



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:43 AM UTC

PDB ID : 5KKU / pdb_00005kku
Title : Crystal structure of an N-terminal dehydratase from difficidin assembly line
Authors : Keatinge-Clay, A.T.; Zeng, J.
Deposited on : 2016-06-22
Resolution : 2.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

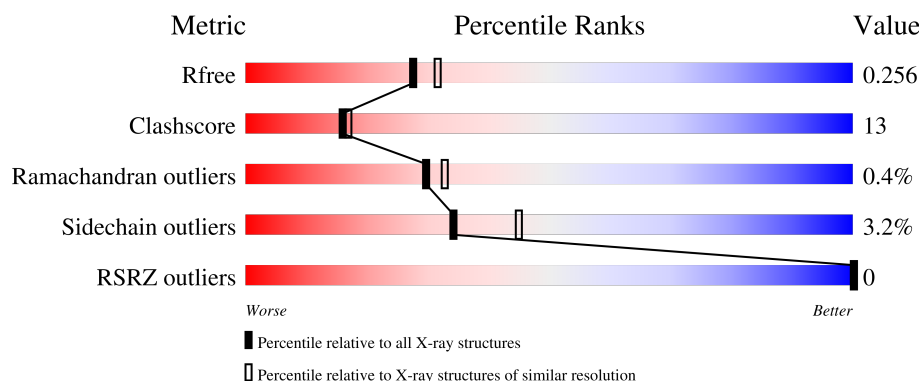
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	300	
1	B	300	
1	C	300	
1	D	300	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9353 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 Polyketide synthase type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2333	1478	409	434	12			
1	B	289	Total	C	N	O	S	0	0	0
			2351	1488	412	439	12			
1	C	289	Total	C	N	O	S	0	0	0
			2351	1488	412	439	12			
1	D	284	Total	C	N	O	S	0	0	0
			2316	1468	407	429	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLU	-	expression tag	UNP Q1RS44
A	295	HIS	-	expression tag	UNP Q1RS44
A	296	HIS	-	expression tag	UNP Q1RS44
A	297	HIS	-	expression tag	UNP Q1RS44
A	298	HIS	-	expression tag	UNP Q1RS44
A	299	HIS	-	expression tag	UNP Q1RS44
A	300	HIS	-	expression tag	UNP Q1RS44
B	294	GLU	-	expression tag	UNP Q1RS44
B	295	HIS	-	expression tag	UNP Q1RS44
B	296	HIS	-	expression tag	UNP Q1RS44
B	297	HIS	-	expression tag	UNP Q1RS44
B	298	HIS	-	expression tag	UNP Q1RS44
B	299	HIS	-	expression tag	UNP Q1RS44
B	300	HIS	-	expression tag	UNP Q1RS44
C	294	GLU	-	expression tag	UNP Q1RS44
C	295	HIS	-	expression tag	UNP Q1RS44
C	296	HIS	-	expression tag	UNP Q1RS44
C	297	HIS	-	expression tag	UNP Q1RS44
C	298	HIS	-	expression tag	UNP Q1RS44
C	299	HIS	-	expression tag	UNP Q1RS44
C	300	HIS	-	expression tag	UNP Q1RS44

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Chain	Residue	Modelled	Actual	Comment	Reference
D	294	GLU	-	expression tag	UNP Q1RS44
D	295	HIS	-	expression tag	UNP Q1RS44
D	296	HIS	-	expression tag	UNP Q1RS44
D	297	HIS	-	expression tag	UNP Q1RS44
D	298	HIS	-	expression tag	UNP Q1RS44
D	299	HIS	-	expression tag	UNP Q1RS44
D	300	HIS	-	expression tag	UNP Q1RS44

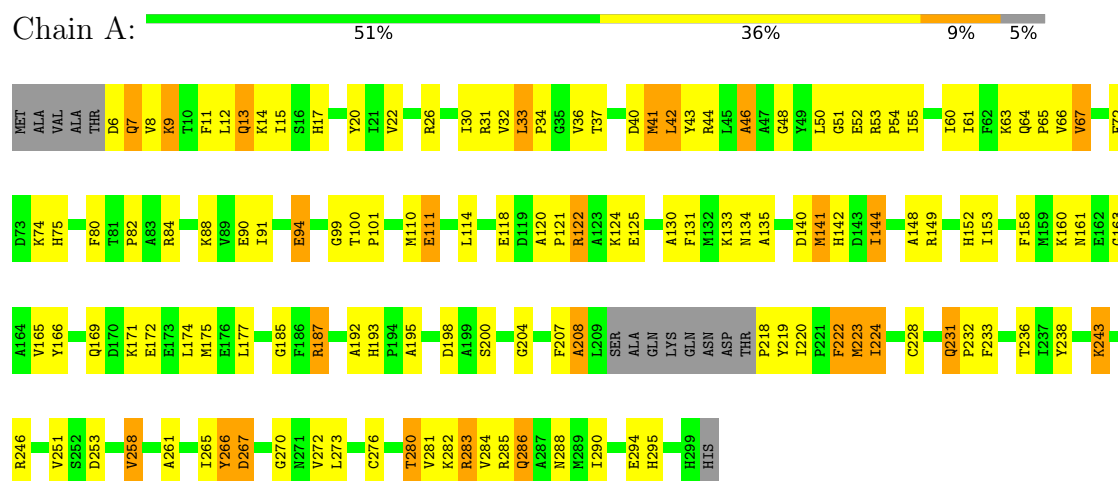
- Molecule 2 is water.

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

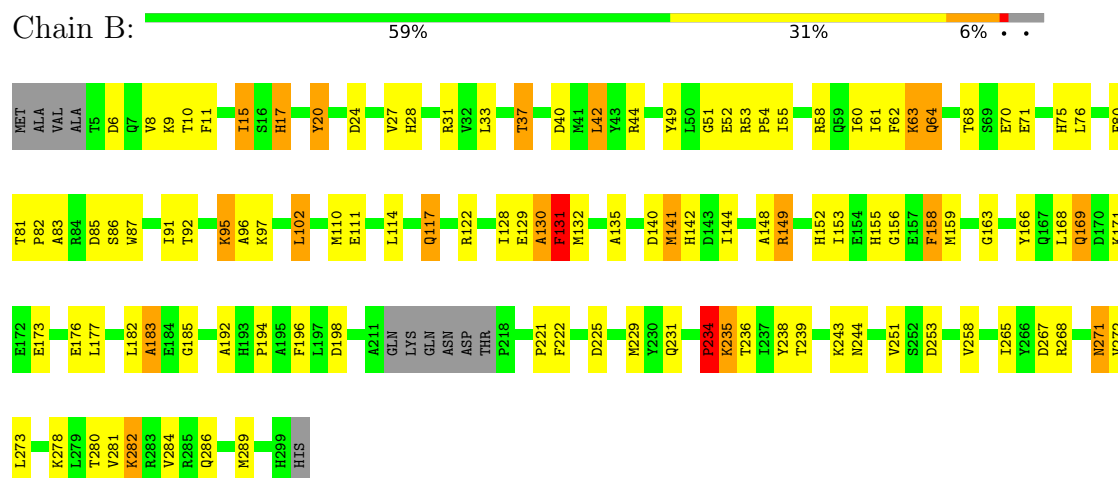
3 Residue-property plots

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: Polyketide synthase type I



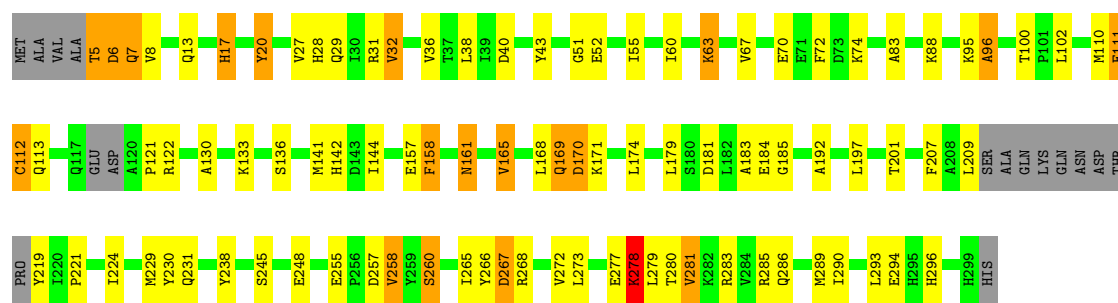
• Molecule 1: Polyketide synthase type I



• Molecule 1: Polyketide synthase type I



- Molecule 1: Polyketide synthase type I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.35Å 73.98Å 94.18Å 90.20° 90.08° 90.66°	Depositor
Resolution (Å)	39.79 – 2.22 39.79 – 2.22	Depositor EDS
% Data completeness (in resolution range)	89.0 (39.79-2.22) 87.3 (39.79-2.22)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.217 , 0.248 0.230 , 0.256	Depositor DCC
R_{free} test set	2513 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 5.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.269 for h,-k,-l 0.012 for -h,k,-l 0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9353	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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	1.94	67/2388 (2.8%)	1.53	40/3222 (1.2%)
1	B	1.89	51/2406 (2.1%)	1.27	21/3247 (0.6%)
1	C	1.93	61/2406 (2.5%)	1.43	14/3247 (0.4%)
1	D	1.89	46/2369 (1.9%)	1.25	21/3195 (0.7%)
All	All	1.91	225/9569 (2.4%)	1.37	96/12911 (0.7%)

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
1	C	0	1
1	D	0	3
All	All	0	6

All (225) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ASP	N-CA	-11.06	1.31	1.45
1	B	131	PHE	C-N	-9.76	1.21	1.33
1	D	267	ASP	N-CA	-9.75	1.33	1.45
1	C	110	MET	C-N	-9.44	1.21	1.33
1	D	267	ASP	C-N	-9.41	1.21	1.33
1	A	288	ASN	C-N	-9.35	1.21	1.33
1	A	261	ALA	C-N	-8.94	1.20	1.33
1	A	258	VAL	CA-C	-8.17	1.42	1.52
1	B	55	ILE	C-N	-7.88	1.23	1.33
1	C	17	HIS	C-O	-7.67	1.14	1.24
1	C	265	ILE	C-O	-7.60	1.15	1.24
1	C	112	CYS	C-O	-7.54	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	THR	C-O	-7.04	1.15	1.24
1	B	42	LEU	C-O	-7.01	1.15	1.24
1	B	253	ASP	C-O	-7.01	1.15	1.24
1	C	128	ILE	C-O	-6.94	1.16	1.24
1	D	165	VAL	C-O	-6.88	1.16	1.24
1	A	63	LYS	C-N	-6.86	1.24	1.33
1	C	291	THR	C-O	-6.81	1.16	1.24
1	A	135	ALA	N-CA	-6.80	1.37	1.46
1	B	251	VAL	C-O	-6.78	1.16	1.24
1	D	157	GLU	C-O	-6.74	1.16	1.24
1	D	281	VAL	C-O	-6.72	1.17	1.24
1	C	200	SER	C-O	-6.66	1.15	1.24
1	A	135	ALA	C-O	-6.64	1.16	1.23
1	D	36	VAL	C-O	-6.59	1.15	1.24
1	A	61	ILE	C-O	-6.59	1.17	1.24
1	C	198	ASP	C-O	-6.57	1.16	1.24
1	D	184	GLU	C-O	-6.52	1.16	1.24
1	B	92	THR	C-O	-6.51	1.15	1.23
1	C	91	ILE	C-O	-6.44	1.17	1.24
1	A	149	ARG	C-O	-6.44	1.16	1.24
1	A	280	THR	C-O	-6.44	1.16	1.24
1	A	111	GLU	C-O	-6.41	1.16	1.23
1	B	37	THR	C-O	-6.38	1.16	1.24
1	C	287	ALA	C-O	-6.36	1.16	1.24
1	C	73	ASP	C-O	-6.34	1.15	1.24
1	C	272	VAL	C-O	-6.33	1.17	1.24
1	C	156	GLY	C-O	-6.32	1.18	1.23
1	C	113	GLN	C-O	-6.30	1.16	1.24
1	B	91	ILE	C-O	-6.28	1.17	1.24
1	C	14	LYS	C-O	-6.27	1.16	1.24
1	B	272	VAL	C-O	-6.25	1.18	1.24
1	C	13	GLN	C-O	-6.23	1.16	1.23
1	D	201	THR	C-O	-6.23	1.16	1.24
1	C	290	ILE	C-O	-6.23	1.17	1.24
1	C	296	HIS	C-O	-6.21	1.16	1.24
1	B	60	ILE	C-O	-6.16	1.17	1.24
1	B	15	ILE	C-O	-6.13	1.16	1.24
1	C	240	TYR	C-O	-6.13	1.16	1.23
1	A	133	LYS	C-O	-6.12	1.16	1.24
1	A	290	ILE	C-O	-6.11	1.17	1.24
1	A	224	ILE	C-O	-6.09	1.17	1.24
1	C	195	ALA	C-O	-6.08	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	ILE	C-O	-6.04	1.17	1.24
1	A	100	THR	C-N	6.03	1.41	1.33
1	D	38	LEU	C-O	-6.02	1.16	1.24
1	A	166	TYR	C-O	-6.00	1.16	1.24
1	B	182	LEU	C-O	-5.99	1.17	1.24
1	D	290	ILE	C-O	-5.99	1.17	1.24
1	A	272	VAL	C-O	-5.98	1.18	1.24
1	C	41	MET	C-O	-5.97	1.17	1.24
1	B	53	ARG	C-N	5.96	1.40	1.33
1	B	27	VAL	C-O	-5.96	1.17	1.24
1	A	198	ASP	C-O	-5.93	1.17	1.24
1	B	96	ALA	C-O	-5.92	1.16	1.23
1	D	17	HIS	C-O	-5.91	1.16	1.24
1	D	83	ALA	C-O	-5.87	1.18	1.24
1	B	194	PRO	C-O	-5.87	1.16	1.24
1	C	81	THR	C-O	-5.82	1.18	1.25
1	D	181	ASP	C-O	-5.81	1.17	1.24
1	D	136	SER	C-O	-5.80	1.17	1.24
1	D	158	PHE	C-O	-5.80	1.17	1.24
1	A	294	GLU	C-O	-5.80	1.17	1.24
1	C	244	ASN	C-O	-5.78	1.17	1.24
1	A	258	VAL	N-CA	-5.78	1.39	1.46
1	D	142	HIS	C-O	-5.78	1.16	1.24
1	D	197	LEU	C-O	-5.78	1.17	1.24
1	B	239	THR	C-O	-5.77	1.17	1.23
1	B	196	PHE	C-O	-5.74	1.17	1.24
1	A	144	ILE	C-O	-5.72	1.17	1.24
1	A	185	GLY	C-O	-5.71	1.17	1.24
1	D	96	ALA	C-O	-5.70	1.16	1.23
1	B	8	VAL	C-O	-5.70	1.18	1.24
1	A	160	LYS	C-O	-5.67	1.17	1.24
1	C	145	TYR	C-O	-5.67	1.16	1.24
1	D	32	VAL	C-O	-5.66	1.18	1.24
1	A	276	CYS	C-O	-5.66	1.17	1.24
1	C	276	CYS	C-O	-5.66	1.17	1.24
1	C	115	TYR	C-N	-5.65	1.25	1.33
1	A	74	LYS	C-O	-5.65	1.17	1.23
1	A	42	LEU	C-O	-5.62	1.17	1.24
1	C	139	TRP	C-O	-5.61	1.16	1.23
1	B	135	ALA	C-O	-5.61	1.17	1.23
1	C	40	ASP	C-O	-5.59	1.17	1.24
1	C	204	GLY	C-O	-5.59	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	ALA	C-O	-5.59	1.17	1.24
1	C	236	THR	C-O	-5.59	1.17	1.24
1	A	54	PRO	C-O	-5.58	1.17	1.23
1	C	253	ASP	C-O	-5.58	1.17	1.24
1	C	284	VAL	C-O	-5.58	1.18	1.24
1	A	130	ALA	C-O	-5.58	1.17	1.24
1	C	286	GLN	C-O	-5.58	1.17	1.24
1	C	174	LEU	C-O	-5.55	1.17	1.23
1	A	172	GLU	C-O	-5.52	1.17	1.23
1	C	129	GLU	C-O	-5.52	1.17	1.24
1	B	70	GLU	C-O	-5.50	1.17	1.24
1	A	14	LYS	C-O	-5.50	1.17	1.24
1	A	67	VAL	C-O	-5.49	1.18	1.24
1	A	243	LYS	C-O	-5.49	1.17	1.24
1	A	94	GLU	C-O	-5.49	1.17	1.23
1	B	152	HIS	C-O	-5.49	1.16	1.23
1	B	102	LEU	C-O	-5.48	1.16	1.24
1	D	293	LEU	C-O	-5.47	1.17	1.24
1	A	75	HIS	C-O	-5.47	1.17	1.24
1	A	26	ARG	C-O	-5.46	1.17	1.24
1	B	173	GLU	C-O	-5.45	1.17	1.23
1	A	281	VAL	C-O	-5.44	1.18	1.24
1	A	295	HIS	C-O	-5.44	1.17	1.24
1	A	265	ILE	C-O	-5.42	1.18	1.24
1	A	65	PRO	C-O	-5.42	1.17	1.23
1	C	288	ASN	C-O	-5.42	1.17	1.24
1	C	189	LYS	C-O	-5.41	1.17	1.24
1	D	43	TYR	C-O	-5.41	1.17	1.24
1	A	270	GLY	C-O	-5.41	1.17	1.24
1	D	40	ASP	C-O	-5.41	1.17	1.24
1	D	231	GLN	C-O	-5.40	1.18	1.24
1	C	60	ILE	C-O	-5.40	1.17	1.24
1	D	294	GLU	C-O	-5.40	1.17	1.24
1	C	297	HIS	C-O	-5.39	1.17	1.24
1	B	284	VAL	C-O	-5.38	1.18	1.24
1	C	243	LYS	C-O	-5.37	1.17	1.24
1	B	156	GLY	C-O	-5.37	1.18	1.23
1	D	258	VAL	C-O	-5.37	1.18	1.23
1	B	225	ASP	C-O	-5.37	1.17	1.24
1	D	161	ASN	C-O	-5.36	1.17	1.23
1	A	43	TYR	C-O	-5.36	1.17	1.24
1	B	158	PHE	C-O	-5.33	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	268	ARG	C-O	-5.33	1.18	1.24
1	A	72	PHE	C-O	-5.33	1.17	1.23
1	B	117	GLN	C-O	-5.33	1.17	1.24
1	B	68	THR	C-O	-5.33	1.17	1.23
1	D	272	VAL	C-O	-5.32	1.18	1.24
1	A	131	PHE	C-O	-5.32	1.18	1.24
1	C	16	SER	C-O	-5.32	1.16	1.23
1	B	222	PHE	C-O	-5.31	1.17	1.24
1	C	280	THR	C-O	-5.31	1.17	1.24
1	B	286	GLN	C-O	-5.31	1.17	1.24
1	A	134	ASN	C-O	-5.30	1.16	1.24
1	C	66	VAL	C-O	-5.30	1.18	1.23
1	C	261	ALA	C-O	-5.30	1.17	1.23
1	A	13	GLN	C-O	-5.29	1.17	1.23
1	C	123	ALA	C-O	-5.29	1.17	1.23
1	A	251	VAL	C-O	-5.29	1.17	1.24
1	B	17	HIS	C-O	-5.29	1.17	1.24
1	B	231	GLN	C-O	-5.28	1.18	1.24
1	B	81	THR	C-O	-5.27	1.19	1.24
1	C	194	PRO	C-O	-5.26	1.17	1.24
1	A	142	HIS	N-CA	-5.26	1.39	1.46
1	D	260	SER	C-O	-5.25	1.17	1.23
1	C	111	GLU	C-N	5.25	1.40	1.33
1	A	261	ALA	C-O	-5.24	1.17	1.23
1	D	257	ASP	C-O	-5.24	1.17	1.24
1	B	44	ARG	C-O	-5.24	1.18	1.24
1	A	36	VAL	C-O	-5.22	1.17	1.24
1	A	20	TYR	C-O	-5.22	1.17	1.24
1	A	233	PHE	C-O	-5.21	1.17	1.24
1	C	153	ILE	C-O	-5.21	1.18	1.24
1	A	99	GLY	C-O	-5.20	1.17	1.24
1	A	114	LEU	C-O	-5.20	1.17	1.24
1	B	149	ARG	C-O	-5.20	1.18	1.24
1	C	62	PHE	C-O	-5.18	1.17	1.24
1	B	62	PHE	C-O	-5.17	1.18	1.24
1	C	251	VAL	C-O	-5.17	1.18	1.24
1	A	41	MET	C-O	-5.17	1.18	1.24
1	C	81	THR	CA-C	-5.17	1.48	1.52
1	B	49	TYR	C-O	-5.16	1.17	1.24
1	C	231	GLN	C-O	-5.16	1.18	1.24
1	A	158	PHE	C-O	-5.15	1.17	1.24
1	C	32	VAL	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	LYS	C-O	-5.14	1.17	1.23
1	A	12	LEU	C-O	-5.14	1.17	1.24
1	A	195	ALA	C-O	-5.14	1.18	1.24
1	D	266	TYR	C-O	-5.13	1.17	1.24
1	A	46	ALA	C-O	-5.13	1.18	1.24
1	A	220	ILE	C-N	5.13	1.40	1.33
1	C	168	LEU	C-O	-5.13	1.18	1.24
1	D	20	TYR	C-O	-5.12	1.17	1.24
1	C	102	LEU	C-O	-5.12	1.17	1.24
1	D	8	VAL	C-O	-5.12	1.18	1.24
1	D	7	GLN	C-O	-5.12	1.17	1.23
1	D	63	LYS	C-O	-5.10	1.18	1.24
1	D	266	TYR	C-N	-5.10	1.26	1.33
1	B	158	PHE	C-N	-5.09	1.26	1.33
1	A	200	SER	C-O	-5.09	1.17	1.24
1	B	58	ARG	C-O	-5.09	1.17	1.23
1	A	120	ALA	C-N	5.08	1.40	1.33
1	A	253	ASP	C-O	-5.08	1.17	1.24
1	B	129	GLU	C-O	-5.07	1.18	1.24
1	D	296	HIS	C-O	-5.07	1.17	1.24
1	A	40	ASP	C-O	-5.07	1.18	1.24
1	B	234	PRO	C-N	-5.07	1.27	1.33
1	D	141	MET	C-O	-5.06	1.18	1.24
1	C	295	HIS	C-O	-5.06	1.18	1.24
1	D	70	GLU	C-O	-5.06	1.17	1.24
1	D	185	GLY	C-O	-5.05	1.17	1.24
1	B	20	TYR	C-O	-5.05	1.17	1.24
1	A	64	GLN	C-O	-5.04	1.17	1.24
1	B	271	ASN	C-O	-5.04	1.17	1.23
1	D	13	GLN	C-O	-5.04	1.17	1.23
1	A	30	ILE	C-O	-5.04	1.18	1.24
1	B	183	ALA	C-O	-5.04	1.17	1.24
1	A	121	PRO	N-CD	5.03	1.54	1.47
1	B	24	ASP	C-O	-5.03	1.17	1.24
1	A	236	THR	C-O	-5.03	1.18	1.24
1	B	185	GLY	C-O	-5.03	1.17	1.24
1	C	294	GLU	C-O	-5.03	1.18	1.24
1	D	100	THR	C-O	-5.03	1.17	1.24
1	D	55	ILE	C-O	-5.03	1.17	1.23
1	C	239	THR	C-O	-5.02	1.18	1.24
1	D	245	SER	C-O	-5.02	1.17	1.24
1	C	255	GLU	C-O	-5.01	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	171	LYS	C-O	-5.01	1.17	1.24
1	C	192	ALA	C-O	-5.01	1.17	1.23
1	C	23	ARG	C-O	-5.00	1.17	1.24

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	MET	CA-C-N	23.89	163.98	121.94
1	C	110	MET	C-N-CA	23.89	163.98	121.94
1	C	110	MET	O-C-N	-21.32	96.09	122.96
1	A	63	LYS	N-CA-C	18.00	137.42	114.56
1	A	63	LYS	CB-CA-C	-14.90	85.88	109.13
1	C	64	GLN	N-CA-CB	12.99	133.50	110.37
1	D	63	LYS	N-CA-C	-12.68	85.19	108.65
1	A	135	ALA	CA-C-O	12.20	134.82	120.92
1	A	261	ALA	CA-C-N	11.57	139.88	122.65
1	A	261	ALA	C-N-CA	11.57	139.88	122.65
1	A	228	CYS	CA-C-N	11.33	138.15	121.72
1	A	228	CYS	C-N-CA	11.33	138.15	121.72
1	B	131	PHE	CA-C-O	11.12	132.66	120.10
1	C	116	LEU	O-C-N	-11.11	110.28	123.16
1	A	222	PHE	CB-CA-C	-10.77	95.27	109.16
1	D	267	ASP	CA-C-N	10.74	135.05	120.44
1	D	267	ASP	C-N-CA	10.74	135.05	120.44
1	D	268	ARG	O-C-N	10.56	133.49	122.09
1	C	63	LYS	N-CA-C	10.51	126.78	111.96
1	D	51	GLY	CA-C-N	-10.32	101.83	121.54
1	D	51	GLY	C-N-CA	-10.32	101.83	121.54
1	A	258	VAL	N-CA-C	-10.18	92.31	108.81
1	C	111	GLU	O-C-N	10.09	135.21	123.41
1	A	208	ALA	N-CA-C	9.59	132.47	113.29
1	B	158	PHE	CA-C-N	9.35	138.83	122.09
1	B	158	PHE	C-N-CA	9.35	138.83	122.09
1	A	261	ALA	O-C-N	-9.35	113.45	123.26
1	A	267	ASP	CA-C-O	9.19	132.27	121.88
1	A	52	GLU	N-CA-C	-9.14	92.57	108.20
1	A	208	ALA	CA-C-N	9.11	138.09	121.70
1	A	208	ALA	C-N-CA	9.11	138.09	121.70
1	A	222	PHE	N-CA-C	9.00	126.09	114.75
1	A	171	LYS	N-CA-C	-8.97	102.92	114.04
1	A	51	GLY	N-CA-C	-8.66	92.64	113.18
1	A	52	GLU	CB-CA-C	8.09	123.73	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	CYS	O-C-N	-7.60	112.93	123.34
1	A	267	ASP	CA-C-N	7.59	131.06	120.29
1	A	267	ASP	C-N-CA	7.59	131.06	120.29
1	B	158	PHE	N-CA-C	7.57	119.61	111.36
1	D	267	ASP	CA-C-O	7.26	130.09	121.88
1	B	53	ARG	CA-C-N	-7.18	112.53	120.14
1	B	53	ARG	C-N-CA	-7.18	112.53	120.14
1	A	223	MET	O-C-N	-7.14	115.48	123.48
1	D	171	LYS	N-CA-C	7.04	121.10	112.23
1	C	163	GLY	N-CA-C	6.50	118.61	110.29
1	B	131	PHE	CA-C-N	6.42	133.71	122.79
1	B	131	PHE	C-N-CA	6.42	133.71	122.79
1	A	100	THR	CA-C-N	-6.37	114.09	120.21
1	A	100	THR	C-N-CA	-6.37	114.09	120.21
1	C	53	ARG	N-CA-C	6.36	117.66	109.65
1	B	61	ILE	CB-CA-C	6.30	121.10	110.95
1	B	244	ASN	N-CA-CB	-6.25	100.68	110.06
1	C	209	LEU	N-CA-C	-6.14	96.80	108.17
1	B	243	LYS	CA-C-N	6.10	128.74	120.38
1	B	243	LYS	C-N-CA	6.10	128.74	120.38
1	C	64	GLN	N-CA-C	-6.09	96.34	109.81
1	A	169	GLN	N-CA-C	5.98	120.16	112.86
1	C	140	ASP	N-CA-C	-5.95	101.48	110.28
1	A	187	ARG	CA-C-N	-5.91	111.68	122.38
1	A	187	ARG	C-N-CA	-5.91	111.68	122.38
1	A	134	ASN	O-C-N	5.91	129.28	122.25
1	A	135	ALA	CA-C-N	5.79	134.30	121.80
1	A	135	ALA	C-N-CA	5.79	134.30	121.80
1	B	6	ASP	N-CA-CB	-5.76	102.18	110.65
1	A	220	ILE	CA-C-N	-5.75	114.04	119.90
1	A	220	ILE	C-N-CA	-5.75	114.04	119.90
1	B	55	ILE	O-C-N	-5.73	116.68	123.04
1	A	120	ALA	CA-C-N	-5.71	113.90	119.78
1	A	120	ALA	C-N-CA	-5.71	113.90	119.78
1	D	63	LYS	CB-CA-C	-5.70	100.20	114.11
1	A	33	LEU	CA-C-N	-5.68	114.11	119.90
1	A	33	LEU	C-N-CA	-5.68	114.11	119.90
1	D	277	GLU	CA-C-N	5.68	132.39	121.54
1	D	277	GLU	C-N-CA	5.68	132.39	121.54
1	D	248	GLU	N-CA-C	5.64	115.99	108.38
1	D	169	GLN	N-CA-C	-5.63	99.67	108.00
1	B	234	PRO	N-CA-C	-5.62	100.88	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	ASP	CB-CA-C	5.60	118.96	109.55
1	B	130	ALA	CA-C-N	5.53	128.24	120.28
1	B	130	ALA	C-N-CA	5.53	128.24	120.28
1	D	72	PHE	N-CA-C	5.51	117.65	108.99
1	A	192	ALA	CB-CA-C	5.49	118.26	110.24
1	C	93	SER	N-CA-C	5.47	117.38	109.07
1	A	72	PHE	N-CA-C	5.38	117.44	108.99
1	B	64	GLN	CA-C-N	-5.37	114.45	120.14
1	B	64	GLN	C-N-CA	-5.37	114.45	120.14
1	B	159	MET	O-C-N	-5.24	114.92	122.36
1	D	63	LYS	CA-C-N	5.22	134.55	121.80
1	D	63	LYS	C-N-CA	5.22	134.55	121.80
1	A	187	ARG	O-C-N	-5.16	116.32	122.20
1	B	51	GLY	N-CA-C	-5.10	103.34	112.22
1	C	62	PHE	N-CA-C	5.09	116.91	108.20
1	D	6	ASP	CA-C-N	-5.05	114.02	122.92
1	D	6	ASP	C-N-CA	-5.05	114.02	122.92
1	D	255	GLU	CA-C-N	-5.02	114.74	119.76
1	D	255	GLU	C-N-CA	-5.02	114.74	119.76

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	TYR	Peptide
1	B	131	PHE	Peptide
1	C	110	MET	Mainchain
1	D	278	LYS	Mainchain
1	D	52	GLU	Mainchain
1	D	63	LYS	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	2333	0	2278	94	0
1	B	2351	0	2296	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2351	0	2295	52	0
1	D	2316	0	2266	38	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	9353	0	9135	243	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 13.

All (243) 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:A:7:GLN:HA	1:A:82:PRO:CG	1.23	1.44
1:A:7:GLN:CA	1:A:82:PRO:HG2	1.52	1.30
1:A:6:ASP:O	1:A:7:GLN:HG2	1.12	1.23
1:C:88:LYS:NZ	1:C:90:GLU:OE1	1.70	1.22
1:A:141:MET:HB2	1:A:163:GLY:C	1.67	1.19
1:A:7:GLN:CA	1:A:82:PRO:CG	2.04	1.18
1:A:141:MET:HB2	1:A:163:GLY:O	1.40	1.17
1:A:7:GLN:HA	1:A:82:PRO:HG3	1.32	1.11
1:A:6:ASP:O	1:A:7:GLN:CG	2.01	1.09
1:C:88:LYS:NZ	1:C:90:GLU:CD	2.11	1.09
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.10	1.08
1:D:278:LYS:O	1:D:278:LYS:HG3	1.54	1.02
1:B:82:PRO:HA	1:B:87:TRP:CD1	2.01	0.96
1:C:88:LYS:HZ2	1:C:90:GLU:CD	1.73	0.95
1:D:260:SER:HB2	1:D:279:LEU:O	1.66	0.95
1:A:219:TYR:CZ	1:A:283:ARG:HB2	2.01	0.95
1:B:82:PRO:HA	1:B:87:TRP:HD1	1.30	0.95
1:B:86:SER:HB2	1:B:114:LEU:O	1.65	0.94
1:B:168:LEU:HG	1:B:169:GLN:HG2	1.50	0.94
1:A:141:MET:CB	1:A:163:GLY:O	2.18	0.91
1:A:246:ARG:NH1	1:A:246:ARG:HB2	1.85	0.90
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.36	0.89
1:C:87:TRP:HZ3	1:C:116:LEU:CD1	1.86	0.89
1:C:91:ILE:HD12	1:C:110:MET:HE2	1.55	0.88
1:C:87:TRP:HZ3	1:C:116:LEU:HD11	1.40	0.87
1:B:141:MET:HE3	1:B:177:LEU:HD21	1.55	0.87
1:A:32:VAL:HG22	1:A:67:VAL:HG22	1.56	0.86
1:B:141:MET:HE3	1:B:177:LEU:CD2	2.04	0.86
1:A:122:ARG:HH11	1:A:122:ARG:CG	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:HB2	1:A:246:ARG:HH11	1.41	0.84
1:A:258:VAL:HG22	1:A:282:LYS:HG3	1.59	0.83
1:C:141:MET:HE1	1:C:175:MET:CE	2.07	0.83
1:A:6:ASP:C	1:A:7:GLN:HG2	2.03	0.83
1:A:218:PRO:O	1:A:283:ARG:HA	1.78	0.83
1:A:285:ARG:HA	1:A:285:ARG:CZ	2.09	0.83
1:A:7:GLN:CA	1:A:82:PRO:HG3	1.95	0.82
1:C:137:ARG:HG3	1:C:137:ARG:NH1	1.94	0.81
1:A:141:MET:HE3	1:A:177:LEU:CD2	2.11	0.80
1:B:33:LEU:HD11	1:B:37:THR:HG21	1.64	0.79
1:D:278:LYS:O	1:D:278:LYS:CG	2.30	0.79
1:D:60:ILE:HG23	1:D:110:MET:HE3	1.62	0.79
1:C:141:MET:HE2	1:C:177:LEU:HD21	1.64	0.78
1:C:87:TRP:CZ3	1:C:116:LEU:HD11	2.18	0.77
1:C:88:LYS:HZ1	1:C:90:GLU:CD	1.84	0.77
1:C:91:ILE:CD1	1:C:110:MET:HE2	2.15	0.76
1:B:142:HIS:O	1:B:149:ARG:NH1	2.17	0.76
1:A:33:LEU:HB3	1:A:66:VAL:HB	1.68	0.75
1:A:140:ASP:OD1	1:A:141:MET:N	2.20	0.75
1:A:33:LEU:HD11	1:A:37:THR:HG21	1.69	0.75
1:A:141:MET:HE3	1:A:177:LEU:HD23	1.68	0.74
1:B:267:ASP:HB3	1:B:273:LEU:HD21	1.69	0.73
1:A:219:TYR:CE2	1:A:283:ARG:HB2	2.23	0.73
1:A:222:PHE:O	1:A:222:PHE:CD1	2.42	0.72
1:D:260:SER:CB	1:D:279:LEU:O	2.38	0.71
1:A:55:ILE:C	1:A:55:ILE:HD12	2.16	0.71
1:A:122:ARG:HG2	1:A:122:ARG:NH1	1.89	0.71
1:A:231:GLN:HG3	1:A:232:PRO:HD2	1.73	0.70
1:A:222:PHE:O	1:A:223:MET:HG3	1.90	0.70
1:A:141:MET:HB3	1:A:163:GLY:H	1.55	0.70
1:A:219:TYR:CE1	1:A:283:ARG:HB2	2.27	0.69
1:A:165:VAL:HG22	1:A:175:MET:HG2	1.73	0.69
1:D:60:ILE:CG2	1:D:110:MET:HE3	2.21	0.69
1:D:144:ILE:HG13	1:D:165:VAL:HG21	1.74	0.69
1:A:7:GLN:HA	1:A:82:PRO:HG2	0.70	0.69
1:A:161:ASN:HD22	1:A:177:LEU:HB3	1.58	0.69
1:B:132:MET:HE3	1:B:166:TYR:CZ	2.28	0.69
1:B:177:LEU:O	1:B:236:THR:HA	1.92	0.69
1:D:170:ASP:O	1:D:207:PHE:CE1	2.46	0.69
1:D:219:TYR:CE2	1:D:283:ARG:HB2	2.28	0.68
1:A:267:ASP:HB3	1:A:273:LEU:HD21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:SER:OG	1:C:239:THR:HG21	1.93	0.68
1:A:285:ARG:HA	1:A:285:ARG:NE	2.08	0.67
1:A:222:PHE:O	1:A:222:PHE:CG	2.44	0.67
1:C:227:PHE:HE1	1:C:229:MET:CE	2.07	0.67
1:B:54:PRO:HB2	1:B:117:GLN:OE1	1.95	0.67
1:A:32:VAL:HG12	1:A:33:LEU:N	2.09	0.67
1:A:141:MET:CB	1:A:163:GLY:H	2.07	0.67
1:C:141:MET:HE1	1:C:175:MET:HE2	1.77	0.67
1:B:158:PHE:O	1:B:183:ALA:HB2	1.95	0.67
1:C:88:LYS:HE3	1:C:90:GLU:HG3	1.76	0.67
1:D:5:THR:HG23	1:D:7:GLN:H	1.59	0.66
1:B:128:ILE:O	1:B:132:MET:HB2	1.96	0.66
1:C:208:ALA:O	1:C:210:SER:N	2.28	0.66
1:D:111:GLU:O	1:D:112:CYS:HB3	1.94	0.66
1:D:168:LEU:HD13	1:D:168:LEU:C	2.21	0.65
1:A:9:LYS:HG2	1:A:11:PHE:CZ	2.32	0.64
1:A:144:ILE:HG13	1:A:165:VAL:HG21	1.79	0.64
1:C:226:ARG:NH2	1:C:275:GLU:OE1	2.31	0.64
1:D:27:VAL:HG11	1:D:289:MET:HE3	1.78	0.64
1:D:174:LEU:HD11	1:D:238:TYR:HB3	1.80	0.64
1:A:13:GLN:OE1	1:A:44:ARG:NH2	2.32	0.62
1:B:258:VAL:CG2	1:B:282:LYS:HG3	2.28	0.62
1:D:60:ILE:HG23	1:D:110:MET:CE	2.28	0.62
1:A:258:VAL:CG1	1:A:280:THR:CG2	2.78	0.62
1:A:141:MET:CB	1:A:163:GLY:N	2.62	0.62
1:A:258:VAL:CG1	1:A:280:THR:HG23	2.30	0.61
1:A:141:MET:HE3	1:A:177:LEU:HD21	1.82	0.61
1:C:209:LEU:N	1:C:209:LEU:HD12	2.16	0.61
1:B:130:ALA:C	1:B:132:MET:H	1.99	0.60
1:A:7:GLN:CB	1:A:82:PRO:HG2	2.30	0.60
1:B:258:VAL:HG13	1:B:280:THR:HG23	1.82	0.60
1:A:94:GLU:OE2	1:A:101:PRO:HB2	2.01	0.59
1:C:128:ILE:HG22	1:C:132:MET:HE2	1.84	0.59
1:A:246:ARG:HH11	1:A:246:ARG:CB	2.12	0.59
1:B:141:MET:HE3	1:B:177:LEU:HD23	1.83	0.59
1:B:258:VAL:HG23	1:B:282:LYS:HG3	1.85	0.58
1:D:265:ILE:HG22	1:D:273:LEU:HD12	1.86	0.58
1:A:204:GLY:HA3	1:A:246:ARG:NH2	2.20	0.57
1:D:192:ALA:HB2	1:D:229:MET:HE2	1.87	0.57
1:C:258:VAL:HG13	1:C:280:THR:HG23	1.86	0.57
1:B:128:ILE:O	1:B:132:MET:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:O	1:A:208:ALA:HB3	2.06	0.55
1:A:266:TYR:HB3	1:A:267:ASP:O	2.06	0.55
1:B:267:ASP:OD2	1:B:271:ASN:ND2	2.29	0.55
1:C:170:ASP:O	1:C:243:LYS:HD3	2.06	0.55
1:C:141:MET:HE2	1:C:177:LEU:CD2	2.35	0.55
1:C:187:ARG:HA	1:C:193:HIS:HD2	1.72	0.53
1:D:96:ALA:HA	1:D:102:LEU:HD13	1.89	0.53
1:A:122:ARG:CG	1:A:122:ARG:NH1	2.53	0.53
1:C:167:GLN:OE1	1:C:170:ASP:OD1	2.27	0.53
1:A:32:VAL:HG12	1:A:33:LEU:H	1.74	0.53
1:B:95:LYS:HB3	1:B:102:LEU:HD12	1.91	0.52
1:C:221:PRO:HA	1:C:281:VAL:HG12	1.90	0.52
1:C:209:LEU:N	1:C:209:LEU:CD1	2.72	0.52
1:A:141:MET:HB2	1:A:163:GLY:CA	2.37	0.52
1:C:227:PHE:HE1	1:C:229:MET:HE1	1.74	0.52
1:C:267:ASP:HB3	1:C:273:LEU:HD21	1.92	0.52
1:C:20:TYR:HB3	1:C:158:PHE:CG	2.44	0.51
1:B:163:GLY:HA3	1:B:176:GLU:O	2.09	0.51
1:D:95:LYS:HB3	1:D:102:LEU:HD22	1.90	0.51
1:A:174:LEU:HD11	1:A:238:TYR:HB3	1.93	0.51
1:D:17:HIS:CE1	1:D:31:ARG:HD2	2.45	0.51
1:B:15:ILE:CD1	1:B:33:LEU:HD22	2.41	0.50
1:B:42:LEU:HD11	1:B:110:MET:HE1	1.93	0.50
1:A:187:ARG:HA	1:A:193:HIS:HD2	1.75	0.50
1:B:221:PRO:HA	1:B:281:VAL:HG12	1.94	0.50
1:C:137:ARG:HH11	1:C:137:ARG:CG	2.14	0.50
1:A:283:ARG:HG2	1:A:284:VAL:N	2.26	0.50
1:A:17:HIS:CE1	1:A:31:ARG:HD2	2.47	0.50
1:A:8:VAL:HA	1:A:80:PHE:O	2.12	0.50
1:A:152:HIS:CE1	1:A:286:GLN:HE22	2.29	0.50
1:C:87:TRP:CZ3	1:C:116:LEU:CD1	2.77	0.49
1:B:132:MET:HE3	1:B:166:TYR:CE1	2.47	0.49
1:A:22:VAL:HB	1:A:31:ARG:HB3	1.94	0.49
1:A:32:VAL:CG1	1:A:33:LEU:N	2.73	0.49
1:A:222:PHE:O	1:A:223:MET:CG	2.59	0.49
1:B:258:VAL:HG22	1:B:282:LYS:HG3	1.95	0.49
1:A:110:MET:HG2	1:A:111:GLU:N	2.28	0.49
1:D:32:VAL:HG22	1:D:67:VAL:HG22	1.95	0.48
1:B:155:HIS:NE2	1:B:198:ASP:OD2	2.46	0.48
1:A:46:ALA:C	1:A:48:GLY:N	2.70	0.48
1:A:219:TYR:CE2	1:A:283:ARG:CB	2.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ALA:HB3	1:B:86:SER:O	2.14	0.48
1:B:9:LYS:HE2	1:B:11:PHE:CZ	2.48	0.48
1:B:28:HIS:CD2	1:B:289:MET:HE2	2.49	0.47
1:D:258:VAL:HG13	1:D:280:THR:HG23	1.97	0.47
1:D:219:TYR:CZ	1:D:283:ARG:HB2	2.49	0.47
1:B:52:GLU:O	1:B:52:GLU:HG2	2.14	0.47
1:C:222:PHE:CE2	1:C:223:MET:HE2	2.50	0.47
1:D:121:PRO:HB3	1:D:230:TYR:CE2	2.49	0.47
1:A:55:ILE:HD12	1:A:55:ILE:O	2.14	0.47
1:D:88:LYS:HG3	1:D:113:GLN:OE1	2.13	0.47
1:A:33:LEU:CB	1:A:66:VAL:HB	2.39	0.47
1:A:42:LEU:HD11	1:A:91:ILE:HD11	1.97	0.47
1:B:141:MET:HB2	1:B:163:GLY:O	2.15	0.47
1:B:168:LEU:HG	1:B:169:GLN:CG	2.32	0.47
1:D:221:PRO:HA	1:D:281:VAL:HG12	1.97	0.47
1:D:224:ILE:HG12	1:D:279:LEU:HD13	1.96	0.47
1:C:148:ALA:HB1	1:C:153:ILE:HB	1.97	0.46
1:B:82:PRO:CA	1:B:87:TRP:HD1	2.15	0.46
1:B:278:LYS:O	1:B:278:LYS:HG2	2.15	0.46
1:A:141:MET:N	1:A:163:GLY:O	2.49	0.46
1:B:267:ASP:OD2	1:B:271:ASN:HB2	2.15	0.46
1:A:148:ALA:HB1	1:A:153:ILE:HB	1.97	0.46
1:A:204:GLY:HA3	1:A:246:ARG:HH21	1.77	0.46
1:C:278:LYS:O	1:C:279:LEU:C	2.59	0.46
1:B:80:PHE:HE2	1:B:114:LEU:HD13	1.80	0.45
1:D:110:MET:HG2	1:D:111:GLU:N	2.31	0.45
1:A:50:LEU:HD12	1:A:55:ILE:HG21	1.98	0.45
1:C:170:ASP:O	1:C:243:LYS:CD	2.65	0.45
1:A:9:LYS:HG2	1:A:11:PHE:CE2	2.51	0.45
1:B:71:GLU:O	1:B:97:LYS:HD2	2.17	0.45
1:A:46:ALA:C	1:A:48:GLY:H	2.24	0.45
1:B:40:ASP:HB2	1:B:192:ALA:O	2.17	0.45
1:B:229:MET:HE3	1:B:229:MET:HB3	1.85	0.44
1:C:205:SER:O	1:C:209:LEU:HD13	2.16	0.44
1:D:28:HIS:O	1:D:29:GLN:HB2	2.16	0.44
1:A:42:LEU:CD1	1:A:91:ILE:HD11	2.47	0.44
1:B:17:HIS:CE1	1:B:31:ARG:HD2	2.53	0.44
1:C:162:GLU:OE1	1:C:162:GLU:HA	2.17	0.44
1:D:267:ASP:HB3	1:D:273:LEU:HD21	1.99	0.44
1:B:140:ASP:O	1:B:142:HIS:N	2.50	0.44
1:C:295:HIS:NE2	1:D:133:LYS:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ALA:HB1	1:B:153:ILE:HB	2.00	0.44
1:B:169:GLN:HE21	1:B:171:LYS:HE2	1.83	0.44
1:B:9:LYS:HE2	1:B:11:PHE:CE2	2.53	0.43
1:C:169:GLN:O	1:C:170:ASP:HB2	2.17	0.43
1:C:16:SER:HA	1:C:73:ASP:HB3	2.00	0.43
1:C:33:LEU:HD11	1:C:37:THR:HG21	2.00	0.43
1:A:219:TYR:HA	1:A:283:ARG:HA	2.00	0.43
1:B:63:LYS:HB2	1:B:64:GLN:H	1.60	0.43
1:A:32:VAL:CG1	1:A:33:LEU:H	2.30	0.43
1:C:207:PHE:CE2	1:C:243:LYS:HG3	2.53	0.43
1:C:235:LYS:HE2	1:C:235:LYS:HB3	1.83	0.43
1:D:20:TYR:HB3	1:D:158:PHE:CG	2.54	0.43
1:D:285:ARG:NH1	1:D:286:GLN:HB2	2.34	0.43
1:B:131:PHE:CD1	1:B:131:PHE:C	2.96	0.43
1:A:41:MET:HE3	1:A:41:MET:HB2	1.87	0.43
1:D:60:ILE:HA	1:D:112:CYS:HB3	2.00	0.43
1:A:55:ILE:C	1:A:55:ILE:CD1	2.86	0.43
1:A:88:LYS:HE3	1:A:90:GLU:CD	2.43	0.43
1:B:141:MET:HB2	1:B:163:GLY:C	2.44	0.43
1:B:282:LYS:HE3	1:B:282:LYS:HB3	1.52	0.42
1:C:55:ILE:C	1:C:55:ILE:HD12	2.45	0.42
1:A:15:ILE:HG13	1:A:33:LEU:HD22	2.01	0.42
1:A:285:ARG:NE	1:A:285:ARG:CA	2.76	0.42
1:B:75:HIS:C	1:B:76:LEU:HD12	2.45	0.42
1:C:88:LYS:HG2	1:C:89:VAL:N	2.34	0.42
1:A:50:LEU:O	1:A:53:ARG:NH2	2.36	0.42
1:B:132:MET:HE3	1:B:166:TYR:OH	2.18	0.42
1:A:34:PRO:O	1:A:37:THR:HB	2.19	0.42
1:B:20:TYR:HB3	1:B:158:PHE:CG	2.55	0.42
1:B:236:THR:O	1:B:238:TYR:CE1	2.73	0.42
1:C:174:LEU:HD11	1:C:238:TYR:HB3	2.01	0.42
1:A:7:GLN:N	1:A:82:PRO:HG3	2.35	0.41
1:D:168:LEU:C	1:D:168:LEU:CD1	2.91	0.41
1:C:96:ALA:HA	1:C:102:LEU:HD13	2.01	0.41
1:C:88:LYS:CE	1:C:90:GLU:CD	2.93	0.41
1:B:176:GLU:HG3	1:B:238:TYR:CE2	2.55	0.41
1:B:234:PRO:HB2	1:B:235:LYS:H	1.61	0.41
1:D:67:VAL:O	1:D:74:LYS:NZ	2.53	0.41
1:A:258:VAL:HG13	1:A:280:THR:CG2	2.50	0.41
1:A:285:ARG:HA	1:A:285:ARG:NH1	2.34	0.41
1:B:63:LYS:NZ	1:B:111:GLU:OE1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:CE	1:C:175:MET:HE2	2.49	0.41
1:A:60:ILE:HB	1:A:224:ILE:HB	2.03	0.41
1:A:219:TYR:CZ	1:A:283:ARG:CB	2.89	0.41
1:C:17:HIS:CE1	1:C:31:ARG:HD2	2.55	0.40
1:D:179:LEU:HB3	1:D:183:ALA:HB3	2.03	0.40
1:B:236:THR:O	1:B:236:THR:HG22	2.21	0.40
1:A:144:ILE:HG13	1:A:165:VAL:CG2	2.49	0.40
1:D:144:ILE:HG13	1:D:165:VAL:CG2	2.47	0.40
1:B:9:LYS:HG2	1:B:11:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

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	282/300 (94%)	266 (94%)	14 (5%)	2 (1%)	18	18
1	B	285/300 (95%)	272 (95%)	11 (4%)	2 (1%)	18	18
1	C	285/300 (95%)	277 (97%)	8 (3%)	0	100	100
1	D	278/300 (93%)	268 (96%)	9 (3%)	1 (0%)	30	33
All	All	1130/1200 (94%)	1083 (96%)	42 (4%)	5 (0%)	30	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	B	141	MET
1	B	234	PRO
1	A	125	GLU
1	D	112	CYS

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	252/263 (96%)	242 (96%)	10 (4%)	28	36
1	B	254/263 (97%)	246 (97%)	8 (3%)	35	46
1	C	254/263 (97%)	248 (98%)	6 (2%)	43	56
1	D	250/263 (95%)	242 (97%)	8 (3%)	34	45
All	All	1010/1052 (96%)	978 (97%)	32 (3%)	34	45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	84	ARG
1	A	118	GLU
1	A	122	ARG
1	A	124	LYS
1	A	141	MET
1	A	231	GLN
1	A	243	LYS
1	A	283	ARG
1	A	286	GLN
1	B	63	LYS
1	B	85	ASP
1	B	122	ARG
1	B	144	ILE
1	B	169	GLN
1	B	235	LYS
1	B	268	ARG
1	B	282	LYS
1	C	153	ILE
1	C	169	GLN
1	C	229	MET
1	C	235	LYS
1	C	278	LYS
1	C	282	LYS

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Mol	Chain	Res	Type
1	D	5	THR
1	D	6	ASP
1	D	111	GLU
1	D	122	ARG
1	D	161	ASN
1	D	169	GLN
1	D	209	LEU
1	D	278	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	28	HIS
1	A	161	ASN
1	A	167	GLN
1	A	286	GLN
1	A	295	HIS
1	A	298	HIS
1	B	75	HIS
1	B	109	ASN
1	B	117	GLN
1	B	169	GLN
1	B	286	GLN
1	B	297	HIS
1	B	298	HIS
1	C	109	ASN
1	C	152	HIS
1	C	299	HIS
1	D	28	HIS
1	D	98	ASN
1	D	296	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	286/300 (95%)	-1.32	0 100 100	20, 28, 48, 61	0
1	B	289/300 (96%)	-1.36	0 100 100	17, 27, 40, 59	0
1	C	289/300 (96%)	-1.37	0 100 100	16, 26, 43, 55	0
1	D	284/300 (94%)	-1.37	0 100 100	19, 27, 43, 52	0
All	All	1148/1200 (95%)	-1.35	0 100 100	16, 27, 44, 61	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.