



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:58 AM UTC

PDB ID : 1R44 / pdb_00001r44
Title : Crystal Structure of VanX
Authors : Pratt, S.D.; Katz, L.; Severin, J.M.; Holzman, T.; Park, C.H.
Deposited on : 2003-10-03
Resolution : 2.25 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

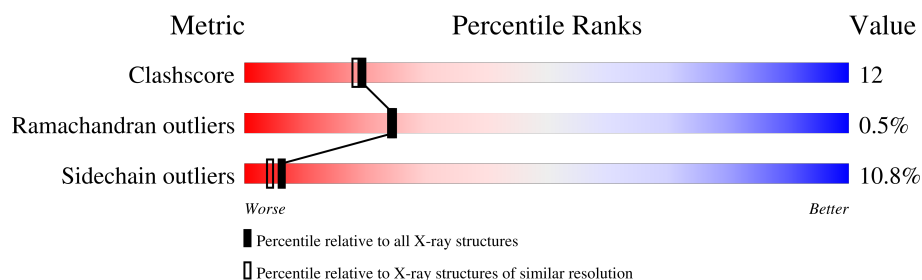
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	61% 27% 8% .
1	B	202	63% 25% 9% .
1	C	202	67% 23% 8% .
1	D	202	66% 24% 7% .
1	E	202	67% 24% 7% .
1	F	202	67% 22% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9924 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 D-alanyl-D-alanine dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1651	1048	284	311	8			
1	B	202	Total	C	N	O	S	0	0	0
			1651	1048	284	311	8			
1	C	202	Total	C	N	O	S	0	0	0
			1651	1048	284	311	8			
1	D	202	Total	C	N	O	S	0	0	0
			1651	1048	284	311	8			
1	E	202	Total	C	N	O	S	0	0	0
			1651	1048	284	311	8			
1	F	202	Total	C	N	O	S	0	0	0
			1651	1048	284	311	8			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

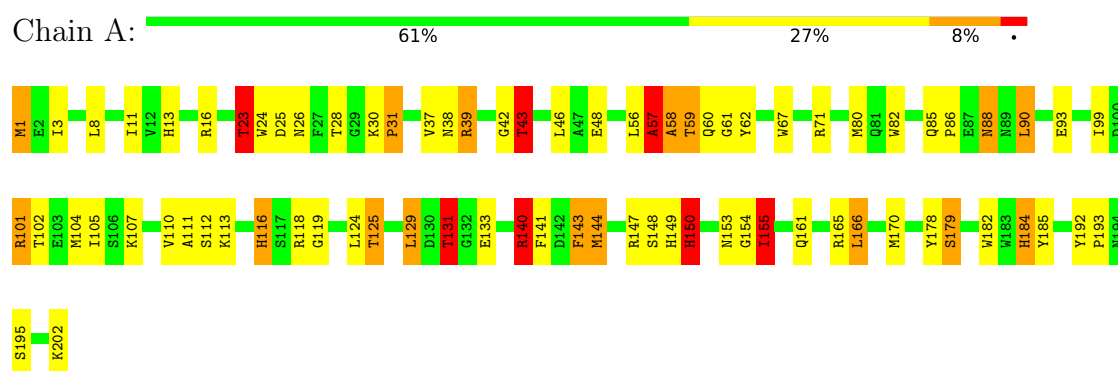
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	2	Total 2	O 2	0	0
3	C	2	Total 2	O 2	0	0
3	D	2	Total 2	O 2	0	0
3	E	2	Total 2	O 2	0	0
3	F	2	Total 2	O 2	0	0

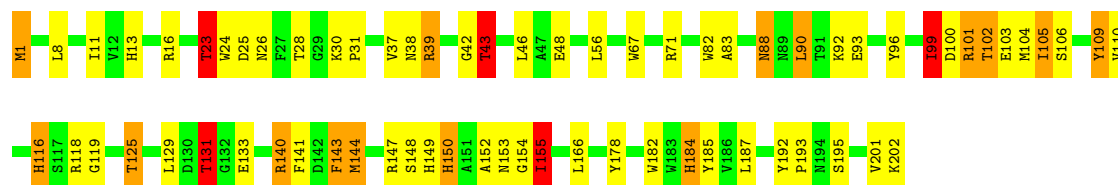
3 Residue-property plots

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. 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. 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.

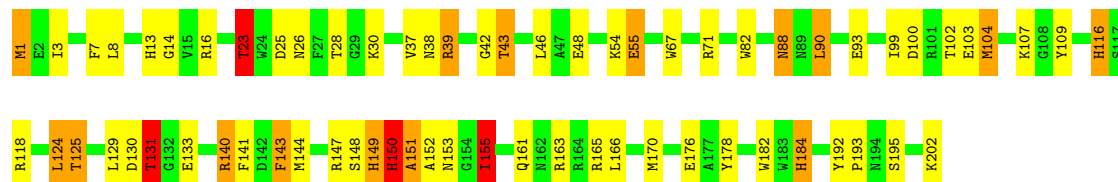
Note EDS was not executed.

- Molecule 1: D-alanyl-D-alanine dipeptidase

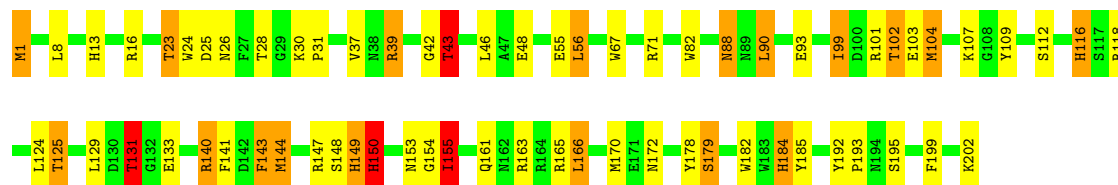




• Molecule 1: D-alanyl-D-alanine dipeptidase



• Molecule 1: D-alanyl-D-alanine dipeptidase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.60Å 44.69Å 169.43Å 90.00° 103.76° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25	Depositor
% Data completeness (in resolution range)	79.2 (50.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.254 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9924	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

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:
ZN

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	1.11	8/1697 (0.5%)	1.66	38/2297 (1.7%)
1	B	1.11	9/1697 (0.5%)	1.62	35/2297 (1.5%)
1	C	1.07	7/1697 (0.4%)	1.58	25/2297 (1.1%)
1	D	1.07	6/1697 (0.4%)	1.62	31/2297 (1.3%)
1	E	1.07	8/1697 (0.5%)	1.58	28/2297 (1.2%)
1	F	1.08	8/1697 (0.5%)	1.58	27/2297 (1.2%)
All	All	1.09	46/10182 (0.5%)	1.61	184/13782 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	149	HIS	ND1-CE1	6.11	1.38	1.32
1	F	150	HIS	CE1-NE2	5.99	1.38	1.32
1	B	149	HIS	ND1-CE1	5.83	1.38	1.32
1	E	149	HIS	CE1-NE2	5.83	1.38	1.32
1	B	149	HIS	CE1-NE2	5.80	1.38	1.32
1	B	59	THR	N-CA	5.80	1.53	1.46
1	F	150	HIS	ND1-CE1	5.79	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	149	HIS	CE1-NE2	5.79	1.38	1.32
1	B	13	HIS	CE1-NE2	5.64	1.38	1.32
1	D	149	HIS	CE1-NE2	5.60	1.38	1.32
1	C	13	HIS	CE1-NE2	5.58	1.38	1.32
1	C	184	HIS	CE1-NE2	5.57	1.38	1.32
1	B	13	HIS	ND1-CE1	5.56	1.38	1.32
1	C	13	HIS	ND1-CE1	5.55	1.38	1.32
1	D	184	HIS	CE1-NE2	5.55	1.38	1.32
1	E	13	HIS	CE1-NE2	5.53	1.38	1.32
1	A	150	HIS	CE1-NE2	5.52	1.38	1.32
1	E	150	HIS	ND1-CE1	5.50	1.38	1.32
1	E	149	HIS	ND1-CE1	5.49	1.38	1.32
1	E	13	HIS	ND1-CE1	5.47	1.38	1.32
1	D	150	HIS	CE1-NE2	5.45	1.38	1.32
1	C	149	HIS	CE1-NE2	5.36	1.38	1.32
1	D	13	HIS	ND1-CE1	5.34	1.37	1.32
1	A	150	HIS	ND1-CE1	5.33	1.37	1.32
1	D	149	HIS	ND1-CE1	5.32	1.37	1.32
1	A	149	HIS	ND1-CE1	5.32	1.37	1.32
1	A	13	HIS	ND1-CE1	5.31	1.37	1.32
1	C	149	HIS	ND1-CE1	5.30	1.37	1.32
1	E	184	HIS	ND1-CE1	5.29	1.37	1.32
1	F	13	HIS	CE1-NE2	5.27	1.37	1.32
1	F	184	HIS	CE1-NE2	5.25	1.37	1.32
1	B	150	HIS	CE1-NE2	5.25	1.37	1.32
1	B	116	HIS	ND1-CE1	5.24	1.37	1.32
1	B	150	HIS	ND1-CE1	5.24	1.37	1.32
1	F	13	HIS	ND1-CE1	5.23	1.37	1.32
1	C	184	HIS	ND1-CE1	5.23	1.37	1.32
1	A	13	HIS	CE1-NE2	5.21	1.37	1.32
1	C	150	HIS	CE1-NE2	5.20	1.37	1.32
1	E	150	HIS	CE1-NE2	5.20	1.37	1.32
1	A	184	HIS	CE1-NE2	5.19	1.37	1.32
1	D	13	HIS	CE1-NE2	5.18	1.37	1.32
1	E	116	HIS	CE1-NE2	5.17	1.37	1.32
1	A	149	HIS	CE1-NE2	5.15	1.37	1.32
1	A	184	HIS	ND1-CE1	5.08	1.37	1.32
1	B	184	HIS	CE1-NE2	5.06	1.37	1.32
1	F	179	SER	CA-CB	-5.05	1.45	1.53

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	HIS	N-CA-C	14.90	127.01	111.07
1	B	13	HIS	N-CA-C	14.45	126.53	111.07
1	E	13	HIS	N-CA-C	13.88	126.13	111.14
1	A	13	HIS	N-CA-C	13.10	125.28	111.14
1	D	13	HIS	N-CA-C	13.02	125.00	111.07
1	C	13	HIS	N-CA-C	12.24	124.36	111.14
1	D	102	THR	CA-CB-OG1	-9.25	95.72	109.60
1	D	99	ILE	CA-CB-CG1	-8.15	96.54	110.40
1	E	30	LYS	CA-CB-CG	8.09	130.28	114.10
1	A	30	LYS	CA-CB-CG	8.03	130.16	114.10
1	E	116	HIS	ND1-CG-CD2	8.01	114.11	106.10
1	C	155	ILE	N-CA-C	-7.98	96.58	108.46
1	D	99	ILE	CA-CB-CG2	7.95	124.02	110.50
1	A	155	ILE	N-CA-C	-7.89	97.12	108.48
1	A	150	HIS	ND1-CG-CD2	7.88	113.98	106.10
1	D	106	SER	N-CA-C	7.87	121.37	111.69
1	E	149	HIS	ND1-CG-CD2	7.69	113.79	106.10
1	A	112	SER	O-C-N	7.66	131.18	122.22
1	C	100	ASP	N-CA-CB	-7.65	99.07	110.85
1	B	57	ALA	N-CA-C	-7.64	103.54	113.17
1	F	155	ILE	N-CA-C	-7.63	97.49	108.48
1	F	102	THR	CA-CB-OG1	-7.61	98.19	109.60
1	C	30	LYS	CA-CB-CG	7.60	129.30	114.10
1	E	155	ILE	N-CA-C	-7.58	97.56	108.48
1	D	30	LYS	CA-CB-CG	7.58	129.26	114.10
1	D	155	ILE	N-CA-C	-7.52	97.65	108.48
1	C	150	HIS	ND1-CG-CD2	7.49	113.59	106.10
1	B	30	LYS	CA-CB-CG	7.49	129.07	114.10
1	D	48	GLU	CA-CB-CG	7.41	128.93	114.10
1	B	155	ILE	N-CA-C	-7.32	97.55	108.46
1	F	30	LYS	CA-CB-CG	7.23	128.55	114.10
1	D	102	THR	CA-CB-CG2	7.21	122.76	110.50
1	D	105	ILE	N-CA-C	-7.21	103.75	110.53
1	E	39	ARG	CA-CB-CG	-7.19	99.72	114.10
1	F	48	GLU	CA-CB-CG	7.17	128.44	114.10
1	F	116	HIS	ND1-CG-CD2	7.16	113.26	106.10
1	A	39	ARG	CA-CB-CG	-7.16	99.78	114.10
1	D	150	HIS	ND1-CG-CD2	7.15	113.25	106.10
1	D	116	HIS	ND1-CG-CD2	7.14	113.25	106.10
1	E	93	GLU	N-CA-C	7.12	119.95	111.33
1	A	116	HIS	ND1-CG-CD2	7.12	113.22	106.10
1	D	39	ARG	CA-CB-CG	-7.11	99.88	114.10
1	A	58	ALA	N-CA-C	-7.10	95.67	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	SER	N-CA-C	7.10	119.02	111.28
1	B	39	ARG	CA-CB-CG	-7.09	99.92	114.10
1	C	149	HIS	ND1-CG-CD2	7.09	113.19	106.10
1	D	149	HIS	ND1-CG-CD2	7.07	113.17	106.10
1	D	93	GLU	N-CA-C	7.05	119.86	111.33
1	C	39	ARG	CA-CB-CG	-7.04	100.01	114.10
1	B	150	HIS	ND1-CG-CD2	7.02	113.12	106.10
1	D	155	ILE	CA-CB-CG2	7.02	122.44	110.50
1	C	48	GLU	CA-CB-CG	7.01	128.12	114.10
1	E	48	GLU	CA-CB-CG	7.00	128.11	114.10
1	F	150	HIS	ND1-CG-CD2	7.00	113.10	106.10
1	D	11	ILE	N-CA-C	-6.99	106.24	111.90
1	B	48	GLU	CA-CB-CG	6.98	128.07	114.10
1	A	155	ILE	CA-CB-CG2	6.96	122.32	110.50
1	A	13	HIS	ND1-CG-CD2	6.93	113.03	106.10
1	A	149	HIS	ND1-CG-CD2	6.92	113.03	106.10
1	B	60	GLN	O-C-N	6.91	131.78	122.59
1	E	143	PHE	CA-C-O	-6.90	112.03	119.97
1	C	116	HIS	ND1-CG-CD2	6.87	112.97	106.10
1	B	116	HIS	ND1-CG-CD2	6.87	112.97	106.10
1	A	143	PHE	CA-C-O	-6.87	112.07	119.97
1	F	155	ILE	CA-CB-CG2	6.84	122.12	110.50
1	B	149	HIS	ND1-CG-CD2	6.81	112.91	106.10
1	E	13	HIS	ND1-CG-CD2	6.80	112.90	106.10
1	C	13	HIS	ND1-CG-CD2	6.79	112.89	106.10
1	F	102	THR	CA-CB-CG2	6.79	122.04	110.50
1	D	13	HIS	ND1-CG-CD2	6.78	112.88	106.10
1	B	131	THR	CA-CB-CG2	6.76	122.00	110.50
1	F	149	HIS	ND1-CG-CD2	6.75	112.85	106.10
1	B	107	LYS	N-CA-C	-6.72	104.34	112.54
1	B	155	ILE	CA-CB-CG2	6.68	121.85	110.50
1	B	23	THR	CA-CB-CG2	6.66	121.81	110.50
1	F	23	THR	CA-CB-OG1	-6.65	99.62	109.60
1	E	155	ILE	CA-CB-CG2	6.62	121.76	110.50
1	D	109	TYR	N-CA-C	-6.61	102.71	111.24
1	A	48	GLU	CA-CB-CG	6.60	127.30	114.10
1	F	39	ARG	CA-CB-CG	-6.60	100.91	114.10
1	B	13	HIS	ND1-CG-CD2	6.58	112.68	106.10
1	E	150	HIS	ND1-CG-CD2	6.56	112.66	106.10
1	E	104	MET	N-CA-C	6.49	122.08	111.37
1	A	93	GLU	N-CA-C	6.47	119.15	111.33
1	F	23	THR	CA-CB-CG2	6.45	121.46	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	LEU	CA-C-O	6.42	129.69	120.51
1	B	93	GLU	N-CA-C	6.41	119.09	111.33
1	F	143	PHE	CA-C-O	-6.37	112.64	119.97
1	A	13	HIS	O-C-N	-6.35	115.23	122.09
1	C	93	GLU	N-CA-C	6.35	119.02	111.33
1	B	131	THR	CA-CB-OG1	-6.33	100.10	109.60
1	A	179	SER	N-CA-C	6.33	118.99	111.71
1	D	155	ILE	CA-CB-CG1	-6.33	99.64	110.40
1	A	57	ALA	CA-C-O	6.32	130.00	122.36
1	E	131	THR	CA-CB-CG2	6.30	121.22	110.50
1	F	93	GLU	N-CA-C	6.30	118.95	111.33
1	B	23	THR	CA-CB-OG1	-6.28	100.19	109.60
1	E	116	HIS	CG-CD2-NE2	-6.26	100.94	107.20
1	C	179	SER	N-CA-C	6.18	118.01	111.28
1	F	155	ILE	CA-CB-CG1	-6.09	100.04	110.40
1	B	13	HIS	O-C-N	-6.09	115.80	122.07
1	C	143	PHE	CA-C-O	-6.04	113.02	119.97
1	A	102	THR	CA-CB-OG1	-6.04	100.54	109.60
1	B	104	MET	O-C-N	6.04	128.52	122.12
1	C	155	ILE	CA-CB-CG2	6.00	120.69	110.50
1	D	131	THR	CA-CB-CG2	5.99	120.68	110.50
1	A	23	THR	CA-CB-CG2	5.96	120.64	110.50
1	A	101	ARG	N-CA-C	5.93	119.34	111.75
1	B	143	PHE	CA-C-O	-5.93	113.16	119.97
1	E	55	GLU	N-CA-CB	-5.92	101.41	110.16
1	E	131	THR	CA-CB-OG1	-5.88	100.78	109.60
1	B	155	ILE	CA-CB-CG1	-5.86	100.45	110.40
1	F	13	HIS	ND1-CG-CD2	5.85	111.95	106.10
1	A	11	ILE	N-CA-C	-5.83	107.18	111.90
1	A	143	PHE	O-C-N	-5.82	115.11	122.27
1	F	131	THR	CA-CB-CG2	5.80	120.35	110.50
1	E	23	THR	CA-CB-CG2	5.79	120.34	110.50
1	B	43	THR	CA-CB-CG2	5.76	120.30	110.50
1	B	154	GLY	N-CA-C	-5.76	106.79	115.32
1	C	103	GLU	CA-CB-CG	5.76	125.62	114.10
1	F	13	HIS	O-C-N	-5.76	116.14	122.07
1	E	23	THR	CA-CB-OG1	-5.76	100.96	109.60
1	C	154	GLY	N-CA-C	-5.73	106.84	115.32
1	F	104	MET	CG-SD-CE	-5.71	88.34	100.90
1	A	155	ILE	CA-CB-CG1	-5.70	100.71	110.40
1	A	131	THR	CA-CB-CG2	5.64	120.09	110.50
1	A	43	THR	CA-CB-CG2	5.62	120.06	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	THR	CA-CB-CG2	5.62	120.05	110.50
1	D	152	ALA	N-CA-C	5.62	118.37	110.23
1	D	143	PHE	O-C-N	-5.59	115.39	122.27
1	C	112	SER	N-CA-C	5.56	118.10	111.71
1	B	7	PHE	N-CA-C	-5.51	101.49	109.59
1	A	59	THR	N-CA-C	-5.50	99.08	110.80
1	A	43	THR	CA-CB-OG1	-5.50	101.36	109.60
1	C	23	THR	CA-CB-CG2	5.49	119.83	110.50
1	A	23	THR	CA-CB-OG1	-5.47	101.40	109.60
1	E	155	ILE	CA-CB-CG1	-5.46	101.12	110.40
1	B	144	MET	CB-CA-C	-5.45	104.56	111.86
1	C	11	ILE	N-CA-C	-5.43	106.89	111.56
1	C	112	SER	CA-C-O	5.43	126.23	120.10
1	E	151	ALA	N-CA-CB	-5.43	101.63	110.42
1	B	179	SER	N-CA-C	5.42	117.19	111.28
1	A	112	SER	CA-C-O	5.40	126.21	120.10
1	F	99	ILE	CA-CB-CG2	5.39	119.66	110.50
1	D	13	HIS	O-C-N	-5.39	116.52	122.07
1	F	116	HIS	CG-CD2-NE2	-5.38	101.82	107.20
1	D	154	GLY	N-CA-C	-5.38	107.36	115.32
1	B	110	VAL	O-C-N	-5.36	115.87	122.57
1	A	140	ARG	N-CA-CB	-5.36	102.31	110.45
1	A	102	THR	CA-CB-CG2	5.35	119.60	110.50
1	A	116	HIS	CG-CD2-NE2	-5.34	101.86	107.20
1	B	143	PHE	O-C-N	-5.33	115.71	122.27
1	B	43	THR	CA-CB-OG1	-5.32	101.62	109.60
1	E	48	GLU	CB-CA-C	-5.32	102.30	110.81
1	D	101	ARG	O-C-N	5.31	127.54	122.07
1	A	86	PRO	N-CA-CB	5.29	108.02	103.31
1	B	104	MET	N-CA-C	5.28	117.03	111.28
1	D	143	PHE	CA-C-O	-5.27	113.91	119.97
1	E	143	PHE	O-C-N	-5.27	115.78	122.27
1	D	23	THR	CA-CB-CG2	5.27	119.45	110.50
1	E	7	PHE	N-CA-C	-5.25	101.22	109.25
1	B	125	THR	CA-C-O	5.19	127.92	120.51
1	F	199	PHE	N-CA-C	-5.18	103.14	110.29
1	A	154	GLY	N-CA-C	-5.18	107.66	115.32
1	A	48	GLU	CB-CA-C	-5.15	102.57	110.81
1	D	43	THR	CA-CB-CG2	5.13	119.22	110.50
1	C	146	GLU	CA-CB-CG	-5.13	103.85	114.10
1	A	107	LYS	N-CA-C	5.10	119.19	112.92
1	E	130	ASP	N-CA-C	5.09	116.64	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	LEU	N-CA-C	5.08	116.57	108.79
1	C	100	ASP	CB-CA-C	5.08	118.86	109.71
1	E	100	ASP	N-CA-C	-5.08	102.54	110.42
1	A	57	ALA	N-CA-CB	-5.07	102.00	110.42
1	F	104	MET	N-CA-C	5.07	117.47	111.33
1	B	37	VAL	CG1-CB-CG2	-5.07	99.65	110.80
1	E	124	LEU	N-CA-C	5.06	116.53	108.79
1	F	43	THR	CA-CB-CG2	5.04	119.07	110.50
1	E	152	ALA	N-CA-C	5.04	117.53	110.23
1	C	13	HIS	O-C-N	-5.02	116.67	122.09
1	C	37	VAL	CG1-CB-CG2	-5.02	99.76	110.80
1	D	201	VAL	N-CA-C	-5.02	100.25	107.37
1	F	154	GLY	N-CA-C	-5.02	108.36	115.43
1	D	48	GLU	CB-CA-C	-5.01	102.79	110.81
1	A	31	PRO	N-CA-CB	5.01	107.77	103.31

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	TYR	Sidechain
1	A	57	ALA	Mainchain
1	B	185	TYR	Sidechain
1	C	185	TYR	Sidechain
1	D	185	TYR	Sidechain
1	F	185	TYR	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	1651	0	1565	47	0
1	B	1651	0	1565	36	0
1	C	1651	0	1565	33	0
1	D	1651	0	1565	40	0
1	E	1651	0	1565	37	0
1	F	1651	0	1565	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	9924	0	9390	224	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 12.

All (224) 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:F:23:THR:HG22	1:F:25:ASP:H	1.28	0.97
1:E:23:THR:HG22	1:E:25:ASP:H	1.30	0.96
1:D:23:THR:HG22	1:D:25:ASP:H	1.32	0.92
1:A:23:THR:HG22	1:A:25:ASP:H	1.30	0.92
1:C:23:THR:HG22	1:C:25:ASP:H	1.32	0.92
1:B:23:THR:HG22	1:B:25:ASP:H	1.33	0.90
1:E:176:GLU:CD	1:F:179:SER:HB3	1.96	0.89
1:D:104:MET:SD	1:D:144:MET:HE3	2.16	0.86
1:F:43:THR:HG22	1:F:46:LEU:H	1.41	0.84
1:D:43:THR:HG22	1:D:46:LEU:H	1.42	0.83
1:A:43:THR:HG22	1:A:46:LEU:H	1.45	0.80
1:F:101:ARG:HA	1:F:104:MET:HE3	1.64	0.80
1:C:43:THR:HG22	1:C:46:LEU:H	1.47	0.79
1:B:43:THR:HG22	1:B:46:LEU:H	1.48	0.78
1:E:151:ALA:HB1	1:F:172:ASN:OD1	1.84	0.76
1:E:43:THR:HG22	1:E:46:LEU:H	1.48	0.76
1:F:26:ASN:HD22	1:F:28:THR:H	1.33	0.76
1:F:147:ARG:HG3	1:F:155:ILE:HD11	1.66	0.75
1:E:26:ASN:HD22	1:E:28:THR:H	1.36	0.73
1:C:147:ARG:HG3	1:C:155:ILE:HD11	1.69	0.73
1:A:147:ARG:HG3	1:A:155:ILE:HD11	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:HD22	1:A:28:THR:H	1.34	0.72
1:D:26:ASN:HD22	1:D:28:THR:H	1.37	0.72
1:F:104:MET:SD	1:F:144:MET:HE3	2.30	0.72
1:B:26:ASN:HD22	1:B:28:THR:H	1.35	0.72
1:C:26:ASN:HD22	1:C:28:THR:H	1.37	0.72
1:B:59:THR:HG22	1:B:60:GLN:H	1.57	0.70
1:D:147:ARG:HG3	1:D:155:ILE:HD11	1.74	0.69
1:E:14:GLY:H	1:E:54:LYS:NZ	1.92	0.68
1:B:147:ARG:HG3	1:B:155:ILE:HD11	1.74	0.68
1:E:8:LEU:HD21	1:E:42:GLY:HA3	1.78	0.66
1:E:103:GLU:HB3	1:E:107:LYS:HD2	1.78	0.66
1:A:104:MET:SD	1:A:144:MET:HE3	2.38	0.64
1:C:8:LEU:HD21	1:C:42:GLY:HA3	1.80	0.64
1:C:131:THR:HG22	1:C:133:GLU:H	1.63	0.64
1:C:125:THR:HG23	1:C:182:TRP:CZ3	2.33	0.63
1:E:147:ARG:HG3	1:E:155:ILE:HD11	1.78	0.63
1:A:131:THR:HG22	1:A:133:GLU:H	1.64	0.63
1:D:118:ARG:HD3	1:D:193:PRO:HA	1.82	0.62
1:A:125:THR:HG23	1:A:182:TRP:CZ3	2.35	0.62
1:D:125:THR:HG23	1:D:182:TRP:CZ3	2.34	0.61
1:E:131:THR:HG22	1:E:133:GLU:H	1.65	0.61
1:E:125:THR:HG23	1:E:182:TRP:CZ3	2.35	0.61
1:A:104:MET:CE	1:A:144:MET:HE3	2.33	0.59
1:A:111:ALA:HB1	1:A:113:LYS:O	2.02	0.59
1:B:59:THR:O	1:B:61:GLY:N	2.33	0.59
1:B:125:THR:HG23	1:B:182:TRP:CZ3	2.38	0.59
1:F:192:TYR:HB3	1:F:195:SER:HB2	1.85	0.59
1:B:131:THR:HG22	1:B:133:GLU:H	1.68	0.58
1:D:192:TYR:HB3	1:D:195:SER:HB2	1.85	0.58
1:A:8:LEU:HD21	1:A:42:GLY:HA3	1.86	0.57
1:E:14:GLY:H	1:E:54:LYS:HZ2	1.52	0.57
1:F:26:ASN:ND2	1:F:28:THR:H	2.02	0.57
1:F:125:THR:HG23	1:F:182:TRP:CZ3	2.39	0.57
1:F:103:GLU:HB3	1:F:107:LYS:HD2	1.87	0.56
1:A:192:TYR:HB3	1:A:195:SER:HB2	1.87	0.56
1:D:131:THR:HG22	1:D:133:GLU:H	1.70	0.56
1:A:71:ARG:HB3	1:A:116:HIS:HB3	1.87	0.56
1:F:131:THR:HG22	1:F:133:GLU:H	1.70	0.56
1:A:26:ASN:ND2	1:A:28:THR:H	2.03	0.56
1:D:88:ASN:HD22	1:D:90:LEU:H	1.54	0.55
1:C:71:ARG:HB3	1:C:116:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:HB3	1:B:116:HIS:HB3	1.89	0.55
1:B:192:TYR:HB3	1:B:195:SER:HB2	1.89	0.55
1:F:71:ARG:HB3	1:F:116:HIS:HB3	1.88	0.54
1:F:88:ASN:HD22	1:F:90:LEU:H	1.55	0.54
1:C:192:TYR:HB3	1:C:195:SER:HB2	1.89	0.54
1:E:176:GLU:OE2	1:F:179:SER:HB3	2.07	0.54
1:E:192:TYR:HB3	1:E:195:SER:HB2	1.89	0.54
1:B:88:ASN:HD22	1:B:90:LEU:H	1.54	0.54
1:F:37:VAL:HG12	1:F:39:ARG:HB2	1.89	0.54
1:B:37:VAL:HG12	1:B:39:ARG:HB2	1.90	0.54
1:D:104:MET:HA	1:D:109:TYR:HD1	1.73	0.54
1:A:37:VAL:HG12	1:A:39:ARG:HB2	1.89	0.54
1:B:26:ASN:ND2	1:B:28:THR:H	2.06	0.54
1:C:125:THR:HG23	1:C:182:TRP:CH2	2.44	0.53
1:E:71:ARG:HB3	1:E:116:HIS:HB3	1.89	0.53
1:E:178:TYR:HB2	1:E:184:HIS:HD2	1.73	0.53
1:A:88:ASN:HD22	1:A:90:LEU:H	1.54	0.53
1:F:118:ARG:HD3	1:F:193:PRO:HA	1.90	0.53
1:D:8:LEU:HD21	1:D:42:GLY:HA3	1.91	0.52
1:F:8:LEU:HD21	1:F:42:GLY:HA3	1.91	0.52
1:C:88:ASN:HD22	1:C:90:LEU:H	1.58	0.52
1:E:26:ASN:ND2	1:E:28:THR:H	2.05	0.52
1:D:104:MET:HG2	1:D:110:VAL:HG22	1.91	0.51
1:B:55:GLU:C	1:B:57:ALA:H	2.18	0.51
1:C:131:THR:CG2	1:C:133:GLU:HB2	2.40	0.51
1:E:131:THR:CG2	1:E:133:GLU:HB2	2.41	0.51
1:A:67:TRP:CH2	1:A:125:THR:OG1	2.63	0.51
1:A:118:ARG:HD3	1:A:193:PRO:HA	1.93	0.51
1:B:131:THR:CG2	1:B:133:GLU:HB2	2.40	0.51
1:B:103:GLU:HG3	1:B:107:LYS:HD2	1.93	0.51
1:E:151:ALA:HB1	1:F:172:ASN:CG	2.35	0.51
1:A:82:TRP:HZ3	1:A:104:MET:CE	2.24	0.51
1:B:124:LEU:HD21	1:B:170:MET:HE2	1.93	0.50
1:E:23:THR:HG22	1:E:25:ASP:N	2.14	0.50
1:D:37:VAL:HG12	1:D:39:ARG:HB2	1.92	0.50
1:E:118:ARG:HD3	1:E:193:PRO:HA	1.94	0.50
1:A:38:ASN:O	1:A:39:ARG:HG3	2.12	0.50
1:B:118:ARG:HD3	1:B:193:PRO:HA	1.94	0.50
1:C:118:ARG:HD3	1:C:193:PRO:HA	1.93	0.50
1:C:26:ASN:ND2	1:C:28:THR:H	2.06	0.50
1:F:131:THR:CG2	1:F:133:GLU:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:GLN:NE2	1:F:165:ARG:HH21	2.10	0.49
1:A:80:MET:SD	1:A:105:ILE:HD13	2.51	0.49
1:D:71:ARG:HB3	1:D:116:HIS:HB3	1.93	0.49
1:D:101:ARG:HA	1:D:104:MET:HE3	1.94	0.49
1:A:179:SER:HB3	1:B:171:GLU:CD	2.37	0.49
1:E:1:MET:HE3	1:E:1:MET:HA	1.94	0.49
1:C:105:ILE:O	1:C:106:SER:HB2	2.13	0.49
1:A:147:ARG:HG3	1:A:155:ILE:CD1	2.41	0.49
1:A:131:THR:CG2	1:A:133:GLU:HB2	2.42	0.49
1:D:82:TRP:HZ3	1:D:104:MET:SD	2.36	0.48
1:C:43:THR:HG22	1:C:46:LEU:N	2.24	0.48
1:E:88:ASN:HD22	1:E:90:LEU:H	1.59	0.48
1:A:125:THR:HG23	1:A:182:TRP:CH2	2.49	0.48
1:A:161:GLN:NE2	1:A:165:ARG:HH21	2.12	0.48
1:D:43:THR:HG22	1:D:46:LEU:N	2.21	0.48
1:A:82:TRP:HZ3	1:A:104:MET:HE1	1.79	0.47
1:D:83:ALA:HB1	1:D:105:ILE:HG13	1.96	0.47
1:D:101:ARG:O	1:D:104:MET:HB3	2.14	0.47
1:E:99:ILE:HD13	1:E:109:TYR:CD1	2.48	0.47
1:F:1:MET:HE3	1:F:1:MET:HA	1.96	0.47
1:B:8:LEU:HD21	1:B:42:GLY:HA3	1.97	0.47
1:A:178:TYR:HB2	1:A:184:HIS:HD2	1.79	0.47
1:D:109:TYR:CG	1:D:144:MET:HG3	2.49	0.47
1:B:38:ASN:O	1:B:39:ARG:HG3	2.15	0.47
1:E:161:GLN:NE2	1:E:165:ARG:HH21	2.13	0.47
1:C:110:VAL:HG13	1:C:111:ALA:N	2.29	0.47
1:C:178:TYR:HB2	1:C:184:HIS:HD2	1.79	0.47
1:E:82:TRP:CZ3	1:E:104:MET:HE3	2.49	0.47
1:A:104:MET:SD	1:A:144:MET:CE	3.03	0.47
1:C:147:ARG:HG3	1:C:155:ILE:CD1	2.43	0.47
1:D:1:MET:HE3	1:D:1:MET:HA	1.97	0.46
1:F:143:PHE:HB3	1:F:148:SER:OG	2.14	0.46
1:F:147:ARG:HG3	1:F:155:ILE:CD1	2.41	0.46
1:C:143:PHE:HB3	1:C:148:SER:OG	2.16	0.46
1:D:131:THR:CG2	1:D:133:GLU:HB2	2.46	0.46
1:C:38:ASN:C	1:C:39:ARG:HG3	2.41	0.46
1:E:140:ARG:HG2	1:E:141:PHE:O	2.16	0.46
1:E:150:HIS:CE1	1:E:182:TRP:HA	2.51	0.46
1:C:161:GLN:NE2	1:C:165:ARG:HH21	2.13	0.46
1:C:124:LEU:HD21	1:C:170:MET:HE2	1.98	0.46
1:D:100:ASP:HB2	1:D:103:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:HIS:O	1:E:163:ARG:NH1	2.49	0.46
1:A:43:THR:HG22	1:A:46:LEU:N	2.24	0.45
1:B:38:ASN:C	1:B:39:ARG:HG3	2.42	0.45
1:D:140:ARG:HG2	1:D:141:PHE:O	2.16	0.45
1:B:125:THR:HG23	1:B:182:TRP:CH2	2.50	0.45
1:C:1:MET:HE3	1:C:1:MET:HA	1.98	0.45
1:B:143:PHE:HB3	1:B:148:SER:OG	2.15	0.45
1:F:140:ARG:HG2	1:F:141:PHE:O	2.16	0.45
1:F:178:TYR:HB2	1:F:184:HIS:HD2	1.80	0.45
1:D:26:ASN:ND2	1:D:28:THR:H	2.07	0.45
1:A:166:LEU:O	1:A:170:MET:HG2	2.16	0.45
1:E:125:THR:HG23	1:E:182:TRP:CH2	2.52	0.45
1:F:109:TYR:CG	1:F:144:MET:HG3	2.52	0.45
1:D:125:THR:HG23	1:D:182:TRP:HZ3	1.80	0.45
1:D:38:ASN:O	1:D:39:ARG:HG3	2.17	0.44
1:A:57:ALA:HB1	1:A:62:TYR:O	2.17	0.44
1:D:23:THR:HG22	1:D:25:ASP:N	2.15	0.44
1:C:37:VAL:HG12	1:C:39:ARG:HB2	1.99	0.44
1:D:99:ILE:HD13	1:D:109:TYR:CE1	2.52	0.44
1:D:125:THR:HG23	1:D:182:TRP:CH2	2.51	0.44
1:B:161:GLN:NE2	1:B:165:ARG:HH21	2.16	0.44
1:C:149:HIS:O	1:C:163:ARG:NH1	2.51	0.44
1:B:178:TYR:HB2	1:B:184:HIS:HD2	1.82	0.44
1:A:38:ASN:C	1:A:39:ARG:HG3	2.43	0.44
1:A:104:MET:HE3	1:A:144:MET:HE3	2.00	0.43
1:C:140:ARG:HG2	1:C:141:PHE:O	2.18	0.43
1:D:38:ASN:C	1:D:39:ARG:HG3	2.43	0.43
1:D:143:PHE:HB3	1:D:148:SER:OG	2.17	0.43
1:B:166:LEU:O	1:B:170:MET:HG2	2.17	0.43
1:F:124:LEU:HD21	1:F:170:MET:HE2	2.00	0.43
1:E:67:TRP:CH2	1:E:125:THR:OG1	2.71	0.43
1:A:43:THR:HB	1:A:119:GLY:O	2.18	0.43
1:B:140:ARG:HG2	1:B:141:PHE:O	2.18	0.43
1:F:149:HIS:O	1:F:163:ARG:NH1	2.51	0.43
1:A:161:GLN:O	1:A:165:ARG:HG3	2.19	0.43
1:B:59:THR:HG22	1:B:60:GLN:N	2.30	0.43
1:A:24:TRP:CE2	1:A:31:PRO:HD3	2.53	0.43
1:C:69:GLY:O	1:C:116:HIS:ND1	2.44	0.43
1:F:24:TRP:CE2	1:F:31:PRO:HD3	2.55	0.42
1:C:43:THR:HB	1:C:119:GLY:O	2.20	0.42
1:A:140:ARG:HG2	1:A:141:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:THR:HG23	1:F:182:TRP:CH2	2.54	0.42
1:E:125:THR:HG23	1:E:182:TRP:HZ3	1.82	0.42
1:A:1:MET:HE3	1:A:1:MET:HA	2.02	0.42
1:F:23:THR:HG22	1:F:25:ASP:N	2.13	0.42
1:A:124:LEU:HD21	1:A:170:MET:HE2	2.02	0.41
1:E:124:LEU:HD21	1:E:170:MET:HE2	2.02	0.41
1:A:56:LEU:O	1:A:58:ALA:N	2.51	0.41
1:A:99:ILE:HD11	1:A:104:MET:HG2	2.02	0.41
1:B:105:ILE:HG22	1:B:110:VAL:O	2.20	0.41
1:F:67:TRP:CZ3	1:F:141:PHE:HB2	2.56	0.41
1:A:143:PHE:HB3	1:A:148:SER:OG	2.20	0.41
1:B:17:TRP:CE2	1:C:38:ASN:HB3	2.55	0.41
1:C:110:VAL:CG1	1:C:111:ALA:N	2.83	0.41
1:D:178:TYR:HB2	1:D:184:HIS:HD2	1.84	0.41
1:E:38:ASN:C	1:E:39:ARG:HG3	2.44	0.41
1:F:150:HIS:CE1	1:F:182:TRP:HA	2.56	0.41
1:D:82:TRP:CH2	1:D:101:ARG:HG2	2.55	0.41
1:A:104:MET:HE3	1:A:110:VAL:HG21	2.03	0.41
1:B:1:MET:HE3	1:B:1:MET:HA	2.03	0.41
1:B:3:ILE:HA	1:B:3:ILE:HD12	1.64	0.41
1:D:187:LEU:HD12	1:D:187:LEU:HA	1.92	0.41
1:F:82:TRP:CH2	1:F:104:MET:HE1	2.56	0.41
1:F:166:LEU:O	1:F:170:MET:HG2	2.21	0.41
1:A:150:HIS:CE1	1:A:182:TRP:HA	2.55	0.41
1:E:3:ILE:HD12	1:E:3:ILE:HA	1.80	0.41
1:E:37:VAL:HG12	1:E:39:ARG:HB2	2.01	0.41
1:E:143:PHE:HB3	1:E:148:SER:OG	2.21	0.41
1:D:24:TRP:CE2	1:D:31:PRO:HD3	2.55	0.41
1:B:150:HIS:CE1	1:B:182:TRP:HA	2.56	0.41
1:C:3:ILE:HD12	1:C:3:ILE:HA	1.91	0.41
1:C:38:ASN:O	1:C:39:ARG:HG3	2.21	0.41
1:D:92:LYS:HG3	1:D:96:TYR:CE1	2.56	0.41
1:B:92:LYS:HG3	1:B:96:TYR:CE1	2.57	0.40
1:A:61:GLY:C	1:A:129:LEU:HB2	2.46	0.40
1:D:43:THR:HB	1:D:119:GLY:O	2.22	0.40
1:A:85:GLN:HB2	1:A:101:ARG:NH1	2.37	0.40
1:B:180:LEU:C	1:B:181:GLU:HG3	2.46	0.40
1:D:67:TRP:CH2	1:D:125:THR:OG1	2.72	0.40
1:A:3:ILE:HD12	1:A:3:ILE:HA	1.85	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	200/202 (99%)	188 (94%)	10 (5%)	2 (1%)	12	10
1	B	200/202 (99%)	185 (92%)	14 (7%)	1 (0%)	24	24
1	C	200/202 (99%)	187 (94%)	11 (6%)	2 (1%)	12	10
1	D	200/202 (99%)	190 (95%)	10 (5%)	0	100	100
1	E	200/202 (99%)	192 (96%)	8 (4%)	0	100	100
1	F	200/202 (99%)	193 (96%)	6 (3%)	1 (0%)	24	24
All	All	1200/1212 (99%)	1135 (95%)	59 (5%)	6 (0%)	24	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	106	SER
1	A	59	THR
1	F	56	LEU
1	B	106	SER
1	C	111	ALA
1	A	60	GLN

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	173/173 (100%)	157 (91%)	16 (9%)	8	6
1	B	173/173 (100%)	154 (89%)	19 (11%)	6	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	173/173 (100%)	153 (88%)	20 (12%)	5	3
1	D	173/173 (100%)	154 (89%)	19 (11%)	6	4
1	E	173/173 (100%)	155 (90%)	18 (10%)	7	5
1	F	173/173 (100%)	153 (88%)	20 (12%)	5	3
All	All	1038/1038 (100%)	926 (89%)	112 (11%)	6	4

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	ARG
1	A	23	THR
1	A	43	THR
1	A	88	ASN
1	A	90	LEU
1	A	125	THR
1	A	129	LEU
1	A	131	THR
1	A	140	ARG
1	A	144	MET
1	A	150	HIS
1	A	153	ASN
1	A	155	ILE
1	A	166	LEU
1	A	202	LYS
1	B	1	MET
1	B	15	VAL
1	B	16	ARG
1	B	43	THR
1	B	54	LYS
1	B	88	ASN
1	B	90	LEU
1	B	99	ILE
1	B	106	SER
1	B	125	THR
1	B	129	LEU
1	B	131	THR
1	B	140	ARG
1	B	144	MET
1	B	150	HIS
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	155	ILE
1	B	166	LEU
1	B	202	LYS
1	C	1	MET
1	C	16	ARG
1	C	23	THR
1	C	26	ASN
1	C	43	THR
1	C	88	ASN
1	C	90	LEU
1	C	99	ILE
1	C	105	ILE
1	C	107	LYS
1	C	125	THR
1	C	129	LEU
1	C	131	THR
1	C	140	ARG
1	C	144	MET
1	C	150	HIS
1	C	153	ASN
1	C	155	ILE
1	C	166	LEU
1	C	202	LYS
1	D	1	MET
1	D	16	ARG
1	D	23	THR
1	D	43	THR
1	D	56	LEU
1	D	88	ASN
1	D	90	LEU
1	D	99	ILE
1	D	102	THR
1	D	125	THR
1	D	129	LEU
1	D	131	THR
1	D	140	ARG
1	D	144	MET
1	D	150	HIS
1	D	153	ASN
1	D	155	ILE
1	D	166	LEU
1	D	202	LYS

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Mol	Chain	Res	Type
1	E	1	MET
1	E	16	ARG
1	E	23	THR
1	E	43	THR
1	E	55	GLU
1	E	88	ASN
1	E	90	LEU
1	E	102	THR
1	E	125	THR
1	E	129	LEU
1	E	131	THR
1	E	140	ARG
1	E	144	MET
1	E	150	HIS
1	E	153	ASN
1	E	155	ILE
1	E	166	LEU
1	E	202	LYS
1	F	1	MET
1	F	16	ARG
1	F	43	THR
1	F	55	GLU
1	F	56	LEU
1	F	88	ASN
1	F	90	LEU
1	F	99	ILE
1	F	102	THR
1	F	112	SER
1	F	125	THR
1	F	129	LEU
1	F	131	THR
1	F	140	ARG
1	F	144	MET
1	F	150	HIS
1	F	153	ASN
1	F	155	ILE
1	F	166	LEU
1	F	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	88	ASN
1	A	161	GLN
1	B	26	ASN
1	B	88	ASN
1	B	161	GLN
1	C	26	ASN
1	C	88	ASN
1	C	149	HIS
1	C	161	GLN
1	D	26	ASN
1	D	88	ASN
1	D	161	GLN
1	E	26	ASN
1	E	88	ASN
1	E	161	GLN
1	F	26	ASN
1	F	88	ASN
1	F	161	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.