



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 3QP9 / pdb_00003qp9
Title : The Structure of a C2-type Ketoreductase from a Modular Polyketide Synthase
Authors : Zheng, J.; Keatinge-Clay, A.T.
Deposited on : 2011-02-11
Resolution : 1.88 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

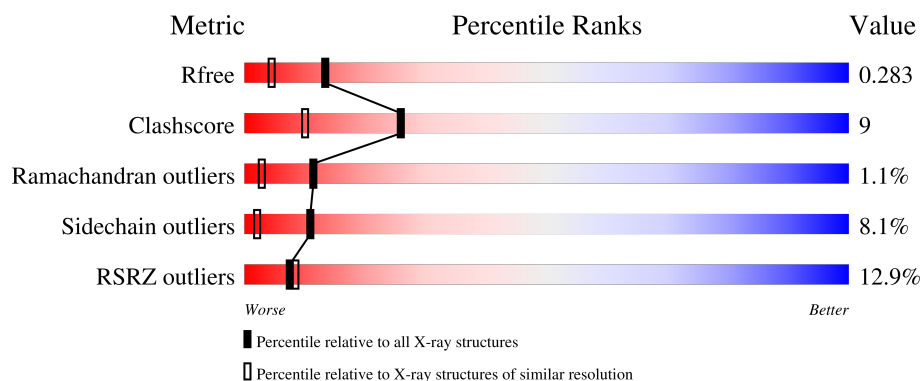
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	525	6% 69% 17% .. 10%
1	B	525	7% 70% 15% .. 12%
1	C	525	15% 71% 16% .. 11%
1	D	525	18% 62% 22% .. 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13673 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 Type I polyketide synthase PikAII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3390	2118	620	647	5			
1	B	460	Total	C	N	O	S	0	0	0
			3317	2075	605	632	5			
1	C	465	Total	C	N	O	S	0	0	0
			3340	2088	609	638	5			
1	D	457	Total	C	N	O	S	0	0	0
			3283	2055	597	626	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9ZGI4
A	-19	GLY	-	expression tag	UNP Q9ZGI4
A	-18	SER	-	expression tag	UNP Q9ZGI4
A	-17	SER	-	expression tag	UNP Q9ZGI4
A	-16	HIS	-	expression tag	UNP Q9ZGI4
A	-15	HIS	-	expression tag	UNP Q9ZGI4
A	-14	HIS	-	expression tag	UNP Q9ZGI4
A	-13	HIS	-	expression tag	UNP Q9ZGI4
A	-12	HIS	-	expression tag	UNP Q9ZGI4
A	-11	HIS	-	expression tag	UNP Q9ZGI4
A	-10	SER	-	expression tag	UNP Q9ZGI4
A	-9	SER	-	expression tag	UNP Q9ZGI4
A	-8	GLY	-	expression tag	UNP Q9ZGI4
A	-7	LEU	-	expression tag	UNP Q9ZGI4
A	-6	VAL	-	expression tag	UNP Q9ZGI4
A	-5	PRO	-	expression tag	UNP Q9ZGI4
A	-4	ARG	-	expression tag	UNP Q9ZGI4
A	-3	GLY	-	expression tag	UNP Q9ZGI4
A	-2	SER	-	expression tag	UNP Q9ZGI4
A	-1	HIS	-	expression tag	UNP Q9ZGI4
A	0	MET	-	expression tag	UNP Q9ZGI4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q9ZGI4
B	-19	GLY	-	expression tag	UNP Q9ZGI4
B	-18	SER	-	expression tag	UNP Q9ZGI4
B	-17	SER	-	expression tag	UNP Q9ZGI4
B	-16	HIS	-	expression tag	UNP Q9ZGI4
B	-15	HIS	-	expression tag	UNP Q9ZGI4
B	-14	HIS	-	expression tag	UNP Q9ZGI4
B	-13	HIS	-	expression tag	UNP Q9ZGI4
B	-12	HIS	-	expression tag	UNP Q9ZGI4
B	-11	HIS	-	expression tag	UNP Q9ZGI4
B	-10	SER	-	expression tag	UNP Q9ZGI4
B	-9	SER	-	expression tag	UNP Q9ZGI4
B	-8	GLY	-	expression tag	UNP Q9ZGI4
B	-7	LEU	-	expression tag	UNP Q9ZGI4
B	-6	VAL	-	expression tag	UNP Q9ZGI4
B	-5	PRO	-	expression tag	UNP Q9ZGI4
B	-4	ARG	-	expression tag	UNP Q9ZGI4
B	-3	GLY	-	expression tag	UNP Q9ZGI4
B	-2	SER	-	expression tag	UNP Q9ZGI4
B	-1	HIS	-	expression tag	UNP Q9ZGI4
B	0	MET	-	expression tag	UNP Q9ZGI4
C	-20	MET	-	expression tag	UNP Q9ZGI4
C	-19	GLY	-	expression tag	UNP Q9ZGI4
C	-18	SER	-	expression tag	UNP Q9ZGI4
C	-17	SER	-	expression tag	UNP Q9ZGI4
C	-16	HIS	-	expression tag	UNP Q9ZGI4
C	-15	HIS	-	expression tag	UNP Q9ZGI4
C	-14	HIS	-	expression tag	UNP Q9ZGI4
C	-13	HIS	-	expression tag	UNP Q9ZGI4
C	-12	HIS	-	expression tag	UNP Q9ZGI4
C	-11	HIS	-	expression tag	UNP Q9ZGI4
C	-10	SER	-	expression tag	UNP Q9ZGI4
C	-9	SER	-	expression tag	UNP Q9ZGI4
C	-8	GLY	-	expression tag	UNP Q9ZGI4
C	-7	LEU	-	expression tag	UNP Q9ZGI4
C	-6	VAL	-	expression tag	UNP Q9ZGI4
C	-5	PRO	-	expression tag	UNP Q9ZGI4
C	-4	ARG	-	expression tag	UNP Q9ZGI4
C	-3	GLY	-	expression tag	UNP Q9ZGI4
C	-2	SER	-	expression tag	UNP Q9ZGI4
C	-1	HIS	-	expression tag	UNP Q9ZGI4
C	0	MET	-	expression tag	UNP Q9ZGI4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q9ZGI4
D	-19	GLY	-	expression tag	UNP Q9ZGI4
D	-18	SER	-	expression tag	UNP Q9ZGI4
D	-17	SER	-	expression tag	UNP Q9ZGI4
D	-16	HIS	-	expression tag	UNP Q9ZGI4
D	-15	HIS	-	expression tag	UNP Q9ZGI4
D	-14	HIS	-	expression tag	UNP Q9ZGI4
D	-13	HIS	-	expression tag	UNP Q9ZGI4
D	-12	HIS	-	expression tag	UNP Q9ZGI4
D	-11	HIS	-	expression tag	UNP Q9ZGI4
D	-10	SER	-	expression tag	UNP Q9ZGI4
D	-9	SER	-	expression tag	UNP Q9ZGI4
D	-8	GLY	-	expression tag	UNP Q9ZGI4
D	-7	LEU	-	expression tag	UNP Q9ZGI4
D	-6	VAL	-	expression tag	UNP Q9ZGI4
D	-5	PRO	-	expression tag	UNP Q9ZGI4
D	-4	ARG	-	expression tag	UNP Q9ZGI4
D	-3	GLY	-	expression tag	UNP Q9ZGI4
D	-2	SER	-	expression tag	UNP Q9ZGI4
D	-1	HIS	-	expression tag	UNP Q9ZGI4
D	0	MET	-	expression tag	UNP Q9ZGI4

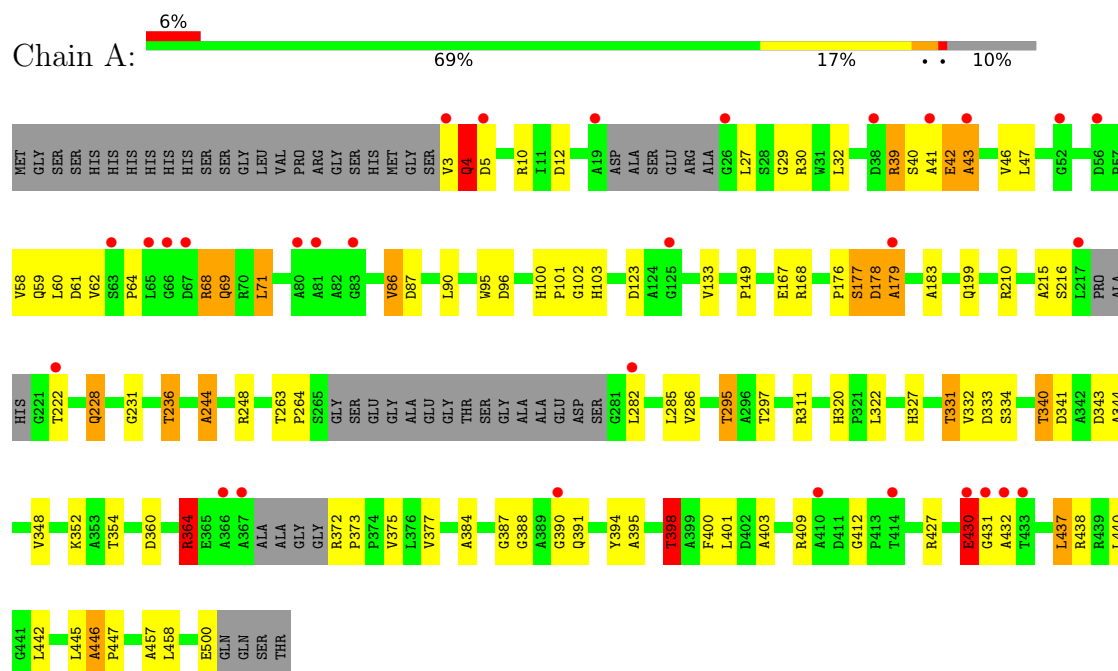
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	120	Total	O	0	0
			120	120		
2	B	99	Total	O	0	0
			99	99		
2	C	69	Total	O	0	0
			69	69		
2	D	55	Total	O	0	0
			55	55		

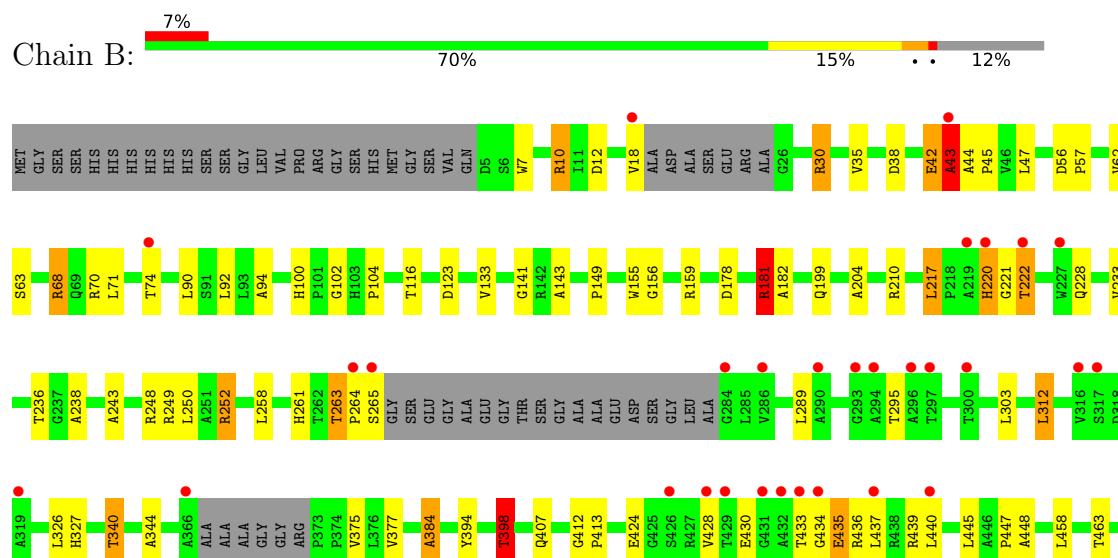
3 Residue-property plots [i](#)

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: Type I polyketide synthase PikAII

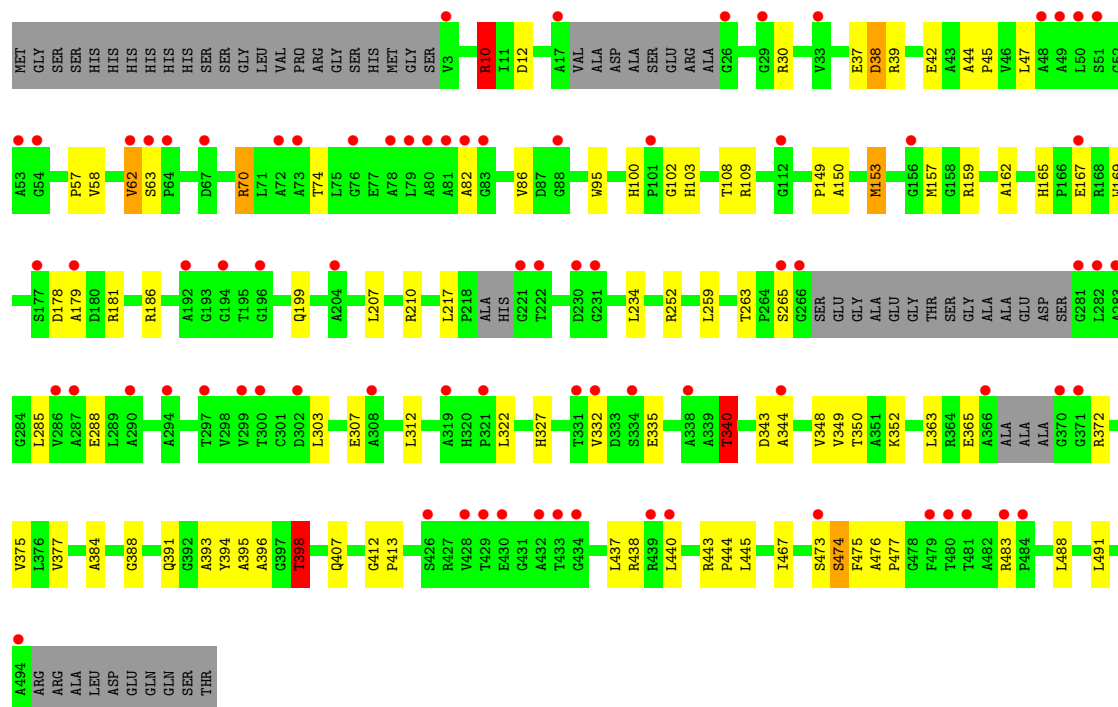


• Molecule 1: Type I polyketide synthase PikAII

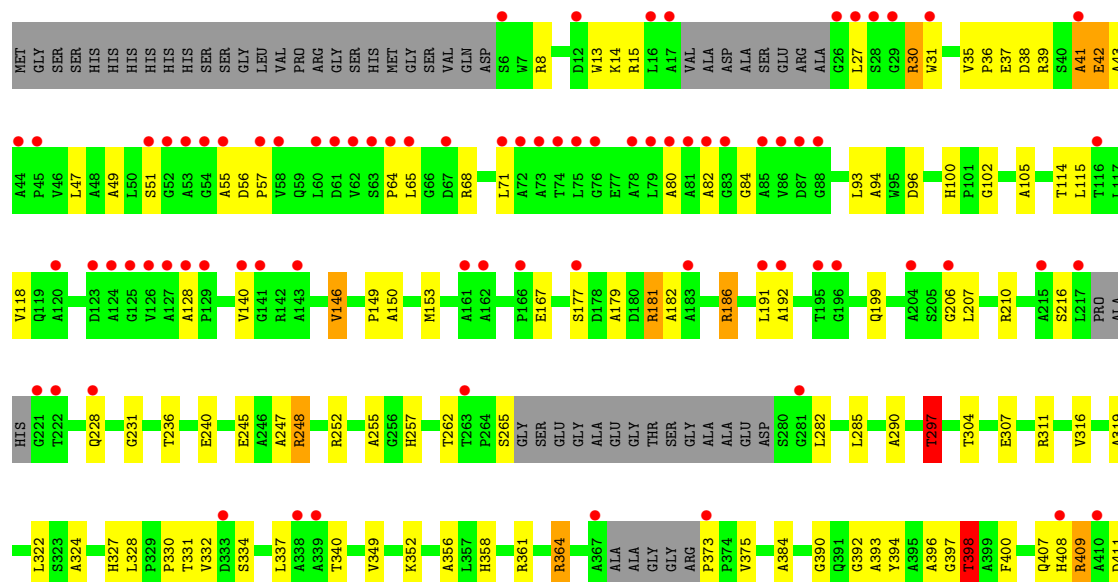




• Molecule 1: Type I polyketide synthase PikAII



• Molecule 1: Type I polyketide synthase PikAII





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.64Å 150.09Å 86.87Å 90.00° 105.12° 90.00°	Depositor
Resolution (Å)	31.23 – 1.88 31.23 – 1.88	Depositor EDS
% Data completeness (in resolution range)	91.0 (31.23-1.88) 90.9 (31.23-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.227 , 0.276 (Not available) , 0.283	Depositor DCC
R_{free} test set	7250 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13673	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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	1.46	16/3457 (0.5%)	1.34	12/4737 (0.3%)
1	B	1.46	16/3387 (0.5%)	1.33	17/4645 (0.4%)
1	C	1.25	4/3408 (0.1%)	1.25	16/4671 (0.3%)
1	D	1.34	16/3350 (0.5%)	1.30	19/4592 (0.4%)
All	All	1.38	52/13602 (0.4%)	1.31	64/18645 (0.3%)

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

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

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	398	THR	CB-CG2	-9.79	1.20	1.52
1	B	156	GLY	N-CA	7.11	1.54	1.45
1	D	316	VAL	CA-CB	6.97	1.62	1.54
1	B	94	ALA	CA-CB	6.93	1.65	1.53
1	D	105	ALA	CA-CB	6.87	1.63	1.53
1	B	141	GLY	N-CA	6.81	1.53	1.45
1	D	375	VAL	CA-CB	6.36	1.62	1.54
1	A	400	PHE	C-O	6.32	1.31	1.24
1	A	387	GLY	N-CA	6.12	1.51	1.45
1	A	377	VAL	N-CA	-6.03	1.38	1.46
1	B	143	ALA	CA-CB	6.00	1.64	1.53
1	C	349	VAL	CA-CB	-5.99	1.47	1.54
1	B	222	THR	CA-CB	5.93	1.63	1.53
1	D	247	ALA	CA-CB	5.88	1.62	1.53
1	A	401	LEU	N-CA	5.74	1.53	1.46
1	A	228	GLN	C-O	-5.74	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	SER	CA-C	5.73	1.60	1.53
1	B	155	TRP	CA-CB	5.67	1.62	1.53
1	A	401	LEU	C-O	5.62	1.30	1.24
1	D	393	ALA	CA-CB	5.59	1.62	1.53
1	B	43	ALA	N-CA	5.55	1.53	1.46
1	B	483	ARG	N-CA	-5.51	1.39	1.46
1	A	149	PRO	N-CA	-5.46	1.40	1.47
1	B	104	PRO	CA-C	5.46	1.59	1.52
1	D	290	ALA	CA-CB	5.46	1.61	1.53
1	D	328	LEU	N-CA	5.46	1.52	1.46
1	D	248	ARG	CA-C	-5.44	1.45	1.52
1	D	94	ALA	N-CA	5.43	1.53	1.46
1	B	30	ARG	CD-NE	5.42	1.53	1.46
1	A	244	ALA	CA-CB	5.41	1.61	1.53
1	A	457	ALA	CA-CB	5.41	1.61	1.53
1	D	455	ASP	CA-C	5.41	1.59	1.52
1	A	236	THR	CA-CB	5.40	1.62	1.53
1	B	182	ALA	CA-CB	5.40	1.61	1.53
1	B	43	ALA	CA-C	-5.39	1.45	1.52
1	C	153	MET	CB-CG	-5.38	1.36	1.52
1	A	46	VAL	CA-C	5.35	1.59	1.52
1	D	255	ALA	CA-CB	-5.33	1.45	1.53
1	C	467	ILE	CA-CB	5.27	1.60	1.53
1	A	286	VAL	C-O	5.26	1.30	1.24
1	B	448	ALA	CA-CB	5.23	1.61	1.53
1	D	319	ALA	CA-CB	5.19	1.62	1.53
1	B	155	TRP	C-O	5.14	1.30	1.24
1	A	354	THR	C-O	5.13	1.30	1.24
1	D	324	ALA	CA-CB	-5.11	1.44	1.53
1	B	384	ALA	C-O	5.11	1.30	1.24
1	A	430	GLU	N-CA	5.07	1.52	1.46
1	C	377	VAL	CA-CB	5.06	1.60	1.54
1	D	332	VAL	N-CA	5.05	1.51	1.46
1	B	204	ALA	CA-CB	5.05	1.61	1.53
1	D	463	THR	CA-CB	5.02	1.61	1.53
1	A	183	ALA	CA-C	5.01	1.59	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	408	HIS	CB-CA-C	8.65	124.96	109.83
1	D	150	ALA	N-CA-C	-7.71	103.32	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	398	THR	N-CA-CB	-7.49	98.77	110.30
1	A	458	LEU	N-CA-C	-7.37	103.33	111.36
1	B	463	THR	N-CA-C	-7.10	103.24	112.68
1	A	320	HIS	CA-C-N	-7.08	113.02	120.03
1	A	320	HIS	C-N-CA	-7.08	113.02	120.03
1	B	42	GLU	N-CA-C	-7.06	101.21	110.53
1	B	217	LEU	CA-C-N	7.02	127.44	119.93
1	B	217	LEU	C-N-CA	7.02	127.44	119.93
1	A	398	THR	CA-CB-CG2	7.01	122.42	110.50
1	D	407	GLN	CA-C-N	-7.00	108.00	122.07
1	D	407	GLN	C-N-CA	-7.00	108.00	122.07
1	D	240	GLU	CA-C-N	-6.92	112.57	119.56
1	D	240	GLU	C-N-CA	-6.92	112.57	119.56
1	B	10	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	C	63	SER	CA-C-N	-6.64	112.96	119.87
1	C	63	SER	C-N-CA	-6.64	112.96	119.87
1	D	483	ARG	CA-C-N	6.59	127.58	120.13
1	D	483	ARG	C-N-CA	6.59	127.58	120.13
1	B	10	ARG	NE-CZ-NH1	-6.39	115.11	121.50
1	D	373	PRO	CA-C-N	-6.20	113.89	120.03
1	D	373	PRO	C-N-CA	-6.20	113.89	120.03
1	C	483	ARG	CA-C-N	6.15	126.47	119.83
1	C	483	ARG	C-N-CA	6.15	126.47	119.83
1	C	263	THR	CA-C-N	-6.06	113.70	119.76
1	C	263	THR	C-N-CA	-6.06	113.70	119.76
1	D	361	ARG	N-CA-C	6.05	117.54	111.07
1	C	10	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	D	207	LEU	N-CA-C	5.96	119.62	110.20
1	B	483	ARG	CA-C-N	-5.94	113.64	119.76
1	B	483	ARG	C-N-CA	-5.94	113.64	119.76
1	B	63	SER	CA-C-N	-5.91	113.59	119.56
1	B	63	SER	C-N-CA	-5.91	113.59	119.56
1	B	155	TRP	N-CA-C	-5.89	104.94	111.36
1	A	331	THR	CB-CA-C	5.83	120.27	109.54
1	B	42	GLU	O-C-N	-5.77	116.22	122.79
1	C	398	THR	CA-CB-CG2	5.75	120.28	110.50
1	B	458	LEU	N-CA-C	-5.63	105.22	111.36
1	B	398	THR	OG1-CB-CG2	5.61	120.52	109.30
1	B	42	GLU	CA-C-N	-5.50	111.03	121.54
1	B	42	GLU	C-N-CA	-5.50	111.03	121.54
1	A	446	ALA	CA-C-N	5.48	124.67	118.97
1	A	446	ALA	C-N-CA	5.48	124.67	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	THR	N-CA-C	5.47	116.98	110.19
1	D	356	ALA	N-CA-C	5.47	117.67	111.11
1	C	350	THR	N-CA-C	5.39	116.84	111.07
1	A	398	THR	N-CA-CB	-5.38	102.01	110.30
1	C	157	MET	N-CA-C	-5.34	105.50	112.23
1	C	150	ALA	N-CA-C	-5.33	105.63	111.82
1	A	403	ALA	N-CA-C	5.31	117.15	111.36
1	D	128	ALA	CA-C-N	5.26	125.52	119.83
1	D	128	ALA	C-N-CA	5.26	125.52	119.83
1	C	398	THR	CB-CA-C	5.26	120.33	110.70
1	C	10	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	C	165	HIS	CA-C-N	5.14	125.43	119.47
1	C	165	HIS	C-N-CA	5.14	125.43	119.47
1	A	231	GLY	N-CA-C	-5.10	103.79	112.51
1	D	297	THR	CA-CB-OG1	-5.08	101.98	109.60
1	D	146	VAL	N-CA-C	-5.07	101.28	108.58
1	A	364	ARG	N-CA-C	-5.06	105.65	111.07
1	B	181	ARG	CG-CD-NE	5.06	123.14	112.00
1	D	464	ALA	N-CA-C	-5.03	99.63	107.93
1	A	295	THR	CB-CA-C	5.01	118.30	110.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	408	HIS	CA

There are no planarity outliers.

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	3390	0	3364	64	0
1	B	3317	0	3287	62	0
1	C	3340	0	3309	58	0
1	D	3283	0	3259	74	0
2	A	120	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	99	0	0	1	0
2	C	69	0	0	1	0
2	D	55	0	0	5	0
All	All	13673	0	13219	251	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 9.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ALA:HB2	1:C:398:THR:HG23	1.16	1.16
1:A:384:ALA:HB2	1:A:398:THR:HG23	1.34	1.08
1:B:384:ALA:HB2	1:B:398:THR:HG23	1.34	1.07
1:A:29:GLY:HA3	1:A:87:ASP:OD2	1.55	1.06
1:D:384:ALA:HB2	1:D:398:THR:CG2	1.90	1.02
1:B:434:GLY:HA2	1:B:436:ARG:N	1.74	1.02
1:D:186:ARG:HH11	1:D:186:ARG:HG3	1.24	1.01
1:A:334:SER:HB2	1:A:390:GLY:O	1.60	0.98
1:C:384:ALA:HB2	1:C:398:THR:CG2	1.93	0.98
1:B:384:ALA:HB2	1:B:398:THR:CG2	1.93	0.97
1:A:384:ALA:HB2	1:A:398:THR:CG2	1.96	0.95
1:D:153:MET:HE3	1:D:400:PHE:HB2	1.45	0.95
1:D:153:MET:HE2	1:D:397:GLY:HA2	1.49	0.94
1:B:42:GLU:O	1:B:43:ALA:HB3	1.64	0.93
1:B:42:GLU:O	1:B:43:ALA:CB	2.12	0.92
1:D:384:ALA:HB2	1:D:398:THR:HG22	1.52	0.90
1:D:49:ALA:HA	1:D:181:ARG:NH2	1.86	0.89
1:C:384:ALA:CB	1:C:398:THR:HG23	2.01	0.88
1:D:199:GLN:NE2	1:D:210:ARG:HD3	1.90	0.86
1:D:49:ALA:HA	1:D:181:ARG:HH21	1.40	0.86
1:B:384:ALA:CB	1:B:398:THR:HG23	2.05	0.86
1:D:228:GLN:HG3	2:D:525:HOH:O	1.77	0.84
1:B:434:GLY:CA	1:B:437:LEU:H	1.92	0.82
1:B:149:PRO:HG3	1:B:407:GLN:NE2	1.94	0.82
1:A:384:ALA:CB	1:A:398:THR:HG23	2.10	0.81
1:D:384:ALA:HB2	1:D:398:THR:HG23	1.62	0.81
1:D:334:SER:HB2	1:D:390:GLY:O	1.81	0.80
1:D:153:MET:HE1	1:D:349:VAL:HG13	1.62	0.79
1:D:153:MET:HE3	1:D:400:PHE:CB	2.13	0.79
1:D:427:ARG:HG2	1:D:427:ARG:HH11	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:GLY:HA2	1:B:435:GLU:C	2.07	0.78
1:D:186:ARG:HH11	1:D:186:ARG:CG	1.97	0.78
1:B:68:ARG:HD2	1:B:123:ASP:OD1	1.82	0.78
1:D:36:PRO:HD3	1:D:93:LEU:HD23	1.66	0.76
1:C:100:HIS:HD2	1:C:102:GLY:H	1.30	0.76
1:C:303:LEU:HD21	1:C:312:LEU:HD22	1.68	0.76
1:B:434:GLY:CA	1:B:436:ARG:N	2.50	0.74
1:C:149:PRO:HG3	1:C:407:GLN:NE2	2.01	0.74
1:A:103:HIS:HE1	1:A:343:ASP:OD2	1.69	0.74
1:A:42:GLU:O	1:A:43:ALA:CB	2.37	0.72
1:D:426:SER:O	1:D:427:ARG:HB3	1.90	0.71
1:B:70:ARG:NH2	1:C:38:ASP:HB3	2.07	0.69
1:A:68:ARG:HD2	1:A:123:ASP:OD1	1.92	0.69
1:A:10:ARG:HG2	1:A:215:ALA:HB2	1.74	0.69
1:D:245:GLU:OE2	1:D:248:ARG:NH2	2.27	0.68
1:C:100:HIS:CD2	1:C:102:GLY:H	2.10	0.68
1:B:489:ALA:O	1:B:495:ARG:NH1	2.27	0.68
1:D:262:THR:HG21	1:D:282:LEU:HD11	1.77	0.66
1:A:236:THR:OG1	1:A:327:HIS:HD2	1.79	0.65
1:D:199:GLN:HE21	1:D:210:ARG:HD3	1.61	0.65
1:B:434:GLY:HA3	1:B:437:LEU:H	1.62	0.65
1:C:340:THR:HG22	1:C:344:ALA:HB3	1.78	0.65
1:C:186:ARG:HB3	1:C:207:LEU:HD21	1.78	0.63
1:D:100:HIS:HD2	1:D:102:GLY:H	1.44	0.63
1:B:236:THR:OG1	1:B:327:HIS:HD2	1.81	0.63
1:B:434:GLY:HA2	1:B:437:LEU:N	2.14	0.62
1:C:30:ARG:HH11	1:C:82:ALA:HA	1.65	0.62
1:C:476:ALA:HB3	1:C:477:PRO:HD3	1.81	0.62
1:D:297:THR:HB	2:D:508:HOH:O	1.98	0.62
1:D:153:MET:CE	1:D:397:GLY:HA2	2.27	0.62
1:D:327:HIS:HE1	2:D:507:HOH:O	1.81	0.61
1:C:234:LEU:HD13	1:C:259:LEU:HD23	1.83	0.61
1:C:303:LEU:HD21	1:C:312:LEU:CD2	2.31	0.61
1:B:70:ARG:HH12	1:C:38:ASP:HA	1.66	0.61
1:A:340:THR:HG22	1:A:344:ALA:HB3	1.83	0.60
1:D:433:THR:O	1:D:437:LEU:HD13	2.01	0.60
1:B:100:HIS:HD2	1:B:102:GLY:H	1.49	0.60
1:C:149:PRO:HG3	1:C:407:GLN:HE21	1.67	0.60
1:D:409:ARG:HD3	1:D:413:PRO:O	2.01	0.60
1:D:394:TYR:O	1:D:398:THR:HB	2.02	0.60
1:A:30:ARG:HD3	1:A:58:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:GLY:CA	1:B:437:LEU:N	2.65	0.59
1:A:90:LEU:HD11	1:A:133:VAL:CG2	2.33	0.59
1:C:335:GLU:OE2	1:C:340:THR:HG23	2.03	0.58
1:C:394:TYR:O	1:C:398:THR:HB	2.03	0.58
1:A:199:GLN:HE21	1:A:210:ARG:HD3	1.66	0.58
1:B:261:HIS:HE1	1:B:263:THR:HG23	1.68	0.58
1:A:69:GLN:HE21	1:A:69:GLN:HA	1.68	0.58
1:A:340:THR:HG22	1:A:341:ASP:H	1.67	0.58
1:A:69:GLN:HA	1:A:69:GLN:NE2	2.18	0.58
1:B:149:PRO:HG3	1:B:407:GLN:HE21	1.65	0.58
1:C:327:HIS:HE1	2:C:509:HOH:O	1.86	0.58
1:A:39:ARG:NH2	1:A:95:TRP:O	2.37	0.58
1:A:427:ARG:O	1:A:430:GLU:HB3	2.04	0.57
1:D:47:LEU:HD22	1:D:57:PRO:HB2	1.85	0.57
1:A:3:VAL:HG12	1:A:4:GLN:N	2.17	0.57
1:D:30:ARG:NH1	1:D:56:ASP:OD2	2.37	0.57
1:D:186:ARG:HG3	1:D:186:ARG:NH1	2.03	0.57
1:B:434:GLY:HA2	1:B:437:LEU:H	1.66	0.57
1:B:220:HIS:CD2	1:B:221:GLY:H	2.23	0.57
1:B:70:ARG:CZ	1:C:38:ASP:HB3	2.35	0.56
1:C:159:ARG:HD3	1:C:199:GLN:HE22	1.71	0.56
1:D:199:GLN:HE22	1:D:210:ARG:HH21	1.53	0.56
1:D:30:ARG:HD3	1:D:56:ASP:O	2.05	0.56
1:B:340:THR:HG22	1:B:344:ALA:HB3	1.87	0.56
1:C:30:ARG:HH21	1:C:58:VAL:HG21	1.71	0.56
1:D:384:ALA:CB	1:D:398:THR:HG23	2.35	0.56
1:A:59:GLN:NE2	1:A:61:ASP:OD1	2.38	0.56
1:A:42:GLU:O	1:A:43:ALA:HB3	2.07	0.55
1:A:100:HIS:CD2	1:A:102:GLY:H	2.24	0.55
1:D:15:ARG:HH21	1:D:206:GLY:HA3	1.71	0.55
1:D:42:GLU:O	1:D:43:ALA:HB3	2.06	0.55
1:B:220:HIS:CG	1:B:221:GLY:H	2.25	0.55
1:A:10:ARG:NH2	1:A:12:ASP:OD1	2.40	0.54
1:A:332:VAL:HG21	1:A:348:VAL:HG13	1.88	0.54
1:C:363:LEU:HB2	1:C:413:PRO:HG3	1.88	0.54
1:D:364:ARG:HG2	1:D:412:GLY:O	2.07	0.54
1:B:7:TRP:CZ3	1:B:445:LEU:HG	2.42	0.54
1:A:100:HIS:HD2	1:A:102:GLY:H	1.54	0.54
1:A:430:GLU:HG3	1:A:432:ALA:H	1.73	0.54
1:B:181:ARG:HH11	1:B:181:ARG:HG3	1.72	0.54
1:D:236:THR:OG1	1:D:327:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ALA:N	1:B:45:PRO:CD	2.72	0.53
1:C:412:GLY:HA2	1:C:413:PRO:C	2.33	0.53
1:D:228:GLN:CG	2:D:525:HOH:O	2.48	0.53
1:D:427:ARG:HH11	1:D:427:ARG:CG	2.21	0.53
1:C:162:ALA:HB2	1:C:169:TRP:CD1	2.45	0.52
1:B:303:LEU:HD21	1:B:312:LEU:HD22	1.90	0.52
1:B:70:ARG:HH22	1:C:38:ASP:HB3	1.72	0.52
1:B:199:GLN:HE21	1:B:210:ARG:HD3	1.75	0.52
1:B:384:ALA:HB2	1:B:398:THR:HG22	1.83	0.52
1:D:186:ARG:CG	1:D:186:ARG:NH1	2.66	0.52
1:B:434:GLY:H	1:B:436:ARG:H	1.57	0.52
1:D:440:LEU:O	1:D:475:PHE:HA	2.10	0.52
1:C:153:MET:HG2	1:C:396:ALA:O	2.10	0.52
1:B:100:HIS:CD2	1:B:102:GLY:H	2.27	0.51
1:C:10:ARG:HD2	1:C:12:ASP:OD2	2.10	0.51
1:A:62:VAL:HG21	1:A:71:LEU:HG	1.93	0.51
1:B:38:ASP:HB2	1:C:70:ARG:NH2	2.24	0.51
1:A:90:LEU:HD11	1:A:133:VAL:HG23	1.93	0.51
1:A:228:GLN:OE1	1:A:372:ARG:HD3	2.11	0.51
1:A:167:GLU:OE2	1:A:168:ARG:HG2	2.10	0.50
1:C:100:HIS:HD2	1:C:102:GLY:N	2.06	0.50
1:B:70:ARG:O	1:B:74:THR:HG23	2.12	0.50
1:A:384:ALA:HB2	1:A:398:THR:HG22	1.88	0.50
1:A:431:GLY:HA2	1:A:438:ARG:HH12	1.77	0.50
1:D:64:PRO:HG2	1:D:96:ASP:OD2	2.11	0.50
1:B:70:ARG:NH1	1:C:38:ASP:HA	2.26	0.49
1:C:167:GLU:CD	1:C:167:GLU:H	2.20	0.49
1:D:199:GLN:HE22	1:D:210:ARG:NH2	2.10	0.49
1:C:199:GLN:NE2	1:C:210:ARG:HD3	2.27	0.49
1:D:182:ALA:O	1:D:186:ARG:HG2	2.12	0.49
1:D:13:TRP:CD1	1:D:140:VAL:HA	2.47	0.49
1:D:146:VAL:HG12	1:D:149:PRO:HD3	1.93	0.49
1:A:437:LEU:HD13	1:A:442:LEU:HD12	1.94	0.49
1:C:30:ARG:NH2	1:C:58:VAL:HG21	2.28	0.49
1:A:431:GLY:HA2	1:A:438:ARG:NH1	2.28	0.48
1:A:30:ARG:HD2	1:A:58:VAL:HG21	1.93	0.48
1:B:90:LEU:HD11	1:B:133:VAL:CG2	2.43	0.48
1:A:236:THR:OG1	1:A:327:HIS:CD2	2.62	0.48
1:C:395:ALA:HA	1:C:398:THR:HG22	1.95	0.48
1:A:327:HIS:HE1	2:A:522:HOH:O	1.97	0.48
1:D:307:GLU:HG2	1:D:311:ARG:HH22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLU:HG3	1:C:62:VAL:O	2.14	0.48
1:B:159:ARG:HD3	1:B:199:GLN:HE22	1.79	0.48
1:B:327:HIS:HE1	2:B:526:HOH:O	1.96	0.48
1:A:395:ALA:HA	1:A:398:THR:HG22	1.96	0.48
1:A:394:TYR:O	1:A:398:THR:HB	2.14	0.47
1:A:178:ASP:O	1:A:179:ALA:HB3	2.15	0.47
1:C:199:GLN:HE22	1:C:210:ARG:NH2	2.13	0.47
1:A:68:ARG:HH11	1:A:123:ASP:CG	2.23	0.47
1:C:39:ARG:HG3	1:C:39:ARG:HH11	1.79	0.47
1:C:44:ALA:HB3	1:C:45:PRO:HD3	1.97	0.47
1:D:477:PRO:C	1:D:479:PHE:H	2.23	0.46
1:B:249:ARG:HD3	1:B:252:ARG:HD2	1.97	0.46
1:B:70:ARG:NH1	1:C:38:ASP:HB3	2.31	0.46
1:A:90:LEU:HD11	1:A:133:VAL:HG21	1.96	0.46
1:D:418:VAL:CG1	1:D:467:ILE:HD12	2.46	0.46
1:B:199:GLN:NE2	1:B:210:ARG:HD3	2.30	0.45
1:D:8:ARG:HG2	2:D:526:HOH:O	2.16	0.45
1:D:337:LEU:HD21	1:D:392:GLY:HA3	1.98	0.45
1:D:80:ALA:C	1:D:82:ALA:H	2.24	0.45
1:B:434:GLY:N	1:B:436:ARG:H	2.14	0.45
1:C:488:LEU:HD12	1:C:488:LEU:N	2.31	0.45
1:A:199:GLN:NE2	1:A:210:ARG:HD3	2.31	0.45
1:A:360:ASP:O	1:A:364:ARG:HB2	2.17	0.45
1:B:326:LEU:HD23	1:B:377:VAL:HB	1.99	0.45
1:C:437:LEU:HA	1:C:440:LEU:HG	1.98	0.45
1:D:153:MET:HE2	1:D:397:GLY:CA	2.35	0.45
1:D:307:GLU:HG2	1:D:311:ARG:NH2	2.32	0.45
1:A:3:VAL:HG12	1:A:4:GLN:H	1.82	0.45
1:D:27:LEU:HD12	1:D:192:ALA:HA	1.99	0.45
1:A:42:GLU:O	1:A:43:ALA:HB2	2.15	0.44
1:A:352:LYS:HE2	1:A:394:TYR:HE1	1.82	0.44
1:B:47:LEU:CD1	1:B:57:PRO:HB2	2.47	0.44
1:B:412:GLY:HA2	1:B:413:PRO:C	2.43	0.44
1:D:153:MET:HG2	1:D:396:ALA:O	2.18	0.44
1:B:424:GLU:HB2	1:B:447:PRO:HD3	2.00	0.44
1:C:47:LEU:HD22	1:C:57:PRO:HB2	1.99	0.44
1:B:10:ARG:HD2	1:B:12:ASP:OD2	2.17	0.44
1:B:394:TYR:O	1:B:398:THR:HB	2.18	0.44
1:C:39:ARG:HD3	1:C:42:GLU:CD	2.42	0.44
1:A:176:PRO:O	1:A:177:SER:C	2.61	0.44
1:C:443:ARG:O	1:C:444:PRO:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HD13	1:B:57:PRO:HB2	1.99	0.43
1:C:443:ARG:HD3	1:C:443:ARG:N	2.33	0.43
1:D:35:VAL:HG12	1:D:36:PRO:O	2.19	0.43
1:D:115:LEU:HD21	1:D:340:THR:HG23	2.00	0.43
1:D:304:THR:O	1:D:358:HIS:HE1	2.01	0.43
1:D:149:PRO:HB2	1:D:400:PHE:CE1	2.53	0.43
1:B:42:GLU:H	1:B:42:GLU:HG3	1.63	0.43
1:B:30:ARG:NH1	1:B:56:ASP:OD2	2.51	0.43
1:B:258:LEU:HD12	1:B:289:LEU:HD13	2.00	0.43
1:C:440:LEU:O	1:C:475:PHE:HA	2.19	0.43
1:A:199:GLN:HE22	1:A:210:ARG:NH2	2.16	0.43
1:C:95:TRP:N	1:C:95:TRP:CD1	2.87	0.43
1:C:473:SER:O	1:C:474:SER:HB3	2.18	0.43
1:B:428:VAL:O	1:B:433:THR:O	2.36	0.43
1:C:332:VAL:HG21	1:C:348:VAL:HG13	2.01	0.43
1:D:39:ARG:NH1	1:D:42:GLU:OE2	2.52	0.42
1:D:418:VAL:HG11	1:D:467:ILE:HD12	2.01	0.42
1:A:388:GLY:HA3	1:A:391:GLN:NE2	2.34	0.42
1:D:37:GLU:C	1:D:39:ARG:H	2.26	0.42
1:D:114:THR:O	1:D:118:VAL:HG23	2.19	0.42
1:D:334:SER:CB	1:D:390:GLY:O	2.60	0.42
1:A:446:ALA:HA	1:A:447:PRO:HD3	1.87	0.42
1:D:55:ALA:O	1:D:57:PRO:HD3	2.19	0.42
1:C:37:GLU:HG3	1:C:62:VAL:C	2.44	0.42
1:D:153:MET:CE	1:D:400:PHE:HB2	2.32	0.42
1:C:159:ARG:HD3	1:C:199:GLN:NE2	2.33	0.42
1:C:332:VAL:HG11	1:C:348:VAL:HG13	2.02	0.42
1:D:416:THR:HA	1:D:463:THR:O	2.20	0.42
1:A:64:PRO:HG2	1:A:96:ASP:OD2	2.20	0.42
1:C:348:VAL:HB	1:C:393:ALA:HB1	2.01	0.42
1:D:186:ARG:CZ	1:D:206:GLY:HA2	2.50	0.41
1:A:32:LEU:HD13	1:A:60:LEU:HD11	2.03	0.41
1:A:263:THR:HA	1:A:264:PRO:HD3	1.92	0.41
1:C:108:THR:O	1:C:109:ARG:C	2.63	0.41
1:D:231:GLY:O	1:D:257:HIS:HB2	2.20	0.41
1:A:199:GLN:HE22	1:A:210:ARG:HH21	1.69	0.41
1:D:31:TRP:CZ3	1:D:191:LEU:HD22	2.55	0.41
1:A:373:PRO:HB3	1:A:412:GLY:HA3	2.02	0.41
1:B:68:ARG:HB2	1:B:116:THR:HG23	2.03	0.41
1:A:372:ARG:HG2	1:A:372:ARG:HH11	1.85	0.41
1:B:35:VAL:HG22	1:B:92:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:HIS:HE1	1:C:343:ASP:OD2	2.04	0.41
1:D:282:LEU:N	1:D:282:LEU:HD12	2.35	0.41
1:A:30:ARG:CD	1:A:58:VAL:HG23	2.49	0.41
1:A:90:LEU:HD12	1:A:90:LEU:HA	1.92	0.41
1:A:244:ALA:O	1:A:248:ARG:HG3	2.21	0.41
1:A:360:ASP:OD2	1:A:409:ARG:NE	2.51	0.41
1:C:388:GLY:HA3	1:C:391:GLN:HE21	1.86	0.41
1:C:388:GLY:CA	1:C:391:GLN:HE21	2.34	0.41
1:D:41:ALA:HB3	1:D:42:GLU:OE1	2.21	0.41
1:A:30:ARG:HG2	1:A:86:VAL:HG22	2.03	0.41
1:B:238:ALA:HA	1:B:243:ALA:CB	2.51	0.41
1:B:258:LEU:CD1	1:B:289:LEU:HD13	2.51	0.41
1:B:233:VAL:HG11	1:B:250:LEU:HD13	2.03	0.40
1:B:238:ALA:HA	1:B:243:ALA:HB3	2.03	0.40
1:D:330:PRO:O	1:D:352:LYS:HE2	2.21	0.40
1:A:100:HIS:HA	1:A:101:PRO:HD3	1.91	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	460/525 (88%)	441 (96%)	13 (3%)	6 (1%)	9	2
1	B	452/525 (86%)	433 (96%)	14 (3%)	5 (1%)	11	3
1	C	455/525 (87%)	441 (97%)	12 (3%)	2 (0%)	30	18
1	D	447/525 (85%)	420 (94%)	20 (4%)	7 (2%)	7	1
All	All	1814/2100 (86%)	1735 (96%)	59 (3%)	20 (1%)	11	3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	430	GLU
1	B	220	HIS
1	B	435	GLU
1	C	179	ALA
1	C	474	SER
1	D	84	GLY
1	D	490	ASP
1	A	41	ALA
1	A	43	ALA
1	B	43	ALA
1	D	42	GLU
1	D	179	ALA
1	D	427	ARG
1	B	222	THR
1	D	41	ALA
1	D	481	THR
1	A	177	SER
1	B	264	PRO
1	A	179	ALA

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	328/365 (90%)	299 (91%)	29 (9%)	9	1
1	B	322/365 (88%)	300 (93%)	22 (7%)	14	3
1	C	323/365 (88%)	299 (93%)	24 (7%)	13	3
1	D	318/365 (87%)	288 (91%)	30 (9%)	8	1
All	All	1291/1460 (88%)	1186 (92%)	105 (8%)	11	2

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	ASP

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	39	ARG
1	A	40	SER
1	A	42	GLU
1	A	47	LEU
1	A	68	ARG
1	A	69	GLN
1	A	71	LEU
1	A	86	VAL
1	A	178	ASP
1	A	222	THR
1	A	282	LEU
1	A	285	LEU
1	A	295	THR
1	A	297	THR
1	A	311	ARG
1	A	322	LEU
1	A	331	THR
1	A	333	ASP
1	A	340	THR
1	A	364	ARG
1	A	375	VAL
1	A	398	THR
1	A	437	LEU
1	A	440	LEU
1	A	445	LEU
1	A	500	GLU
1	B	18	VAL
1	B	62	VAL
1	B	68	ARG
1	B	71	LEU
1	B	178	ASP
1	B	181	ARG
1	B	217	LEU
1	B	228	GLN
1	B	248	ARG
1	B	252	ARG
1	B	263	THR
1	B	265	SER
1	B	295	THR
1	B	312	LEU
1	B	340	THR

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Mol	Chain	Res	Type
1	B	375	VAL
1	B	398	THR
1	B	430	GLU
1	B	439	ARG
1	B	440	LEU
1	B	493	GLU
1	B	495	ARG
1	C	10	ARG
1	C	38	ASP
1	C	62	VAL
1	C	70	ARG
1	C	74	THR
1	C	86	VAL
1	C	178	ASP
1	C	181	ARG
1	C	217	LEU
1	C	252	ARG
1	C	265	SER
1	C	285	LEU
1	C	288	GLU
1	C	307	GLU
1	C	322	LEU
1	C	340	THR
1	C	352	LYS
1	C	365	GLU
1	C	372	ARG
1	C	375	VAL
1	C	398	THR
1	C	438	ARG
1	C	445	LEU
1	C	491	LEU
1	D	14	LYS
1	D	30	ARG
1	D	38	ASP
1	D	51	SER
1	D	65	LEU
1	D	68	ARG
1	D	71	LEU
1	D	167	GLU
1	D	177	SER
1	D	181	ARG
1	D	186	ARG

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Mol	Chain	Res	Type
1	D	216	SER
1	D	252	ARG
1	D	265	SER
1	D	285	LEU
1	D	297	THR
1	D	322	LEU
1	D	331	THR
1	D	364	ARG
1	D	398	THR
1	D	409	ARG
1	D	411	ASP
1	D	427	ARG
1	D	428	VAL
1	D	438	ARG
1	D	440	LEU
1	D	445	LEU
1	D	463	THR
1	D	473	SER
1	D	490	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	100	HIS
1	A	103	HIS
1	A	199	GLN
1	A	228	GLN
1	A	257	HIS
1	A	327	HIS
1	A	358	HIS
1	A	391	GLN
1	B	100	HIS
1	B	103	HIS
1	B	199	GLN
1	B	228	GLN
1	B	257	HIS
1	B	320	HIS
1	B	327	HIS
1	B	358	HIS
1	B	407	GLN
1	C	100	HIS

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Mol	Chain	Res	Type
1	C	103	HIS
1	C	145	HIS
1	C	199	GLN
1	C	257	HIS
1	C	320	HIS
1	C	327	HIS
1	C	391	GLN
1	C	407	GLN
1	D	100	HIS
1	D	199	GLN
1	D	257	HIS
1	D	327	HIS
1	D	358	HIS
1	D	460	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	470/525 (89%)	0.51	30 (6%) 25 28	21, 36, 59, 75	0
1	B	460/525 (87%)	0.55	35 (7%) 20 22	19, 37, 63, 72	0
1	C	465/525 (88%)	0.99	79 (16%) 4 5	24, 47, 68, 80	0
1	D	457/525 (87%)	1.09	95 (20%) 2 2	22, 48, 80, 88	0
All	All	1852/2100 (88%)	0.78	239 (12%) 7 8	19, 40, 70, 88	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	GLY	6.8
1	A	282	LEU	6.1
1	D	162	ALA	5.9
1	A	3	VAL	5.7
1	A	432	ALA	5.2
1	D	41	ALA	5.2
1	B	290	ALA	5.0
1	D	82	ALA	4.7
1	D	482	ALA	4.7
1	C	300	THR	4.7
1	D	480	THR	4.4
1	D	72	ALA	4.3
1	B	433	THR	4.3
1	D	76	GLY	4.3
1	C	432	ALA	4.2
1	D	62	VAL	4.1
1	D	73	ALA	4.1
1	B	284	GLY	4.1
1	D	410	ALA	4.0
1	C	428	VAL	3.9
1	D	55	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	141	GLY	3.9
1	D	64	PRO	3.9
1	D	492	PRO	3.9
1	B	220	HIS	3.8
1	C	434	GLY	3.8
1	D	367	ALA	3.8
1	D	221	GLY	3.8
1	D	484	PRO	3.8
1	B	478	GLY	3.7
1	D	27	LEU	3.7
1	C	266	GLY	3.7
1	C	494	ALA	3.7
1	D	65	LEU	3.6
1	D	83	GLY	3.6
1	B	286	VAL	3.6
1	D	481	THR	3.6
1	B	434	GLY	3.5
1	C	282	LEU	3.5
1	B	481	THR	3.5
1	D	58	VAL	3.5
1	B	480	THR	3.4
1	B	432	ALA	3.4
1	C	221	GLY	3.4
1	B	219	ALA	3.4
1	C	82	ALA	3.4
1	C	76	GLY	3.4
1	C	433	THR	3.4
1	B	222	THR	3.3
1	B	484	PRO	3.3
1	A	66	GLY	3.3
1	D	60	LEU	3.3
1	D	12	ASP	3.3
1	C	371	GLY	3.3
1	D	206	GLY	3.3
1	C	484	PRO	3.2
1	A	367	ALA	3.2
1	D	222	THR	3.2
1	B	264	PRO	3.2
1	D	63	SER	3.2
1	C	51	SER	3.2
1	D	26	GLY	3.2
1	C	480	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	339	ALA	3.1
1	C	83	GLY	3.1
1	C	196	GLY	3.1
1	A	81	ALA	3.1
1	A	83	GLY	3.1
1	C	290	ALA	3.1
1	A	52	GLY	3.1
1	C	79	LEU	3.1
1	B	479	PHE	3.1
1	C	177	SER	3.1
1	D	80	ALA	3.1
1	B	317	SER	3.0
1	D	143	ALA	3.0
1	B	437	LEU	3.0
1	D	16	LEU	3.0
1	C	479	PHE	3.0
1	D	177	SER	3.0
1	C	481	THR	3.0
1	C	194	GLY	3.0
1	D	217	LEU	2.9
1	B	296	ALA	2.9
1	B	366	ALA	2.9
1	C	53	ALA	2.9
1	C	78	ALA	2.9
1	D	478	GLY	2.9
1	C	334	SER	2.9
1	A	179	ALA	2.9
1	B	428	VAL	2.8
1	B	429	THR	2.8
1	A	80	ALA	2.8
1	D	53	ALA	2.8
1	D	88	GLY	2.8
1	C	429	THR	2.8
1	D	204	ALA	2.8
1	D	412	GLY	2.8
1	B	227	TRP	2.8
1	B	18	VAL	2.8
1	D	192	ALA	2.8
1	C	370	GLY	2.8
1	B	440	LEU	2.8
1	D	126	VAL	2.8
1	A	19	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	41	ALA	2.7
1	A	222	THR	2.7
1	A	414	THR	2.7
1	C	440	LEU	2.7
1	D	45	PRO	2.7
1	D	57	PRO	2.7
1	C	48	ALA	2.7
1	C	167	GLU	2.7
1	C	294	ALA	2.7
1	B	300	THR	2.7
1	C	72	ALA	2.7
1	C	112	GLY	2.7
1	A	67	ASP	2.7
1	C	63	SER	2.7
1	C	286	VAL	2.7
1	D	281	GLY	2.6
1	D	433	THR	2.6
1	D	6	SER	2.6
1	D	166	PRO	2.6
1	C	29	GLY	2.6
1	C	80	ALA	2.6
1	D	85	ALA	2.6
1	C	439	ARG	2.5
1	A	65	LEU	2.5
1	D	61	ASP	2.5
1	D	52	GLY	2.5
1	D	51	SER	2.5
1	A	217	LEU	2.5
1	A	125	GLY	2.5
1	B	294	ALA	2.5
1	C	287	ALA	2.5
1	C	344	ALA	2.5
1	A	430	GLU	2.5
1	C	321	PRO	2.5
1	D	125	GLY	2.5
1	D	124	ALA	2.5
1	B	297	THR	2.5
1	D	427	ARG	2.4
1	D	431	GLY	2.4
1	C	299	VAL	2.4
1	D	491	LEU	2.4
1	D	215	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	373	PRO	2.4
1	C	54	GLY	2.4
1	C	156	GLY	2.4
1	C	281	GLY	2.4
1	C	50	LEU	2.4
1	D	67	ASP	2.4
1	B	74	THR	2.4
1	C	222	THR	2.4
1	C	283	ALA	2.4
1	D	120	ALA	2.4
1	D	128	ALA	2.4
1	D	489	ALA	2.4
1	D	54	GLY	2.4
1	D	31	TRP	2.4
1	C	331	THR	2.3
1	A	43	ALA	2.3
1	D	44	ALA	2.3
1	C	88	GLY	2.3
1	C	231	GLY	2.3
1	C	62	VAL	2.3
1	C	230	ASP	2.3
1	D	408	HIS	2.3
1	A	410	ALA	2.3
1	C	192	ALA	2.3
1	D	78	ALA	2.3
1	B	431	GLY	2.3
1	C	426	SER	2.3
1	C	473	SER	2.3
1	A	5	ASP	2.3
1	C	302	ASP	2.3
1	C	319	ALA	2.3
1	D	17	ALA	2.3
1	D	127	ALA	2.3
1	D	129	PRO	2.3
1	C	483	ARG	2.3
1	C	67	ASP	2.3
1	C	101	PRO	2.2
1	C	338	ALA	2.2
1	C	366	ALA	2.2
1	D	29	GLY	2.2
1	D	479	PHE	2.2
1	A	38	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	86	VAL	2.2
1	A	56	ASP	2.2
1	D	28	SER	2.2
1	A	366	ALA	2.2
1	C	81	ALA	2.2
1	D	161	ALA	2.2
1	C	297	THR	2.2
1	D	263	THR	2.2
1	D	463	THR	2.2
1	B	43	ALA	2.2
1	D	81	ALA	2.2
1	D	87	ASP	2.2
1	A	63	SER	2.2
1	B	293	GLY	2.2
1	D	191	LEU	2.2
1	C	49	ALA	2.2
1	C	179	ALA	2.2
1	D	228	GLN	2.1
1	D	333	ASP	2.1
1	C	3	VAL	2.1
1	D	140	VAL	2.1
1	B	426	SER	2.1
1	C	265	SER	2.1
1	C	73	ALA	2.1
1	C	204	ALA	2.1
1	D	183	ALA	2.1
1	D	116	THR	2.1
1	D	195	THR	2.1
1	C	33	VAL	2.1
1	D	196	GLY	2.1
1	D	75	LEU	2.1
1	C	17	ALA	2.1
1	D	338	ALA	2.1
1	D	436	ARG	2.1
1	C	430	GLU	2.1
1	A	26	GLY	2.1
1	A	390	GLY	2.1
1	B	316	VAL	2.1
1	D	71	LEU	2.1
1	D	79	LEU	2.1
1	B	265	SER	2.0
1	A	433	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	74	THR	2.0
1	C	26	GLY	2.0
1	C	332	VAL	2.0
1	B	319	ALA	2.0
1	C	308	ALA	2.0
1	D	123	ASP	2.0
1	D	485	GLY	2.0
1	C	64	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.