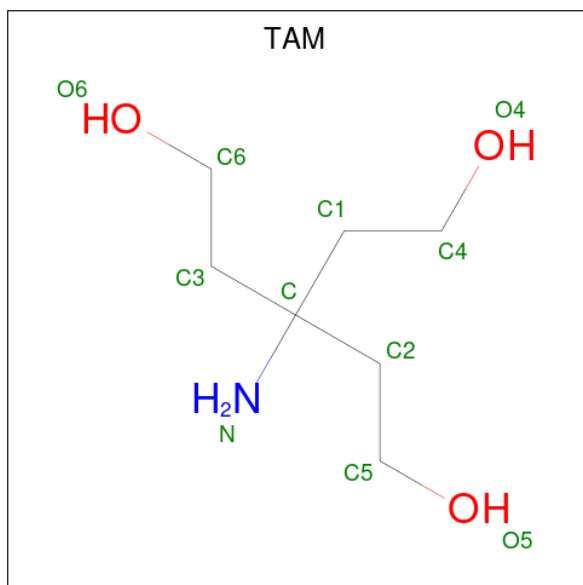
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	Cl 4	0	0

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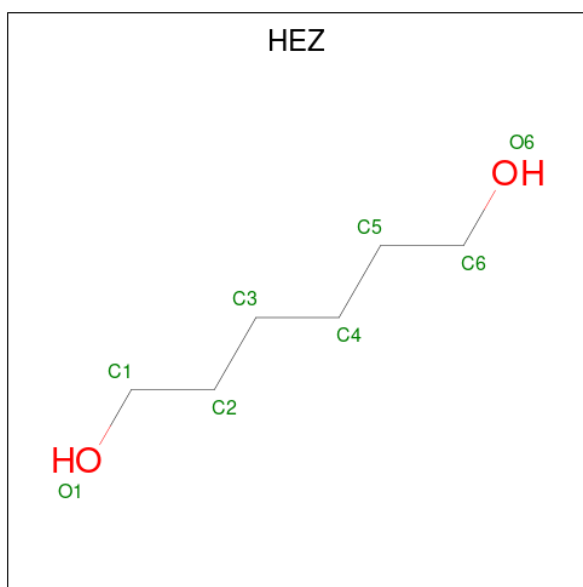
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total Cl 4 4	0	0

- Molecule 5 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 11 7 1 3	0	0
5	A	1	Total C N O 11 7 1 3	0	0
5	B	1	Total C N O 11 7 1 3	0	0
5	B	1	Total C N O 11 7 1 3	0	0

- Molecule 6 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



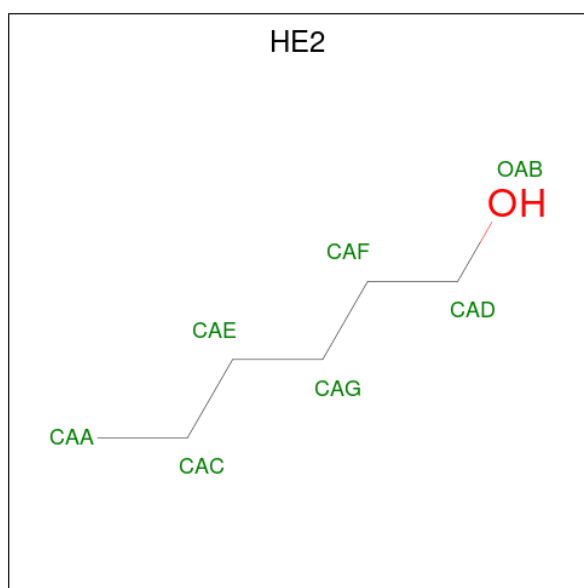
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is HEXAN-1-OL (three-letter code: HE2) (formula: C₆H₁₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	6	1		
7	B	1	Total	C	O	0	0
			7	6	1		

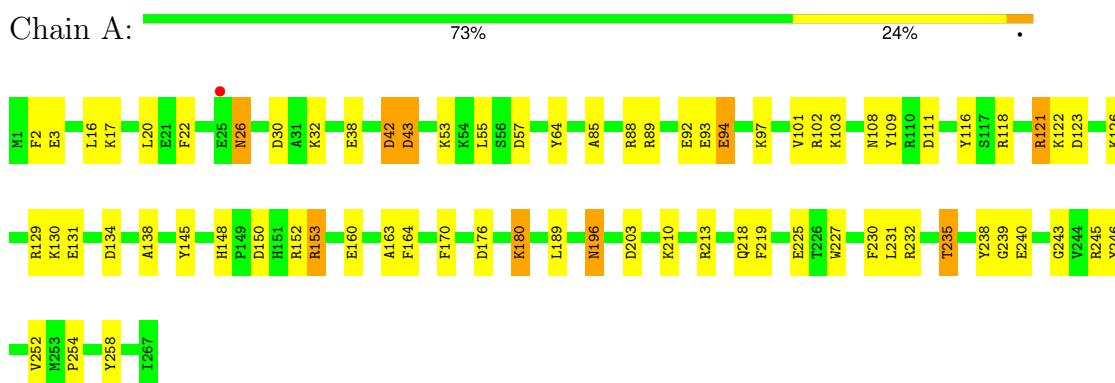
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	165	Total 165	O 165	0	0
8	B	156	Total 156	O 156	0	0

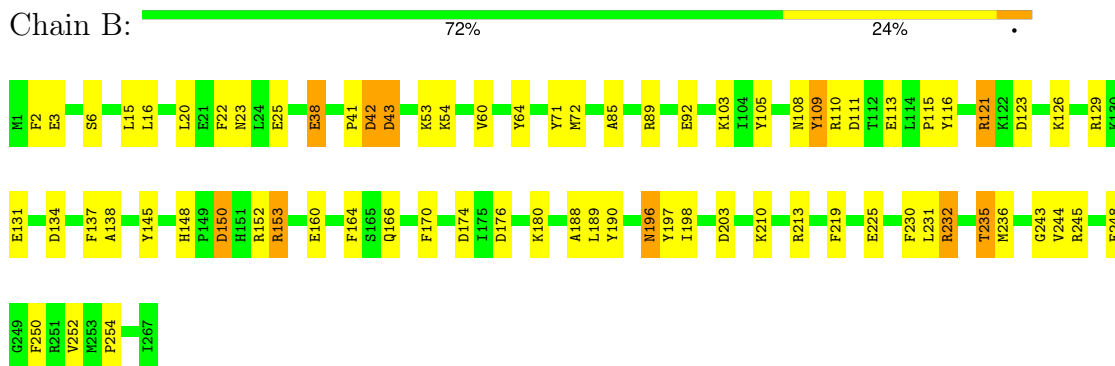
3 Residue-property plots [i](#)

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	113.89Å 113.89Å 201.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.40 – 1.54 26.40 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.40-1.54) 99.8 (26.40-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 1.54Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.154 , 0.169 0.153 , 0.168	Depositor DCC
R_{free} test set	7197 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.476 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4941	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CA, CL, HEZ, TAM, HE2

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	1.74	25/2242 (1.1%)	1.74	51/3023 (1.7%)
1	B	1.77	31/2242 (1.4%)	1.70	41/3023 (1.4%)
All	All	1.76	56/4484 (1.2%)	1.72	92/6046 (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	A	0	1
1	B	0	1
All	All	0	2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	GLU	CG-CD	10.14	1.67	1.51
1	A	94	GLU	CD-OE1	9.15	1.35	1.25
1	B	166	GLN	CB-CG	-8.81	1.28	1.52
1	A	225	GLU	CG-CD	7.69	1.63	1.51
1	B	225	GLU	CG-CD	7.49	1.63	1.51
1	B	126	LYS	CD-CE	-7.39	1.32	1.51
1	B	197	TYR	CD1-CE1	6.89	1.49	1.39
1	A	93	GLU	CB-CG	6.77	1.65	1.52
1	B	85	ALA	CA-CB	6.71	1.66	1.52
1	B	38	GLU	CD-OE1	-6.62	1.18	1.25
1	B	131	GLU	CD-OE2	-6.62	1.18	1.25
1	A	53	LYS	CB-CG	6.45	1.70	1.52
1	B	53	LYS	CB-CG	6.40	1.69	1.52
1	B	108	ASN	CG-ND2	-6.34	1.17	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	GLU	CG-CD	-6.28	1.42	1.51
1	B	64	TYR	CD1-CE1	6.25	1.48	1.39
1	A	219	PHE	N-CA	6.20	1.58	1.46
1	B	198	ILE	CB-CG1	6.14	1.71	1.54
1	A	64	TYR	CD1-CE1	6.04	1.48	1.39
1	B	213	ARG	CZ-NH1	6.03	1.40	1.33
1	B	103	LYS	CE-NZ	5.99	1.64	1.49
1	B	219	PHE	CE1-CZ	5.83	1.48	1.37
1	A	213	ARG	CZ-NH1	5.82	1.40	1.33
1	B	2	PHE	CE2-CZ	5.81	1.48	1.37
1	A	2	PHE	CE2-CZ	5.78	1.48	1.37
1	A	258	TYR	CE2-CZ	-5.71	1.31	1.38
1	A	108	ASN	CG-ND2	-5.67	1.18	1.32
1	B	188	ALA	CA-CB	5.63	1.64	1.52
1	B	243	GLY	N-CA	5.61	1.54	1.46
1	A	160	GLU	CG-CD	5.59	1.60	1.51
1	B	166	GLN	CG-CD	5.52	1.63	1.51
1	A	122	LYS	CE-NZ	5.50	1.62	1.49
1	A	103	LYS	CE-NZ	5.47	1.62	1.49
1	A	180	LYS	CE-NZ	5.44	1.62	1.49
1	B	160	GLU	CD-OE1	-5.43	1.19	1.25
1	B	180	LYS	CD-CE	5.43	1.64	1.51
1	B	197	TYR	CD2-CE2	5.41	1.47	1.39
1	B	6	SER	CA-CB	5.41	1.61	1.52
1	B	219	PHE	N-CA	5.33	1.57	1.46
1	A	53	LYS	CD-CE	5.28	1.64	1.51
1	B	54	LYS	CD-CE	5.24	1.64	1.51
1	A	239	GLY	N-CA	5.23	1.53	1.46
1	A	213	ARG	CG-CD	5.22	1.65	1.51
1	A	3	GLU	CG-CD	-5.22	1.44	1.51
1	A	130	LYS	CD-CE	5.18	1.64	1.51
1	A	97	LYS	CD-CE	5.17	1.64	1.51
1	A	101	VAL	CB-CG1	5.17	1.63	1.52
1	A	134	ASP	CA-CB	5.13	1.65	1.53
1	B	126	LYS	CE-NZ	5.13	1.61	1.49
1	A	85	ALA	CA-CB	5.11	1.63	1.52
1	B	105	TYR	CG-CD2	5.08	1.45	1.39
1	A	180	LYS	CD-CE	5.06	1.64	1.51
1	B	244	VAL	CB-CG2	5.05	1.63	1.52
1	B	60	VAL	N-CA	5.05	1.56	1.46
1	B	134	ASP	CA-CB	5.03	1.65	1.53
1	B	250	PHE	CE1-CZ	5.00	1.46	1.37

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PHE	CB-CG-CD1	-11.50	112.75	120.80
1	A	232	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	A	153	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	B	232	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	64	TYR	CB-CG-CD2	-10.18	114.89	121.00
1	B	152	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	A	121	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	153	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	B	164	PHE	CB-CG-CD2	-9.61	114.07	120.80
1	B	64	TYR	CB-CG-CD2	-9.34	115.40	121.00
1	A	245	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	A	102	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	B	170	PHE	CB-CG-CD1	-8.80	114.64	120.80
1	A	164	PHE	CB-CG-CD2	-8.32	114.98	120.80
1	B	89	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	B	111	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	16	LEU	CB-CG-CD1	-7.89	97.58	111.00
1	B	153	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	121	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	180	LYS	CD-CE-NZ	7.54	129.05	111.70
1	A	57	ASP	CB-CG-OD1	7.44	125.00	118.30
1	B	109	TYR	CZ-CE2-CD2	-7.42	113.12	119.80
1	A	88	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	B	129	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	B	22	PHE	CG-CD1-CE1	-7.20	112.89	120.80
1	A	92	GLU	OE1-CD-OE2	-7.07	114.81	123.30
1	A	164	PHE	CB-CG-CD1	7.05	125.73	120.80
1	B	137	PHE	CB-CG-CD2	-7.03	115.88	120.80
1	A	246	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	A	43	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	164	PHE	CB-CG-CD1	6.83	125.58	120.80
1	B	150	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	89	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	B	92	GLU	OE1-CD-OE2	-6.73	115.23	123.30
1	B	245	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	111	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	131	GLU	OE1-CD-OE2	6.57	131.18	123.30
1	A	210	LYS	CD-CE-NZ	-6.54	96.66	111.70
1	B	203	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	230	PHE	CB-CG-CD2	-6.42	116.31	120.80
1	A	88	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	B	230	PHE	CB-CG-CD2	-6.33	116.37	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	121	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	235	THR	CA-CB-CG2	-6.24	103.67	112.40
1	B	16	LEU	CB-CG-CD1	-6.22	100.42	111.00
1	A	118	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	64	TYR	CD1-CE1-CZ	-6.15	114.27	119.80
1	A	126	LYS	CD-CE-NZ	-6.14	97.58	111.70
1	A	235	THR	CA-CB-CG2	-6.12	103.83	112.40
1	A	203	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	130	LYS	CD-CE-NZ	-6.10	97.68	111.70
1	B	198	ILE	CA-CB-CG1	-6.05	99.50	111.00
1	B	15	LEU	CB-CG-CD2	-6.04	100.73	111.00
1	B	43	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	145	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	B	121	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	210	LYS	CD-CE-NZ	-5.94	98.03	111.70
1	A	123	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	123	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	B	225	GLU	CG-CD-OE2	5.82	129.95	118.30
1	B	123	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	238	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	55	LEU	CB-CG-CD1	-5.74	101.25	111.00
1	A	64	TYR	CD1-CE1-CZ	-5.71	114.66	119.80
1	B	126	LYS	CD-CE-NZ	-5.71	98.57	111.70
1	A	111	ASP	N-CA-CB	-5.67	100.39	110.60
1	B	174	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	176	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	152	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	227	TRP	CA-CB-CG	-5.58	103.09	113.70
1	A	109	TYR	CZ-CE2-CD2	-5.55	114.80	119.80
1	A	53	LYS	CD-CE-NZ	-5.50	99.05	111.70
1	B	190	TYR	CG-CD1-CE1	-5.45	116.94	121.30
1	A	109	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	B	111	ASP	N-CA-CB	-5.39	100.90	110.60
1	A	176	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	225	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	64	TYR	CE1-CZ-CE2	5.29	128.26	119.80
1	B	22	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	A	89	ARG	CA-CB-CG	-5.27	101.81	113.40
1	A	102	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	258	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	225	GLU	CG-CD-OE2	5.20	128.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	A	102	ARG	CD-NE-CZ	5.17	130.84	123.60
1	B	145	TYR	CG-CD1-CE1	-5.16	117.17	121.30
1	A	129	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	17	LYS	CD-CE-NZ	-5.08	100.01	111.70
1	A	145	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	B	71	TYR	CD1-CE1-CZ	-5.04	115.26	119.80
1	A	170	PHE	CD1-CG-CD2	5.01	124.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	B	121	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2190	0	2161	38	0
1	B	2190	0	2161	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	22	0	31	14	0
5	B	22	0	32	11	0
6	A	72	0	125	25	0
6	B	96	0	168	27	0
7	A	7	0	14	0	0
7	B	7	0	13	4	0
8	A	165	0	0	9	0
8	B	156	0	0	7	0
All	All	4941	0	4705	107	0

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 11.

All (107) 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)
6:B:313:HEZ:H62	8:B:536:HOH:O	1.25	1.29
5:A:309:TAM:H52	5:A:309:TAM:C4	1.74	1.16
6:A:316:HEZ:C2	8:A:532:HOH:O	1.95	1.12
5:A:309:TAM:C4	5:A:309:TAM:C5	2.29	1.09
5:A:309:TAM:H52	5:A:309:TAM:H42	1.11	1.09
5:A:309:TAM:C5	5:A:309:TAM:H42	1.75	1.08
5:A:308:TAM:O6	5:A:308:TAM:H12	1.30	1.07
1:A:243:GLY:HA2	6:A:318:HEZ:H62	1.06	1.06
1:B:113:GLU:OE1	6:B:320:HEZ:H22	1.56	1.04
5:A:308:TAM:O6	5:A:308:TAM:C1	2.05	1.03
6:B:320:HEZ:H62	8:B:431:HOH:O	1.59	1.00
1:A:180:LYS:HE3	8:A:499:HOH:O	1.60	1.00
1:B:43:ASP:OD1	5:B:309:TAM:H42	1.59	1.00
1:B:42:ASP:OD2	5:B:309:TAM:H51	1.63	0.97
1:B:110:ARG:H	6:B:320:HEZ:H41	1.32	0.95
6:A:316:HEZ:H21	8:A:532:HOH:O	1.56	0.93
1:B:116:TYR:H	6:B:313:HEZ:H32	1.31	0.93
1:A:180:LYS:CE	8:A:499:HOH:O	2.17	0.90
1:B:196:ASN:HD21	1:B:252:VAL:H	1.20	0.90
5:A:308:TAM:H12	5:A:308:TAM:HO6	1.37	0.88
1:B:153:ARG:HH12	6:B:313:HEZ:H41	1.41	0.85
1:A:196:ASN:HD21	1:A:252:VAL:H	1.19	0.85
6:B:318:HEZ:H41	8:B:452:HOH:O	1.80	0.82
1:A:26:ASN:H	1:A:26:ASN:HD22	1.27	0.82
1:A:243:GLY:CA	6:A:318:HEZ:H62	2.02	0.82
6:A:316:HEZ:H22	8:A:532:HOH:O	1.71	0.81
5:B:309:TAM:H62	5:B:309:TAM:O4	1.80	0.81
1:B:254:PRO:HB3	6:B:319:HEZ:H22	1.64	0.79
6:B:320:HEZ:H21	6:B:320:HEZ:O6	1.82	0.79
1:A:243:GLY:HA2	6:A:318:HEZ:C6	2.01	0.78
5:B:309:TAM:O4	5:B:309:TAM:C6	2.33	0.76
1:A:26:ASN:HD22	1:A:26:ASN:N	1.82	0.74
6:A:317:HEZ:H41	6:A:319:HEZ:H12	1.71	0.72
1:B:115:PRO:HD3	6:B:320:HEZ:H61	1.72	0.72
1:B:235:THR:HG22	7:B:316:HE2:HAA3	1.71	0.72
1:A:148:HIS:HD2	1:A:150:ASP:H	1.36	0.71
6:B:320:HEZ:C6	8:B:431:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:H	6:B:320:HEZ:C4	2.03	0.70
1:B:148:HIS:HD2	1:B:150:ASP:H	1.40	0.67
1:A:42:ASP:OD2	5:A:309:TAM:H61	1.94	0.67
5:A:308:TAM:H62	8:A:463:HOH:O	1.94	0.67
1:B:72:MSE:HB2	6:B:318:HEZ:H61	1.76	0.66
1:A:148:HIS:HE1	8:A:408:HOH:O	1.80	0.64
1:A:116:TYR:H	6:A:314:HEZ:H62	1.63	0.64
1:A:254:PRO:HB3	6:A:316:HEZ:H32	1.79	0.64
1:A:218:GLN:O	6:A:315:HEZ:H61	1.99	0.63
1:B:110:ARG:N	6:B:320:HEZ:H41	2.10	0.62
6:B:319:HEZ:H12	8:B:426:HOH:O	1.98	0.62
1:B:148:HIS:HE1	6:B:318:HEZ:O6	1.82	0.62
1:B:235:THR:HG22	7:B:316:HE2:CAA	2.31	0.60
5:B:308:TAM:C3	5:B:308:TAM:O5	2.50	0.59
1:B:110:ARG:H	6:B:320:HEZ:C5	2.14	0.59
1:B:20:LEU:O	6:B:319:HEZ:H31	2.03	0.58
1:B:231:LEU:HD23	7:B:316:HE2:HAF1	1.86	0.58
1:A:94:GLU:HG3	8:A:521:HOH:O	2.04	0.56
1:B:113:GLU:OE1	6:B:320:HEZ:C2	2.44	0.56
1:B:116:TYR:N	6:B:313:HEZ:H32	2.12	0.55
1:A:42:ASP:OD2	5:A:309:TAM:C6	2.53	0.55
1:B:196:ASN:ND2	1:B:252:VAL:H	1.97	0.55
5:B:308:TAM:H62	8:B:531:HOH:O	2.07	0.55
1:A:26:ASN:N	1:A:26:ASN:ND2	2.49	0.55
1:A:196:ASN:ND2	1:A:252:VAL:H	1.98	0.55
1:B:23:ASN:ND2	1:B:25:GLU:HB2	2.23	0.54
5:B:308:TAM:O5	5:B:308:TAM:H32	2.07	0.54
1:A:254:PRO:HA	6:A:316:HEZ:H32	1.90	0.54
1:B:38:GLU:HB2	1:B:43:ASP:HB2	1.89	0.53
1:B:109:TYR:HD1	6:B:320:HEZ:C6	2.21	0.53
1:A:38:GLU:HB2	1:A:43:ASP:HB2	1.90	0.53
1:B:254:PRO:CB	6:B:319:HEZ:H22	2.37	0.53
1:A:20:LEU:O	6:A:316:HEZ:H41	2.08	0.53
1:B:110:ARG:H	6:B:320:HEZ:H52	1.74	0.52
1:A:148:HIS:CD2	1:A:150:ASP:H	2.24	0.50
1:A:116:TYR:H	6:A:314:HEZ:C6	2.25	0.50
5:A:308:TAM:O4	5:A:308:TAM:H22	2.11	0.50
5:B:308:TAM:O5	5:B:308:TAM:H62	2.11	0.50
1:A:153:ARG:HH12	6:A:314:HEZ:H42	1.76	0.50
1:B:153:ARG:HH12	6:B:313:HEZ:C4	2.20	0.50
1:A:163:ALA:HB2	6:A:319:HEZ:H31	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:NH1	6:B:313:HEZ:H41	2.18	0.49
1:A:231:LEU:O	1:A:235:THR:HG23	2.13	0.48
1:A:254:PRO:CB	6:A:316:HEZ:H32	2.43	0.48
1:A:254:PRO:CA	6:A:316:HEZ:H32	2.45	0.46
6:A:311:HEZ:H21	6:A:311:HEZ:H52	1.17	0.46
1:B:148:HIS:CD2	1:B:150:ASP:H	2.26	0.46
5:B:308:TAM:O5	5:B:308:TAM:C6	2.64	0.46
1:A:240:GLU:HA	6:A:318:HEZ:H42	1.97	0.45
5:B:309:TAM:O5	8:B:463:HOH:O	2.18	0.45
1:A:20:LEU:HB3	6:A:316:HEZ:H31	1.97	0.45
5:A:309:TAM:H52	5:A:309:TAM:O4	2.08	0.45
1:B:231:LEU:O	1:B:235:THR:HG23	2.16	0.45
1:B:109:TYR:HB3	6:B:320:HEZ:H52	1.99	0.44
6:A:316:HEZ:H21	8:A:530:HOH:O	2.18	0.43
1:B:110:ARG:N	6:B:320:HEZ:H52	2.33	0.43
1:A:240:GLU:OE1	6:A:318:HEZ:H21	2.18	0.43
1:B:138:ALA:O	1:B:189:LEU:HA	2.18	0.43
1:B:43:ASP:OD1	5:B:309:TAM:C4	2.49	0.43
1:A:153:ARG:HH21	5:A:308:TAM:H61	1.84	0.42
1:B:23:ASN:HD22	1:B:25:GLU:H	1.66	0.42
1:B:41:PRO:O	1:B:42:ASP:CG	2.58	0.42
1:A:22:PHE:HD1	6:A:316:HEZ:H61	1.85	0.41
1:A:32:LYS:HB3	1:A:32:LYS:HE2	1.94	0.41
1:B:248:GLU:HA	7:B:316:HE2:HAA1	2.02	0.41
1:A:22:PHE:HD1	6:A:316:HEZ:H42	1.86	0.41
1:B:232:ARG:O	1:B:236:MSE:HG3	2.20	0.41
1:A:153:ARG:HH12	6:A:314:HEZ:C4	2.34	0.40
1:A:153:ARG:NH2	5:A:308:TAM:H61	2.36	0.40
1:A:138:ALA:O	1:A:189:LEU:HA	2.21	0.40

There are no symmetry-related clashes.

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	265/267 (99%)	259 (98%)	5 (2%)	1 (0%)	34	13
1	B	265/267 (99%)	260 (98%)	4 (2%)	1 (0%)	34	13
All	All	530/534 (99%)	519 (98%)	9 (2%)	2 (0%)	34	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	B	42	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/232 (103%)	237 (99%)	2 (1%)	81	64
1	B	239/232 (103%)	238 (100%)	1 (0%)	91	82
All	All	478/464 (103%)	475 (99%)	3 (1%)	86	72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	196	ASN
1	B	196	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	148	HIS
1	A	169	ASN
1	A	172	ASN
1	A	196	ASN
1	A	218	GLN

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Mol	Chain	Res	Type
1	B	23	ASN
1	B	148	HIS
1	B	169	ASN
1	B	172	ASN
1	B	196	ASN
1	B	218	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 14 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	HEZ	A	318	-	7,7,7	1.35	0	6,6,6	1.21	0
7	HE2	A	313	-	6,6,6	0.99	1 (16%)	5,5,5	0.85	0
6	HEZ	B	317	-	7,7,7	1.19	1 (14%)	6,6,6	0.97	0
5	TAM	B	308	-	10,10,10	1.72	1 (10%)	12,12,12	4.33	9 (75%)
5	TAM	A	309	2	10,10,10	3.19	9 (90%)	12,12,12	6.03	8 (66%)
6	HEZ	B	310	-	7,7,7	1.00	0	6,6,6	0.85	0
6	HEZ	A	315	-	7,7,7	0.55	0	6,6,6	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEZ	A	319	-	7,7,7	0.78	0	6,6,6	1.60	2 (33%)
6	HEZ	A	316	-	7,7,7	0.95	0	6,6,6	0.99	0
6	HEZ	B	320	-	7,7,7	0.83	0	6,6,6	1.96	2 (33%)
6	HEZ	B	322	-	7,7,7	0.30	0	6,6,6	1.52	1 (16%)
6	HEZ	A	311	-	7,7,7	0.29	0	6,6,6	1.76	2 (33%)
5	TAM	A	308	-	10,10,10	1.38	2 (20%)	12,12,12	6.09	8 (66%)
6	HEZ	B	318	-	7,7,7	1.06	0	6,6,6	2.00	3 (50%)
6	HEZ	B	314	-	7,7,7	1.34	1 (14%)	6,6,6	0.84	0
6	HEZ	A	314	-	7,7,7	0.99	0	6,6,6	2.00	2 (33%)
5	TAM	B	309	2	10,10,10	3.07	7 (70%)	12,12,12	6.27	7 (58%)
6	HEZ	B	319	-	7,7,7	1.32	1 (14%)	6,6,6	0.55	0
6	HEZ	B	311	-	7,7,7	0.70	0	6,6,6	1.27	1 (16%)
6	HEZ	A	312	-	7,7,7	0.28	0	6,6,6	1.07	0
6	HEZ	A	310	-	7,7,7	1.12	0	6,6,6	1.03	0
6	HEZ	B	312	-	7,7,7	1.05	0	6,6,6	0.95	0
6	HEZ	B	321	-	7,7,7	0.58	0	6,6,6	1.14	0
6	HEZ	B	313	-	7,7,7	1.93	2 (28%)	6,6,6	1.22	1 (16%)
6	HEZ	A	317	-	7,7,7	1.28	1 (14%)	6,6,6	1.99	2 (33%)
7	HE2	B	316	-	6,6,6	1.11	0	5,5,5	1.42	1 (20%)
6	HEZ	B	315	-	7,7,7	0.48	0	6,6,6	1.20	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEZ	A	318	-	-	3/5/5/5	-
7	HE2	A	313	-	-	2/4/4/4	-
6	HEZ	B	317	-	-	4/5/5/5	-
5	TAM	B	308	-	-	7/12/12/12	-
5	TAM	A	309	2	-	3/12/12/12	-
6	HEZ	B	310	-	-	0/5/5/5	-
6	HEZ	A	315	-	-	3/5/5/5	-
6	HEZ	A	319	-	-	1/5/5/5	-
6	HEZ	A	316	-	-	4/5/5/5	-
6	HEZ	B	320	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEZ	B	322	-	-	2/5/5/5	-
6	HEZ	A	311	-	-	2/5/5/5	-
5	TAM	A	308	-	-	4/12/12/12	-
6	HEZ	B	318	-	-	2/5/5/5	-
6	HEZ	B	314	-	-	2/5/5/5	-
6	HEZ	A	314	-	-	3/5/5/5	-
5	TAM	B	309	2	-	8/12/12/12	-
6	HEZ	B	319	-	-	3/5/5/5	-
6	HEZ	B	311	-	-	3/5/5/5	-
6	HEZ	A	312	-	-	0/5/5/5	-
6	HEZ	A	310	-	-	0/5/5/5	-
6	HEZ	B	312	-	-	0/5/5/5	-
6	HEZ	B	321	-	-	4/5/5/5	-
6	HEZ	B	313	-	-	4/5/5/5	-
6	HEZ	A	317	-	-	4/5/5/5	-
7	HE2	B	316	-	-	2/4/4/4	-
6	HEZ	B	315	-	-	1/5/5/5	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	309	TAM	C2-C5	-4.75	1.43	1.52
6	B	313	HEZ	C4-C3	4.37	1.73	1.51
5	B	309	TAM	C3-C6	-4.17	1.44	1.52
5	A	309	TAM	C3-C6	-4.16	1.44	1.52
5	A	309	TAM	C2-C	-4.15	1.47	1.53
5	B	308	TAM	C2-C	-3.98	1.48	1.53
5	A	309	TAM	C3-C	-3.90	1.48	1.53
5	B	309	TAM	C1-C	-3.79	1.48	1.53
5	B	309	TAM	C2-C	-3.69	1.48	1.53
5	A	309	TAM	C-N	3.60	1.61	1.49
5	B	309	TAM	C-N	3.17	1.59	1.49
5	A	309	TAM	C1-C4	-2.95	1.46	1.52
5	A	309	TAM	O5-C5	-2.91	1.27	1.42
5	A	309	TAM	C1-C	-2.85	1.49	1.53
5	B	309	TAM	O4-C4	-2.76	1.28	1.42
5	A	308	TAM	C2-C5	2.69	1.56	1.52
6	B	319	HEZ	O1-C1	2.59	1.55	1.42
5	A	309	TAM	O4-C4	2.57	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	309	TAM	O6-C6	2.47	1.54	1.42
6	A	317	HEZ	O6-C6	2.44	1.54	1.42
5	A	308	TAM	C1-C4	2.36	1.56	1.52
5	A	309	TAM	C2-C5	2.23	1.56	1.52
6	B	317	HEZ	O1-C1	2.18	1.53	1.42
6	B	314	HEZ	C5-C4	2.18	1.62	1.51
7	A	313	HE2	CAA-CAC	2.17	1.65	1.50
6	B	313	HEZ	C5-C6	2.05	1.62	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	309	TAM	C5-C2-C	-12.67	101.02	115.97
5	B	309	TAM	O4-C4-C1	-10.77	81.10	111.33
5	A	308	TAM	C6-C3-C	-10.62	103.44	115.97
5	B	309	TAM	C6-C3-C	-10.35	103.77	115.97
5	B	309	TAM	C4-C1-C	10.21	128.01	115.97
5	A	308	TAM	C5-C2-C	-9.95	104.23	115.97
5	A	309	TAM	C4-C1-C	-9.46	104.81	115.97
5	A	308	TAM	C4-C1-C	-9.25	105.06	115.97
5	B	308	TAM	C2-C-C1	-8.91	94.79	110.50
5	A	308	TAM	C3-C-C2	-8.44	95.62	110.50
5	B	309	TAM	C2-C-C1	-7.16	97.88	110.50
5	A	309	TAM	O5-C5-C2	-7.04	91.58	111.33
5	A	309	TAM	O4-C4-C1	-6.88	92.02	111.33
5	A	309	TAM	C2-C-C1	6.69	122.30	110.50
5	B	309	TAM	O5-C5-C2	6.30	129.01	111.33
5	B	309	TAM	C3-C-C1	5.46	120.14	110.50
5	B	308	TAM	C5-C2-C	-5.30	109.72	115.97
5	A	309	TAM	O6-C6-C3	4.93	125.18	111.33
5	B	308	TAM	C3-C-N	4.69	120.00	108.22
5	A	308	TAM	O4-C4-C1	-4.58	98.48	111.33
5	B	308	TAM	C1-C-N	4.49	119.49	108.22
5	A	308	TAM	C2-C-C1	4.44	118.34	110.50
5	A	308	TAM	O5-C5-C2	4.33	123.50	111.33
5	B	309	TAM	O6-C6-C3	-4.32	99.21	111.33
5	B	308	TAM	C4-C1-C	-4.30	110.90	115.97
5	B	308	TAM	C6-C3-C	-4.19	111.03	115.97
5	B	308	TAM	O6-C6-C3	-3.80	100.67	111.33
5	B	308	TAM	C3-C-C2	-3.76	103.88	110.50
6	B	320	HEZ	O6-C6-C5	-3.61	88.50	111.44
6	A	314	HEZ	C4-C3-C2	-3.48	96.80	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	317	HEZ	C5-C4-C3	-3.25	97.93	114.37
6	A	311	HEZ	C4-C3-C2	-3.14	98.48	114.37
5	A	308	TAM	C2-C-N	3.12	116.06	108.22
6	B	318	HEZ	C4-C5-C6	-2.89	96.60	113.83
6	B	313	HEZ	O1-C1-C2	-2.79	93.70	111.44
7	B	316	HE2	CAF-CAG-CAE	2.79	128.47	114.37
5	A	309	TAM	C3-C-C2	-2.76	105.64	110.50
6	A	311	HEZ	C5-C4-C3	-2.70	100.71	114.37
6	A	319	HEZ	C4-C5-C6	-2.61	98.22	113.83
6	B	318	HEZ	C4-C3-C2	-2.60	101.21	114.37
6	A	319	HEZ	C3-C2-C1	-2.57	98.48	113.83
6	B	311	HEZ	C4-C3-C2	-2.42	102.15	114.37
5	A	309	TAM	C1-C-N	-2.38	102.24	108.22
6	B	318	HEZ	C5-C4-C3	2.36	126.32	114.37
6	A	317	HEZ	C4-C5-C6	2.34	127.77	113.83
5	B	308	TAM	O5-C5-C2	2.24	117.64	111.33
6	B	315	HEZ	C5-C4-C3	-2.22	103.17	114.37
6	B	320	HEZ	C4-C3-C2	-2.18	103.34	114.37
6	A	314	HEZ	C4-C5-C6	-2.07	101.46	113.83
6	B	322	HEZ	C5-C4-C3	-2.03	104.10	114.37

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	308	TAM	C1-C-C2-C5
5	A	308	TAM	C3-C-C2-C5
5	A	308	TAM	N-C-C2-C5
5	A	308	TAM	C-C3-C6-O6
5	A	309	TAM	C2-C-C1-C4
5	A	309	TAM	C3-C-C1-C4
5	A	309	TAM	N-C-C1-C4
5	B	308	TAM	C2-C-C1-C4
5	B	308	TAM	N-C-C1-C4
5	B	308	TAM	C1-C-C3-C6
5	B	308	TAM	C2-C-C3-C6
5	B	308	TAM	N-C-C3-C6
5	B	308	TAM	C-C2-C5-O5
5	B	309	TAM	C2-C-C1-C4
5	B	309	TAM	C3-C-C1-C4
5	B	309	TAM	N-C-C1-C4
5	B	309	TAM	C2-C-C3-C6

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Mol	Chain	Res	Type	Atoms
5	B	309	TAM	N-C-C3-C6
5	B	309	TAM	C-C2-C5-O5
6	A	314	HEZ	C1-C2-C3-C4
6	B	320	HEZ	C2-C3-C4-C5
6	B	319	HEZ	C1-C2-C3-C4
6	A	316	HEZ	C2-C3-C4-C5
6	A	311	HEZ	C2-C3-C4-C5
6	B	321	HEZ	C2-C3-C4-C5
6	A	315	HEZ	C2-C3-C4-C5
6	B	317	HEZ	C1-C2-C3-C4
6	B	322	HEZ	C1-C2-C3-C4
6	A	316	HEZ	C1-C2-C3-C4
6	A	315	HEZ	C1-C2-C3-C4
6	B	314	HEZ	C1-C2-C3-C4
6	B	319	HEZ	C3-C4-C5-C6
6	B	313	HEZ	C3-C4-C5-C6
6	B	320	HEZ	C1-C2-C3-C4
6	A	317	HEZ	C1-C2-C3-C4
6	A	317	HEZ	C2-C3-C4-C5
6	B	318	HEZ	C2-C3-C4-C5
6	A	316	HEZ	C3-C4-C5-C6
6	B	321	HEZ	C3-C4-C5-C6
7	B	316	HE2	CAC-CAE-CAG-CAF
6	A	318	HEZ	C4-C5-C6-O6
6	B	318	HEZ	O1-C1-C2-C3
6	B	322	HEZ	O1-C1-C2-C3
6	A	314	HEZ	O1-C1-C2-C3
6	A	315	HEZ	C4-C5-C6-O6
6	B	311	HEZ	O1-C1-C2-C3
6	B	317	HEZ	C4-C5-C6-O6
6	B	321	HEZ	C4-C5-C6-O6
5	B	308	TAM	C3-C-C1-C4
5	B	309	TAM	C1-C-C3-C6
6	A	317	HEZ	O1-C1-C2-C3
6	B	315	HEZ	O1-C1-C2-C3
7	A	313	HE2	OAB-CAD-CAF-CAG
7	B	316	HE2	CAD-CAF-CAG-CAE
6	B	317	HEZ	O1-C1-C2-C3
6	B	320	HEZ	C4-C5-C6-O6
6	B	313	HEZ	C2-C3-C4-C5
6	B	313	HEZ	O1-C1-C2-C3
6	B	321	HEZ	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	318	HEZ	C1-C2-C3-C4
6	A	316	HEZ	O1-C1-C2-C3
6	B	319	HEZ	C4-C5-C6-O6
6	A	317	HEZ	C3-C4-C5-C6
6	A	311	HEZ	C4-C5-C6-O6
6	B	313	HEZ	C1-C2-C3-C4
6	B	311	HEZ	C4-C5-C6-O6
5	B	309	TAM	C-C1-C4-O4
6	A	319	HEZ	O1-C1-C2-C3
6	B	317	HEZ	C2-C3-C4-C5
6	A	318	HEZ	C2-C3-C4-C5
7	A	313	HE2	CAA-CAC-CAE-CAG
6	A	314	HEZ	C4-C5-C6-O6
6	B	314	HEZ	C3-C4-C5-C6
6	B	320	HEZ	C3-C4-C5-C6
6	B	311	HEZ	C2-C3-C4-C5

There are no ring outliers.

16 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	318	HEZ	5	0
5	B	308	TAM	5	0
5	A	309	TAM	7	0
6	A	315	HEZ	1	0
6	A	319	HEZ	2	0
6	A	316	HEZ	12	0
6	B	320	HEZ	14	0
6	A	311	HEZ	1	0
5	A	308	TAM	7	0
6	B	318	HEZ	3	0
6	A	314	HEZ	4	0
5	B	309	TAM	6	0
6	B	319	HEZ	4	0
6	B	313	HEZ	6	0
6	A	317	HEZ	1	0
7	B	316	HE2	4	0

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/267 (97%)	-0.77	1 (0%) 92 94	13, 19, 37, 52	0
1	B	260/267 (97%)	-0.77	0 100 100	13, 19, 36, 53	0
All	All	520/534 (97%)	-0.77	1 (0%) 95 95	13, 19, 36, 53	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	GLU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	HEZ	A	316	8/8	0.75	0.21	32,51,58,60	0
6	HEZ	B	314	8/8	0.77	0.10	33,41,43,50	0
6	HEZ	B	317	8/8	0.83	0.16	39,48,51,56	0
6	HEZ	B	321	8/8	0.83	0.18	45,62,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	HEZ	A	315	8/8	0.86	0.17	40,56,69,71	0
6	HEZ	A	319	8/8	0.86	0.12	33,39,41,42	0
6	HEZ	B	313	8/8	0.86	0.18	16,38,49,52	0
6	HEZ	A	311	8/8	0.88	0.12	25,44,48,49	0
6	HEZ	B	315	8/8	0.88	0.16	28,32,37,41	0
6	HEZ	B	319	8/8	0.89	0.25	30,40,71,74	0
6	HEZ	A	318	8/8	0.89	0.23	31,40,48,51	0
6	HEZ	B	311	8/8	0.90	0.18	25,41,52,54	0
7	HE2	A	313	7/7	0.90	0.17	27,30,38,40	0
6	HEZ	B	320	8/8	0.91	0.20	18,28,43,47	0
5	TAM	A	309	11/11	0.92	0.12	15,19,41,48	0
5	TAM	B	308	11/11	0.93	0.15	13,17,24,24	11
6	HEZ	A	314	8/8	0.93	0.16	16,35,40,40	0
5	TAM	B	309	11/11	0.93	0.14	16,22,33,44	0
6	HEZ	A	317	8/8	0.94	0.11	22,35,41,42	0
6	HEZ	B	322	8/8	0.94	0.15	31,43,56,56	0
6	HEZ	A	312	8/8	0.94	0.18	30,45,54,57	0
6	HEZ	B	312	8/8	0.95	0.07	22,26,32,33	0
6	HEZ	B	310	8/8	0.95	0.09	22,30,32,34	0
6	HEZ	B	318	8/8	0.95	0.14	17,34,47,48	0
6	HEZ	A	310	8/8	0.95	0.10	23,26,33,34	0
5	TAM	A	308	11/11	0.96	0.21	14,19,21,27	11
7	HE2	B	316	7/7	0.97	0.11	21,27,34,34	0
4	CL	B	306	1/1	0.98	0.06	23,23,23,23	0
4	CL	B	307	1/1	0.99	0.08	20,20,20,20	0
2	CD	B	302	1/1	0.99	0.07	20,20,20,20	0
4	CL	A	305	1/1	0.99	0.07	20,20,20,20	0
4	CL	A	306	1/1	0.99	0.04	22,22,22,22	0
4	CL	A	307	1/1	0.99	0.06	23,23,23,23	0
4	CL	B	305	1/1	0.99	0.05	22,22,22,22	0
2	CD	A	302	1/1	0.99	0.07	20,20,20,20	0
3	CA	B	303	1/1	1.00	0.11	16,16,16,16	0
4	CL	A	304	1/1	1.00	0.04	19,19,19,19	0
2	CD	B	301	1/1	1.00	0.07	16,16,16,16	0
2	CD	A	301	1/1	1.00	0.08	16,16,16,16	0
3	CA	A	303	1/1	1.00	0.11	17,17,17,17	0
4	CL	B	304	1/1	1.00	0.04	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.