



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 PM UTC

PDB ID : 3B2Z / pdb_00003b2z
Title : Crystal Structure of ADAMTS4 (apo form)
Authors : Mosyak, L.; Stahl, M.; Somers, W.
Deposited on : 2007-10-19
Resolution : 2.80 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

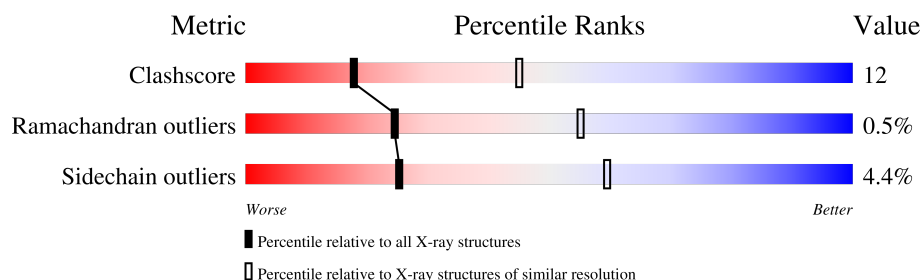
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	316	
1	B	316	
1	C	316	
1	D	316	
1	E	316	
1	F	316	
1	G	316	
1	H	316	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17609 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 ADAMTS-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2176	1359	386	407	24			
1	B	287	Total	C	N	O	S	0	0	0
			2158	1351	384	399	24			
1	C	289	Total	C	N	O	S	0	0	0
			2166	1353	383	406	24			
1	D	287	Total	C	N	O	S	0	0	0
			2158	1351	384	399	24			
1	E	282	Total	C	N	O	S	0	0	0
			2131	1335	381	390	25			
1	F	293	Total	C	N	O	S	0	0	0
			2195	1371	390	410	24			
1	G	291	Total	C	N	O	S	0	0	0
			2180	1361	387	408	24			
1	H	281	Total	C	N	O	S	0	0	0
			2122	1328	380	390	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173

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Chain	Residue	Modelled	Actual	Comment	Reference
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173

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Chain	Residue	Modelled	Actual	Comment	Reference
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173

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

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

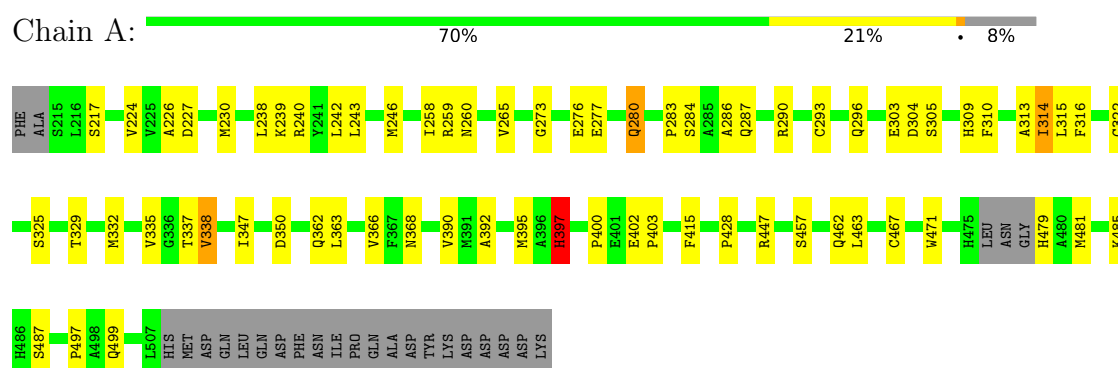
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0
4	B	37	Total O 37 37	0	0
4	C	36	Total O 36 36	0	0
4	D	63	Total O 63 63	0	0
4	E	22	Total O 22 22	0	0
4	F	26	Total O 26 26	0	0
4	G	28	Total O 28 28	0	0
4	H	36	Total O 36 36	0	0

3 Residue-property plots

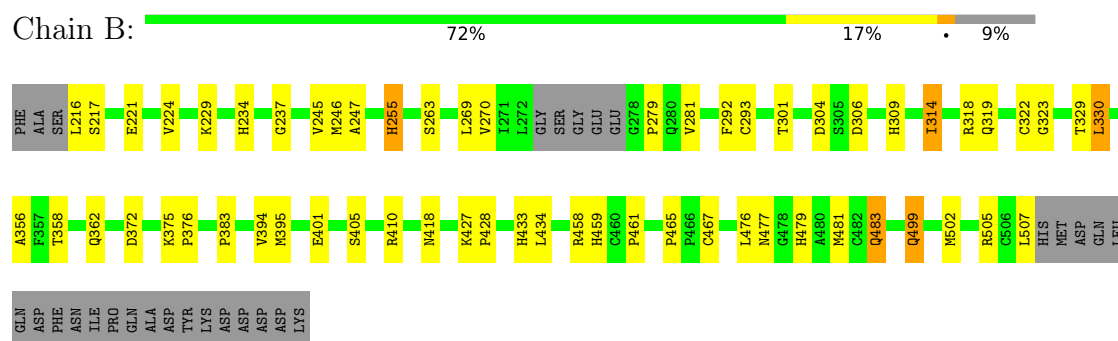
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

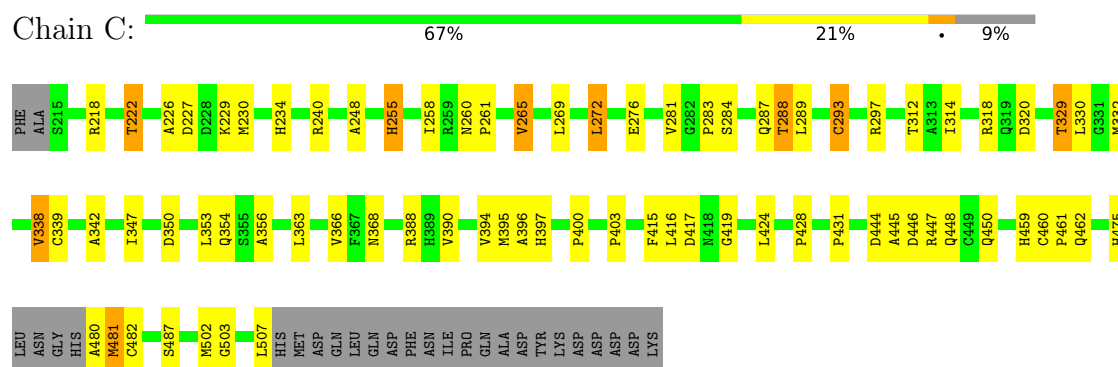
• Molecule 1: ADAMTS-4

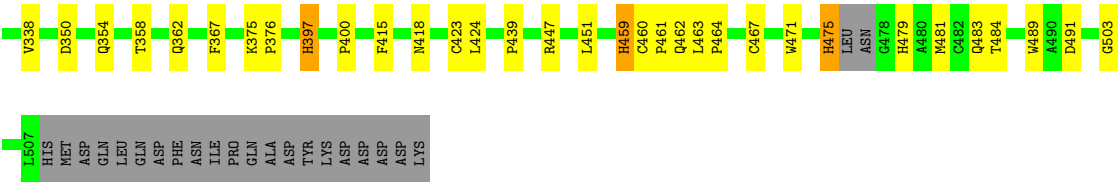


• Molecule 1: ADAMTS-4

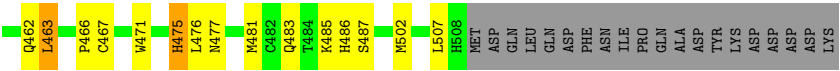
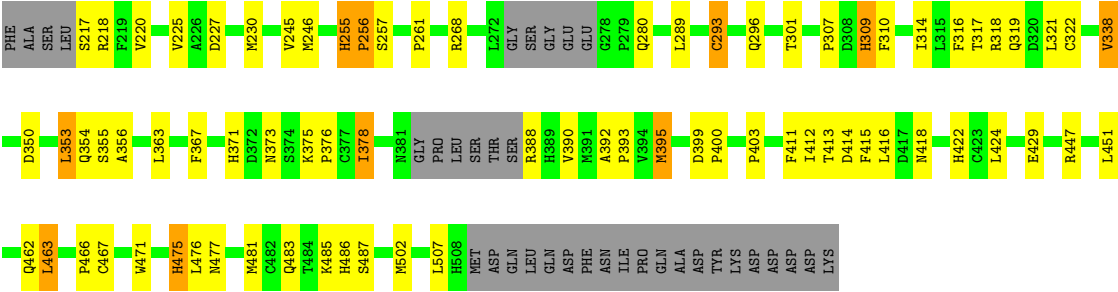


• Molecule 1: ADAMTS-4





● Molecule 1: ADAMTS-4



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	128.33Å 84.31Å 150.15Å 90.00° 112.23° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.6 (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17609	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.64	4/2236 (0.2%)	0.90	4/3049 (0.1%)
1	B	0.66	7/2218 (0.3%)	0.90	6/3026 (0.2%)
1	C	0.58	2/2225 (0.1%)	0.88	4/3034 (0.1%)
1	D	0.73	7/2218 (0.3%)	0.95	11/3026 (0.4%)
1	E	0.83	11/2191 (0.5%)	1.08	16/2986 (0.5%)
1	F	0.64	6/2256 (0.3%)	0.92	9/3078 (0.3%)
1	G	0.67	6/2240 (0.3%)	0.93	10/3054 (0.3%)
1	H	0.67	8/2181 (0.4%)	0.95	10/2973 (0.3%)
All	All	0.68	51/17765 (0.3%)	0.94	70/24226 (0.3%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	418	ASN	CG-OD1	6.47	1.35	1.23
1	H	280	GLN	CD-OE1	6.10	1.35	1.23
1	D	418	ASN	CG-OD1	5.88	1.34	1.23
1	E	483	GLN	CD-OE1	5.75	1.34	1.23
1	E	397	HIS	ND1-CE1	5.69	1.38	1.32
1	E	477	ASN	CG-OD1	5.56	1.34	1.23
1	E	508	HIS	ND1-CE1	5.56	1.38	1.32
1	E	479	HIS	ND1-CE1	5.55	1.38	1.32
1	D	433	HIS	ND1-CE1	5.49	1.38	1.32
1	E	389	HIS	ND1-CE1	5.46	1.38	1.32
1	F	477	ASN	CG-OD1	5.46	1.33	1.23
1	D	309	HIS	ND1-CE1	5.42	1.38	1.32
1	E	362	GLN	CD-OE1	5.39	1.33	1.23
1	H	422	HIS	ND1-CE1	5.39	1.38	1.32
1	G	475	HIS	ND1-CE1	5.39	1.38	1.32
1	D	422	HIS	ND1-CE1	5.38	1.38	1.32
1	G	459	HIS	ND1-CE1	5.37	1.38	1.32
1	H	475	HIS	ND1-CE1	5.37	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	418	ASN	CG-OD1	5.36	1.33	1.23
1	H	319	GLN	CD-OE1	5.35	1.33	1.23
1	G	397	HIS	ND1-CE1	5.35	1.37	1.32
1	B	309	HIS	ND1-CE1	5.35	1.37	1.32
1	A	397	HIS	ND1-CE1	5.34	1.37	1.32
1	H	309	HIS	ND1-CE1	5.34	1.37	1.32
1	H	486	HIS	ND1-CE1	5.33	1.37	1.32
1	F	459	HIS	ND1-CE1	5.33	1.37	1.32
1	B	255	HIS	ND1-CE1	5.31	1.37	1.32
1	A	362	GLN	CD-OE1	5.30	1.33	1.23
1	F	255	HIS	ND1-CE1	5.29	1.37	1.32
1	H	255	HIS	ND1-CE1	5.28	1.37	1.32
1	D	234	HIS	ND1-CE1	5.27	1.37	1.32
1	B	477	ASN	CG-OD1	5.26	1.33	1.23
1	E	418	ASN	CG-OD1	5.26	1.33	1.23
1	B	483	GLN	CD-OE1	5.25	1.33	1.23
1	G	309	HIS	ND1-CE1	5.25	1.37	1.32
1	G	418	ASN	CG-OD1	5.25	1.33	1.23
1	D	483	GLN	CD-OE1	5.24	1.33	1.23
1	F	234	HIS	ND1-CE1	5.23	1.37	1.32
1	F	309	HIS	ND1-CE1	5.22	1.37	1.32
1	C	255	HIS	ND1-CE1	5.21	1.37	1.32
1	G	296	GLN	CD-OE1	5.20	1.33	1.23
1	D	255	HIS	ND1-CE1	5.20	1.37	1.32
1	E	309	HIS	ND1-CE1	5.20	1.37	1.32
1	F	418	ASN	CG-OD1	5.20	1.33	1.23
1	E	255	HIS	ND1-CE1	5.19	1.37	1.32
1	C	234	HIS	ND1-CE1	5.16	1.37	1.32
1	E	499	GLN	CD-OE1	5.14	1.33	1.23
1	A	309	HIS	ND1-CE1	5.13	1.37	1.32
1	B	234	HIS	ND1-CE1	5.10	1.37	1.32
1	B	499	GLN	CD-OE1	5.06	1.33	1.23
1	A	499	GLN	CD-OE1	5.06	1.33	1.23

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	441	LYS	N-CA-C	-7.50	104.36	113.97
1	G	459	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	H	475	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	B	234	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	C	255	HIS	CB-CG-CD2	-6.65	122.56	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	389	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	H	486	HIS	CB-CG-CD2	-6.61	122.60	131.20
1	G	255	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	F	309	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	B	255	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	H	422	HIS	CB-CG-CD2	-6.57	122.65	131.20
1	F	234	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	F	459	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	H	309	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	309	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	D	433	HIS	CB-CG-CD2	-6.56	122.68	131.20
1	E	508	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	D	422	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	G	309	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	G	475	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	D	234	HIS	CB-CG-CD2	-6.53	122.72	131.20
1	E	309	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	A	397	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	F	255	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	C	234	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	H	255	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	E	479	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	E	255	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	E	397	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	D	255	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	B	309	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	G	397	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	D	309	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	F	478	GLY	N-CA-C	-5.85	106.38	115.67
1	E	508	HIS	CB-CG-ND1	5.76	131.34	122.70
1	G	459	HIS	CB-CG-ND1	5.76	131.34	122.70
1	H	475	HIS	CB-CG-ND1	5.75	131.33	122.70
1	C	255	HIS	CB-CG-ND1	5.72	131.28	122.70
1	F	309	HIS	CB-CG-ND1	5.70	131.24	122.70
1	E	397	HIS	CB-CG-ND1	5.69	131.24	122.70
1	H	255	HIS	CB-CG-ND1	5.69	131.24	122.70
1	B	255	HIS	CB-CG-ND1	5.69	131.23	122.70
1	E	389	HIS	CB-CG-ND1	5.69	131.23	122.70
1	F	459	HIS	CB-CG-ND1	5.68	131.22	122.70
1	H	309	HIS	CB-CG-ND1	5.68	131.22	122.70
1	G	475	HIS	CB-CG-ND1	5.68	131.22	122.70
1	F	255	HIS	CB-CG-ND1	5.67	131.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	422	HIS	CB-CG-ND1	5.66	131.19	122.70
1	B	309	HIS	CB-CG-ND1	5.66	131.19	122.70
1	D	309	HIS	CB-CG-ND1	5.66	131.18	122.70
1	D	433	HIS	CB-CG-ND1	5.66	131.18	122.70
1	G	255	HIS	CB-CG-ND1	5.66	131.18	122.70
1	G	309	HIS	CB-CG-ND1	5.65	131.18	122.70
1	B	234	HIS	CB-CG-ND1	5.64	131.16	122.70
1	A	397	HIS	CB-CG-ND1	5.63	131.14	122.70
1	A	309	HIS	CB-CG-ND1	5.62	131.13	122.70
1	H	422	HIS	CB-CG-ND1	5.61	131.12	122.70
1	C	234	HIS	CB-CG-ND1	5.61	131.11	122.70
1	E	255	HIS	CB-CG-ND1	5.60	131.10	122.70
1	F	234	HIS	CB-CG-ND1	5.59	131.08	122.70
1	D	234	HIS	CB-CG-ND1	5.58	131.07	122.70
1	D	255	HIS	CB-CG-ND1	5.57	131.06	122.70
1	E	309	HIS	CB-CG-ND1	5.57	131.05	122.70
1	H	486	HIS	CB-CG-ND1	5.56	131.03	122.70
1	E	479	HIS	CB-CG-ND1	5.56	131.03	122.70
1	G	397	HIS	CB-CG-ND1	5.51	130.96	122.70
1	D	338	VAL	N-CA-C	5.17	115.89	110.62
1	E	225	VAL	N-CA-C	5.14	115.67	108.17
1	E	282	GLY	CA-C-N	5.03	124.47	119.24
1	E	282	GLY	C-N-CA	5.03	124.47	119.24

There are no chirality outliers.

There are no planarity outliers.

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	2176	0	2075	54	0
1	B	2158	0	2067	36	0
1	C	2166	0	2068	61	0
1	D	2158	0	2067	82	0
1	E	2131	0	2036	48	0
1	F	2195	0	2093	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2180	0	2078	51	0
1	H	2122	0	2024	58	0
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
2	G	1	0	0	0	0
2	H	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
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	51	0	0	22	0
4	B	37	0	0	11	0
4	C	36	0	0	14	0
4	D	63	0	0	35	0
4	E	22	0	0	8	0
4	F	26	0	0	6	0
4	G	28	0	0	9	0
4	H	36	0	0	20	0
All	All	17609	0	16508	415	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 (415) 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:D:332:MET:HE2	4:D:545:HOH:O	1.20	1.27
1:C:395:MET:HB3	1:C:396:ALA:HB2	1.31	1.09
1:E:259:ARG:HG2	4:E:517:HOH:O	1.52	1.08
1:E:488:PRO:O	4:E:525:HOH:O	1.76	1.03
1:C:320:ASP:HB3	4:C:527:HOH:O	1.57	1.03
1:A:259:ARG:HG2	4:A:553:HOH:O	1.66	0.95
1:A:479:HIS:HB2	4:A:554:HOH:O	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:MET:HE1	1:A:314:ILE:HD12	1.52	0.92
1:A:283:PRO:HD2	1:A:287:GLN:OE1	1.69	0.92
1:C:481:MET:HG3	1:H:481:MET:HE3	1.53	0.91
1:A:303:GLU:HG3	4:A:530:HOH:O	1.74	0.87
1:B:246:MET:HE1	1:B:314:ILE:HD12	1.56	0.87
1:H:246:MET:HE2	1:H:246:MET:HA	1.56	0.87
1:A:332:MET:HE2	4:A:544:HOH:O	1.75	0.86
1:B:410:ARG:HD2	4:B:523:HOH:O	1.74	0.86
1:D:251:LYS:HB2	4:D:563:HOH:O	1.74	0.86
1:H:322:CYS:HB2	4:H:537:HOH:O	1.76	0.85
1:D:297:ARG:HD2	4:D:517:HOH:O	1.79	0.82
1:F:338:VAL:HG22	1:F:366:VAL:HG12	1.62	0.81
1:H:392:ALA:CB	4:H:529:HOH:O	2.28	0.81
1:B:458:ARG:HD2	4:B:534:HOH:O	1.80	0.80
1:E:284:SER:OG	1:E:287:GLN:HB2	1.82	0.79
1:A:395:MET:HE1	4:A:548:HOH:O	1.83	0.79
1:D:481:MET:HE2	1:D:483:GLN:HB3	1.65	0.78
1:F:274:SER:N	1:F:275:GLY:HA3	1.99	0.77
1:D:355:SER:HB2	4:D:523:HOH:O	1.82	0.77
1:E:400:PRO:HG2	4:E:516:HOH:O	1.84	0.77
1:H:476:LEU:HG	1:H:477:ASN:H	1.50	0.76
1:E:364:GLY:O	1:E:369:MET:HB2	1.84	0.76
1:G:246:MET:HA	1:G:246:MET:HE2	1.68	0.76
1:E:329:THR:HG21	1:E:395:MET:HB2	1.67	0.75
1:B:237:GLY:HA2	4:B:513:HOH:O	1.87	0.74
1:D:261:PRO:HA	4:D:565:HOH:O	1.86	0.74
1:E:338:VAL:HG23	1:E:415:PHE:HE1	1.52	0.74
1:E:481:MET:HE1	1:E:483:GLN:HB3	1.69	0.74
1:A:497:PRO:HD2	4:A:546:HOH:O	1.87	0.73
1:H:388:ARG:N	4:H:529:HOH:O	2.20	0.73
1:B:481:MET:HE3	1:F:481:MET:SD	2.29	0.72
1:E:320:ASP:HB3	4:E:521:HOH:O	1.88	0.72
1:C:354:GLN:HG2	1:C:487:SER:OG	1.88	0.72
1:C:502:MET:HB2	1:C:507:LEU:HD12	1.69	0.72
1:A:322:CYS:HB2	4:A:550:HOH:O	1.88	0.72
1:E:296:GLN:HE21	1:E:310:PHE:HE1	1.38	0.72
1:H:481:MET:HE2	1:H:483:GLN:HB3	1.71	0.72
1:A:315:LEU:HD23	1:A:347:ILE:HD12	1.72	0.71
1:F:459:HIS:O	1:F:461:PRO:HD3	1.90	0.71
1:A:329:THR:HA	4:A:529:HOH:O	1.89	0.71
1:D:251:LYS:HG3	4:D:568:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:HA	4:A:539:HOH:O	1.90	0.71
1:F:444:ASP:HB2	4:F:528:HOH:O	1.91	0.71
1:E:314:ILE:HD11	1:E:363:LEU:HD11	1.74	0.69
1:A:338:VAL:HG23	1:A:415:PHE:HE1	1.57	0.69
1:A:447:ARG:HD3	4:A:525:HOH:O	1.92	0.69
1:C:276:GLU:HB3	4:C:517:HOH:O	1.91	0.69
1:G:459:HIS:O	1:G:461:PRO:HD3	1.92	0.69
1:D:379:SER:CB	4:D:550:HOH:O	2.40	0.69
1:A:226:ALA:HB2	1:A:242:LEU:HD11	1.75	0.68
1:B:358:THR:CG2	1:B:395:MET:HE2	2.24	0.68
1:D:216:LEU:HA	4:D:536:HOH:O	1.92	0.68
1:A:286:ALA:HA	4:A:544:HOH:O	1.94	0.68
1:G:479:HIS:HA	4:G:532:HOH:O	1.93	0.68
1:H:268:ARG:HD3	4:H:514:HOH:O	1.94	0.67
1:A:240:ARG:HG2	4:A:531:HOH:O	1.93	0.67
1:H:255:HIS:ND1	1:H:257:SER:HB2	2.09	0.67
1:F:230:MET:HE1	1:F:350:ASP:OD2	1.95	0.67
1:D:229:LYS:HD2	1:D:319:GLN:HB2	1.75	0.67
1:C:240:ARG:HD3	4:C:533:HOH:O	1.95	0.67
1:F:225:VAL:HG22	1:F:270:VAL:HG22	1.76	0.66
1:C:289:LEU:HA	1:C:347:ILE:HD12	1.77	0.66
1:E:466:PRO:O	1:E:467:CYS:HB2	1.95	0.66
1:D:281:VAL:HG12	1:D:281:VAL:O	1.96	0.65
1:D:297:ARG:HB2	4:D:557:HOH:O	1.96	0.65
1:C:281:VAL:HA	1:C:288:THR:HG23	1.78	0.65
1:D:379:SER:HB2	4:D:550:HOH:O	1.95	0.65
1:D:473:SER:HB2	4:D:544:HOH:O	1.98	0.64
1:H:230:MET:HE3	1:H:316:PHE:HB3	1.78	0.64
1:C:395:MET:CB	1:C:396:ALA:HB2	2.18	0.64
1:D:481:MET:HE3	1:G:481:MET:HE3	1.79	0.64
1:C:265:VAL:HG13	1:C:431:PRO:HB3	1.80	0.64
1:G:296:GLN:HG3	1:G:313:ALA:CB	2.28	0.64
1:H:392:ALA:HB3	4:H:529:HOH:O	1.92	0.63
1:G:354:GLN:HB2	4:G:516:HOH:O	1.97	0.63
1:D:324:VAL:HG12	4:D:515:HOH:O	1.98	0.63
1:H:375:LYS:HG3	1:H:376:PRO:HD3	1.78	0.63
1:H:392:ALA:HB2	4:H:529:HOH:O	1.96	0.63
1:C:289:LEU:HA	1:C:347:ILE:CD1	2.29	0.63
1:E:255:HIS:O	1:E:258:ILE:HG22	1.99	0.63
1:E:369:MET:HE2	1:E:412:ILE:HB	1.79	0.63
1:G:217:SER:HA	1:G:261:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:HIS:N	1:A:397:HIS:CD2	2.66	0.62
1:C:395:MET:HB3	1:C:396:ALA:CB	2.20	0.62
1:F:329:THR:HG22	1:F:330:LEU:N	2.13	0.62
1:H:413:THR:HG21	4:H:534:HOH:O	1.98	0.62
1:B:433:HIS:HB3	4:B:517:HOH:O	2.01	0.61
1:D:428:PRO:HG2	4:D:561:HOH:O	2.00	0.61
1:C:297:ARG:HD3	1:C:342:ALA:HA	1.82	0.61
1:E:281:VAL:HA	1:E:288:THR:HG23	1.83	0.61
1:A:325:SER:HB3	4:A:539:HOH:O	2.00	0.61
1:G:423:CYS:SG	1:G:424:LEU:HD12	2.40	0.61
1:A:487:SER:HB2	4:A:526:HOH:O	2.01	0.61
1:D:369:MET:HE2	1:D:408:SER:HB3	1.83	0.61
1:C:329:THR:HG22	1:C:330:LEU:N	2.16	0.60
1:F:357:PHE:HB3	1:F:395:MET:CE	2.32	0.60
1:D:354:GLN:HG3	4:D:546:HOH:O	2.01	0.59
1:E:457:SER:OG	1:E:472:CYS:HB3	2.00	0.59
1:D:321:LEU:HD22	4:D:542:HOH:O	2.02	0.59
1:F:338:VAL:HG23	1:F:366:VAL:O	2.03	0.59
1:B:270:VAL:HA	4:B:531:HOH:O	2.02	0.58
1:G:358:THR:O	1:G:362:GLN:HG2	2.01	0.58
1:F:462:GLN:O	1:F:464:PRO:HD3	2.04	0.58
1:A:462:GLN:HG2	1:A:463:LEU:HD12	1.84	0.58
1:B:358:THR:HG22	1:B:395:MET:HE2	1.84	0.58
1:D:349:GLU:HG3	4:D:562:HOH:O	2.02	0.58
1:H:227:ASP:OD1	1:H:230:MET:HB2	2.02	0.58
1:E:315:LEU:HD12	1:E:316:PHE:N	2.19	0.58
1:F:385:SER:HA	4:F:530:HOH:O	2.03	0.57
1:F:502:MET:C	1:F:504:GLY:H	2.12	0.57
1:E:348:VAL:HG21	1:E:359:ALA:HA	1.86	0.57
1:D:321:LEU:HA	4:D:512:HOH:O	2.03	0.57
1:A:481:MET:HB3	4:A:533:HOH:O	2.04	0.57
1:C:318:ARG:HD2	1:C:350:ASP:HB3	1.85	0.57
1:A:296:GLN:HE21	1:A:310:PHE:HE1	1.52	0.57
1:H:399:ASP:OD1	1:H:400:PRO:HD2	2.04	0.57
1:D:254:LYS:HG3	4:D:570:HOH:O	2.05	0.56
1:C:481:MET:HG2	1:C:482:CYS:N	2.19	0.56
1:F:255:HIS:CE1	1:F:401:GLU:O	2.58	0.56
1:G:463:LEU:HD12	1:G:471:TRP:CD1	2.41	0.56
1:B:481:MET:HE2	1:B:483:GLN:HG3	1.88	0.56
1:E:362:GLN:O	1:E:365:HIS:HB2	2.05	0.56
1:F:246:MET:HE1	1:F:314:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ARG:HG3	4:D:554:HOH:O	2.04	0.56
1:C:329:THR:HG21	1:C:395:MET:HG3	1.87	0.55
1:D:463:LEU:HG	1:D:471:TRP:CD1	2.41	0.55
1:D:502:MET:HB2	1:D:507:LEU:HD12	1.87	0.55
1:A:296:GLN:HG3	1:A:313:ALA:CB	2.37	0.55
1:D:329:THR:HG21	1:D:395:MET:HG2	1.89	0.55
1:A:428:PRO:HB2	4:A:528:HOH:O	2.05	0.55
1:H:476:LEU:O	1:H:477:ASN:C	2.49	0.55
1:D:349:GLU:CG	4:D:562:HOH:O	2.55	0.55
1:D:459:HIS:CE1	1:D:461:PRO:HA	2.42	0.55
1:B:465:PRO:HG3	4:B:539:HOH:O	2.07	0.55
1:H:230:MET:HE1	1:H:350:ASP:CB	2.36	0.55
1:H:217:SER:N	4:H:540:HOH:O	2.40	0.54
1:G:322:CYS:SG	1:G:330:LEU:HA	2.46	0.54
1:G:367:PHE:HE2	1:G:424:LEU:HD21	1.72	0.54
1:D:348:VAL:HG21	1:D:359:ALA:HA	1.89	0.54
1:D:476:LEU:HD22	1:G:481:MET:HE1	1.88	0.54
1:D:387:SER:OG	1:D:392:ALA:HB1	2.08	0.54
1:H:477:ASN:HB3	4:H:521:HOH:O	2.07	0.54
1:A:338:VAL:CG2	1:A:415:PHE:HE1	2.21	0.54
1:D:290:ARG:HG3	4:D:513:HOH:O	2.08	0.53
1:A:463:LEU:HD11	1:E:463:LEU:HD21	1.90	0.53
1:D:357:PHE:HB3	1:D:395:MET:HE2	1.90	0.53
1:H:261:PRO:HD3	4:H:531:HOH:O	2.07	0.53
1:A:276:GLU:HG2	1:B:383:PRO:HG2	1.90	0.53
1:E:463:LEU:HD13	1:E:471:TRP:CG	2.43	0.53
1:F:307:PRO:HG3	1:F:429:GLU:OE1	2.08	0.53
1:E:314:ILE:HD11	1:E:363:LEU:CD1	2.37	0.53
1:F:437:THR:HG23	4:F:517:HOH:O	2.09	0.53
1:E:231:ALA:HA	1:E:238:LEU:HD22	1.90	0.53
1:C:338:VAL:HG23	1:C:415:PHE:HE1	1.73	0.53
1:B:427:LYS:HE2	4:B:516:HOH:O	2.09	0.52
1:C:388:ARG:HG2	1:C:397:HIS:CD2	2.44	0.52
1:D:283:PRO:HD2	1:D:287:GLN:OE1	2.09	0.52
1:A:258:ILE:HG23	1:A:260:ASN:H	1.74	0.52
1:B:323:GLY:N	4:B:525:HOH:O	2.42	0.52
1:D:485:LYS:O	1:D:486:HIS:HB2	2.08	0.52
1:G:251:LYS:HE3	4:G:517:HOH:O	2.09	0.52
1:G:367:PHE:CE2	1:G:424:LEU:HD21	2.45	0.52
1:D:339:CYS:O	1:D:341:PRO:HD3	2.10	0.52
1:F:272:LEU:HD21	1:F:279:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLN:CD	4:C:520:HOH:O	2.52	0.52
1:D:318:ARG:NH1	1:D:350:ASP:OD2	2.42	0.52
1:C:222:THR:HG23	1:C:312:THR:HG23	1.92	0.52
1:D:431:PRO:HD2	4:D:548:HOH:O	2.09	0.52
1:E:380:LEU:HB2	1:E:407:CYS:HB3	1.91	0.52
1:A:397:HIS:CD2	1:A:397:HIS:H	2.27	0.51
1:G:242:LEU:HD13	1:G:269:LEU:HD11	1.92	0.51
1:D:216:LEU:N	4:D:521:HOH:O	2.43	0.51
1:E:258:ILE:HB	1:E:404:TRP:CD1	2.45	0.51
1:C:297:ARG:HD2	4:C:534:HOH:O	2.11	0.51
1:E:220:VAL:HG21	1:E:367:PHE:HZ	1.75	0.51
1:E:348:VAL:HG22	1:E:358:THR:HG22	1.92	0.51
1:A:338:VAL:HG23	1:A:415:PHE:CE1	2.44	0.51
1:B:281:VAL:HG22	4:B:521:HOH:O	2.09	0.51
1:C:400:PRO:HD3	1:C:503:GLY:HA3	1.93	0.51
1:E:247:ALA:HB2	1:E:435:PRO:HD2	1.93	0.51
1:G:327:CYS:HA	1:G:332:MET:HE3	1.93	0.51
1:C:255:HIS:O	1:C:258:ILE:HG22	2.10	0.51
1:G:296:GLN:HG3	1:G:313:ALA:HB2	1.93	0.51
1:H:355:SER:HA	4:H:512:HOH:O	2.11	0.51
1:A:230:MET:HE3	1:A:316:PHE:C	2.36	0.50
1:F:450:GLN:HE21	1:F:458:ARG:NH1	2.09	0.50
1:H:393:PRO:HB2	4:H:518:HOH:O	2.11	0.50
1:B:375:LYS:HB3	1:B:376:PRO:HD3	1.92	0.50
1:B:304:ASP:HB2	4:B:510:HOH:O	2.10	0.50
1:C:276:GLU:CB	4:C:517:HOH:O	2.55	0.50
1:C:284:SER:HA	4:C:528:HOH:O	2.12	0.50
1:H:301:THR:OG1	1:H:309:HIS:HB2	2.10	0.50
1:C:218:ARG:HD2	1:C:416:LEU:HD13	1.94	0.50
1:C:446:ASP:O	1:C:450:GLN:HG3	2.11	0.50
1:D:282:GLY:C	4:D:543:HOH:O	2.54	0.50
1:E:427:LYS:HG2	1:E:428:PRO:HD2	1.93	0.50
1:G:264:LEU:HD23	1:G:265:VAL:N	2.26	0.50
1:H:218:ARG:NH2	1:H:416:LEU:HB3	2.26	0.50
1:H:227:ASP:OD1	1:H:317:THR:HA	2.11	0.50
1:H:246:MET:HA	1:H:246:MET:CE	2.36	0.50
1:G:218:ARG:HB3	1:G:424:LEU:HD23	1.94	0.49
1:G:246:MET:HE3	1:G:316:PHE:HZ	1.75	0.49
1:H:395:MET:HE1	4:H:525:HOH:O	2.12	0.49
1:H:230:MET:HE1	1:H:350:ASP:HB3	1.93	0.49
1:C:329:THR:CG2	1:C:395:MET:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LYS:HB3	1:B:318:ARG:HB2	1.94	0.49
1:E:481:MET:CE	1:E:483:GLN:HB3	2.40	0.49
1:C:289:LEU:HD22	1:C:332:MET:HG3	1.94	0.49
1:D:284:SER:N	4:D:543:HOH:O	2.46	0.49
1:C:447:ARG:NH2	4:C:520:HOH:O	2.05	0.49
1:H:255:HIS:CE1	1:H:403:PRO:HD2	2.47	0.49
1:H:393:PRO:CB	4:H:518:HOH:O	2.61	0.49
1:D:285:ALA:HB1	1:D:332:MET:HG3	1.94	0.49
1:D:464:PRO:HD2	1:G:462:GLN:HB3	1.93	0.49
1:E:239:LYS:O	1:E:243:LEU:HD22	2.13	0.49
1:A:303:GLU:C	1:A:305:SER:H	2.20	0.49
1:A:332:MET:HG3	4:A:544:HOH:O	2.13	0.49
1:B:459:HIS:CE1	1:B:461:PRO:HA	2.48	0.49
1:D:410:ARG:CG	4:D:554:HOH:O	2.60	0.49
1:F:329:THR:HG22	1:F:330:LEU:H	1.76	0.49
1:D:296:GLN:HG3	1:D:313:ALA:CB	2.43	0.48
1:D:429:GLU:HB3	1:E:394:VAL:HG11	1.95	0.48
1:C:248:ALA:HB3	1:C:356:ALA:HB1	1.95	0.48
1:E:306:ASP:N	1:E:306:ASP:OD1	2.46	0.48
1:G:322:CYS:HB2	4:G:523:HOH:O	2.12	0.48
1:H:314:ILE:HD11	1:H:363:LEU:HD21	1.95	0.48
1:H:414:ASP:HB3	4:H:516:HOH:O	2.13	0.48
1:F:296:GLN:HE21	1:F:310:PHE:HE1	1.62	0.48
1:D:319:GLN:HA	4:D:538:HOH:O	2.11	0.48
1:F:218:ARG:NH1	1:F:421:GLY:O	2.47	0.48
1:C:338:VAL:HG23	1:C:415:PHE:CE1	2.49	0.48
1:D:463:LEU:HD13	1:G:463:LEU:HD21	1.95	0.48
1:B:224:VAL:HG22	1:B:246:MET:HE3	1.96	0.48
1:F:337:THR:O	1:F:344:SER:HB2	2.14	0.48
1:D:255:HIS:CE1	1:D:257:SER:HG	2.29	0.48
1:D:355:SER:CB	4:D:523:HOH:O	2.48	0.47
1:H:447:ARG:HD2	4:H:527:HOH:O	2.15	0.47
1:E:489:TRP:CD1	1:E:489:TRP:N	2.82	0.47
1:F:367:PHE:HB3	1:F:412:ILE:HG13	1.95	0.47
1:G:301:THR:OG1	1:G:309:HIS:HB2	2.14	0.47
1:B:476:LEU:HD13	1:F:476:LEU:HD13	1.96	0.47
1:C:289:LEU:O	1:C:293:CYS:HB2	2.14	0.47
1:A:400:PRO:HG3	4:A:518:HOH:O	2.15	0.47
1:B:217:SER:HB2	4:B:520:HOH:O	2.15	0.47
1:B:322:CYS:SG	1:B:330:LEU:HA	2.55	0.47
1:B:502:MET:HB3	1:B:507:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ILE:HG23	1:C:260:ASN:H	1.80	0.47
1:D:293:CYS:SG	1:D:343:ARG:HA	2.54	0.47
1:F:339:CYS:SG	1:F:424:LEU:HD13	2.55	0.47
1:G:447:ARG:HD2	4:G:510:HOH:O	2.14	0.47
1:F:450:GLN:HA	1:F:454:GLY:O	2.15	0.47
1:B:479:HIS:HB2	1:F:484:THR:O	2.15	0.47
1:G:304:ASP:HA	1:G:309:HIS:CD2	2.49	0.47
1:E:246:MET:HE3	1:E:316:PHE:CZ	2.49	0.46
1:E:400:PRO:CD	4:E:516:HOH:O	2.63	0.46
1:F:265:VAL:HG11	1:F:428:PRO:HG2	1.98	0.46
1:H:268:ARG:CD	4:H:514:HOH:O	2.56	0.46
1:D:369:MET:HE2	1:D:408:SER:CB	2.45	0.46
1:H:378:ILE:HG13	4:H:522:HOH:O	2.13	0.46
1:B:247:ALA:HA	1:B:434:LEU:HD13	1.98	0.46
1:D:462:GLN:HG2	1:D:463:LEU:HD22	1.97	0.46
1:A:280:GLN:HG2	4:A:549:HOH:O	2.16	0.46
1:F:231:ALA:HA	1:F:238:LEU:HD22	1.96	0.46
1:G:246:MET:HE2	1:G:246:MET:CA	2.43	0.46
1:A:230:MET:HE1	1:A:350:ASP:HB2	1.97	0.46
1:E:400:PRO:CG	4:E:516:HOH:O	2.53	0.46
1:C:428:PRO:HB2	4:C:536:HOH:O	2.14	0.46
1:D:368:ASN:HB2	1:D:415:PHE:CD2	2.51	0.46
1:G:309:HIS:HB3	4:G:521:HOH:O	2.16	0.46
1:H:318:ARG:NH2	1:H:451:LEU:O	2.40	0.46
1:A:390:VAL:HG23	1:A:403:PRO:O	2.16	0.46
1:C:339:CYS:SG	1:C:424:LEU:HD13	2.56	0.46
1:D:297:ARG:N	4:D:557:HOH:O	2.43	0.46
1:G:246:MET:HE3	1:G:316:PHE:CZ	2.51	0.45
1:H:230:MET:HE1	1:H:350:ASP:HB2	1.98	0.45
1:D:479:HIS:HB2	1:G:484:THR:O	2.17	0.45
1:A:335:VAL:HG12	1:A:368:ASN:HA	1.98	0.45
1:C:265:VAL:CG1	1:C:431:PRO:HB3	2.46	0.45
1:H:354:GLN:HG2	1:H:487:SER:CB	2.47	0.45
1:A:463:LEU:HD22	1:A:471:TRP:CD2	2.52	0.45
1:G:280:GLN:HG3	4:G:519:HOH:O	2.15	0.45
1:A:238:LEU:O	1:A:239:LYS:C	2.60	0.45
1:C:445:ALA:HB1	1:C:459:HIS:CG	2.51	0.45
1:F:427:LYS:HE2	4:F:524:HOH:O	2.16	0.45
1:A:290:ARG:HD3	1:A:290:ARG:HA	1.62	0.45
1:D:369:MET:CE	1:D:408:SER:HB3	2.47	0.45
1:H:255:HIS:HA	1:H:256:PRO:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:HD13	1:F:476:LEU:CD1	2.47	0.44
1:C:314:ILE:HD11	1:C:363:LEU:HD11	1.99	0.44
1:D:335:VAL:HA	1:D:365:HIS:O	2.17	0.44
1:F:301:THR:HB	1:F:302:PRO:HD2	1.99	0.44
1:H:463:LEU:HD13	1:H:471:TRP:CG	2.53	0.44
1:A:230:MET:HE1	1:A:350:ASP:CB	2.47	0.44
1:C:354:GLN:HG2	1:C:487:SER:CB	2.46	0.44
1:G:400:PRO:HG3	1:G:503:GLY:HA3	1.99	0.44
1:A:273:GLY:H	1:A:276:GLU:HB2	1.83	0.44
1:E:443:TYR:HB3	1:E:447:ARG:HB2	1.98	0.44
1:G:471:TRP:HA	1:G:483:GLN:O	2.17	0.44
1:C:394:VAL:HG23	1:C:394:VAL:O	2.18	0.44
1:F:227:ASP:OD1	1:F:317:THR:HA	2.17	0.44
1:H:289:LEU:O	1:H:293:CYS:HB2	2.18	0.44
1:D:286:ALA:HA	4:D:545:HOH:O	2.16	0.44
1:G:375:LYS:N	1:G:376:PRO:HD2	2.33	0.44
1:A:337:THR:O	1:A:338:VAL:C	2.61	0.44
1:D:337:THR:HG22	1:D:366:VAL:HG13	2.00	0.44
1:D:255:HIS:ND1	1:D:257:SER:OG	2.36	0.44
1:E:230:MET:HE1	1:E:350:ASP:HB2	1.99	0.44
1:E:397:HIS:CE1	4:E:513:HOH:O	2.71	0.44
1:H:220:VAL:HG21	1:H:367:PHE:HZ	1.83	0.44
1:B:245:VAL:HG13	1:B:356:ALA:HA	1.99	0.43
1:H:390:VAL:HG23	1:H:403:PRO:O	2.17	0.43
1:H:502:MET:HB2	1:H:507:LEU:HD12	2.00	0.43
1:A:224:VAL:HG22	1:A:246:MET:HE3	2.00	0.43
1:C:329:THR:HG22	1:C:330:LEU:H	1.80	0.43
1:H:296:GLN:HE21	1:H:310:PHE:HE1	1.66	0.43
1:B:221:GLU:HG2	1:B:428:PRO:HB3	1.99	0.43
1:D:463:LEU:HD13	1:G:463:LEU:CD2	2.49	0.43
1:G:280:GLN:HG2	1:G:291:SER:OG	2.18	0.43
1:C:261:PRO:HA	4:C:529:HOH:O	2.17	0.43
1:C:368:ASN:HB2	1:C:415:PHE:CD2	2.53	0.43
1:E:332:MET:HB2	1:E:347:ILE:HG22	2.01	0.43
1:D:281:VAL:O	1:D:281:VAL:CG1	2.65	0.43
1:G:475:HIS:HA	1:G:479:HIS:O	2.19	0.43
1:C:444:ASP:O	1:C:448:GLN:HG3	2.19	0.43
1:D:258:ILE:HG23	1:D:260:ASN:H	1.83	0.43
1:H:463:LEU:HD13	1:H:471:TRP:CD2	2.53	0.43
1:E:445:ALA:HB1	1:E:459:HIS:CG	2.54	0.43
1:H:353:LEU:HD13	1:H:451:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LEU:CA	4:D:536:HOH:O	2.60	0.43
1:D:321:LEU:HD11	4:D:526:HOH:O	2.18	0.43
1:D:375:LYS:HB3	1:D:376:PRO:HD3	2.00	0.43
1:G:329:THR:HG22	1:G:330:LEU:N	2.34	0.43
1:D:247:ALA:HA	1:D:434:LEU:HD13	2.00	0.43
1:D:301:THR:OG1	1:D:309:HIS:HB2	2.18	0.43
1:H:338:VAL:HG23	1:H:415:PHE:HE1	1.83	0.43
1:F:255:HIS:HE1	1:F:401:GLU:O	1.99	0.42
1:F:338:VAL:CG1	1:F:424:LEU:HD11	2.49	0.42
1:G:338:VAL:HG12	1:G:415:PHE:HE1	1.84	0.42
1:H:307:PRO:HB3	1:H:429:GLU:HG2	2.01	0.42
1:A:485:LYS:HE2	1:E:479:HIS:NE2	2.34	0.42
1:A:497:PRO:CD	4:A:546:HOH:O	2.57	0.42
1:B:358:THR:O	1:B:362:GLN:HG2	2.19	0.42
1:C:502:MET:HE1	4:C:539:HOH:O	2.19	0.42
1:D:246:MET:HE3	1:D:316:PHE:HZ	1.84	0.42
1:G:245:VAL:HG12	1:G:246:MET:CE	2.49	0.42
1:H:475:HIS:CE1	4:H:542:HOH:O	2.72	0.42
1:H:466:PRO:O	1:H:467:CYS:HB2	2.19	0.42
1:B:255:HIS:CE1	1:B:401:GLU:O	2.72	0.42
1:B:372:ASP:OD1	1:B:405:SER:OG	2.31	0.42
1:C:338:VAL:HG22	1:C:366:VAL:HG12	2.02	0.42
1:C:480:ALA:HB3	4:C:535:HOH:O	2.20	0.42
1:D:227:ASP:OD1	1:D:317:THR:HA	2.20	0.42
1:B:229:LYS:HE2	1:B:319:GLN:HG3	2.02	0.42
1:G:397:HIS:CD2	4:G:530:HOH:O	2.72	0.42
1:F:491:ASP:HA	1:F:501:CYS:O	2.19	0.42
1:H:371:HIS:C	1:H:373:ASN:H	2.27	0.42
1:D:458:ARG:NE	4:D:534:HOH:O	2.53	0.42
1:E:473:SER:HA	1:E:481:MET:O	2.20	0.42
1:C:265:VAL:HG11	1:C:428:PRO:HG3	2.02	0.41
1:C:480:ALA:N	4:C:512:HOH:O	2.52	0.41
1:A:230:MET:HE2	1:A:230:MET:HB2	1.93	0.41
1:C:227:ASP:HA	1:C:272:LEU:HD12	2.01	0.41
1:C:283:PRO:HD2	1:C:287:GLN:HG2	2.02	0.41
1:G:462:GLN:O	1:G:464:PRO:HD3	2.20	0.41
1:A:363:LEU:O	1:A:366:VAL:HB	2.21	0.41
1:B:467:CYS:HB2	1:B:505:ARG:HA	2.02	0.41
1:D:285:ALA:HB1	1:D:332:MET:CG	2.49	0.41
1:E:400:PRO:HD2	4:E:516:HOH:O	2.20	0.41
1:G:289:LEU:O	1:G:293:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:485:LYS:HE3	4:H:533:HOH:O	2.20	0.41
1:D:296:GLN:HG3	1:D:313:ALA:HB3	2.01	0.41
1:E:481:MET:HE3	1:E:481:MET:HB2	1.96	0.41
1:F:254:LYS:HE3	4:F:514:HOH:O	2.20	0.41
1:G:246:MET:HA	1:G:246:MET:CE	2.42	0.41
1:E:365:HIS:CD2	1:E:391:MET:HE1	2.55	0.41
1:G:230:MET:HE1	1:G:350:ASP:OD2	2.21	0.41
1:G:251:LYS:CE	4:G:517:HOH:O	2.66	0.41
1:C:226:ALA:HB1	1:C:230:MET:HG2	2.03	0.41
1:D:312:THR:HB	4:D:551:HOH:O	2.21	0.41
1:E:447:ARG:O	1:E:451:LEU:HG	2.21	0.41
1:G:241:TYR:CE2	1:G:451:LEU:HD22	2.56	0.41
1:G:439:PRO:HD2	1:G:491:ASP:O	2.21	0.41
1:H:245:VAL:HG13	1:H:356:ALA:HA	2.03	0.41
1:A:335:VAL:CG1	1:A:368:ASN:HA	2.51	0.41
1:G:467:CYS:HA	1:G:489:TRP:CG	2.56	0.41
1:A:402:GLU:N	1:A:403:PRO:HD3	2.36	0.40
1:F:354:GLN:HG2	1:F:487:SER:OG	2.20	0.40
1:F:357:PHE:HB3	1:F:395:MET:HE1	2.01	0.40
1:H:476:LEU:HG	1:H:477:ASN:N	2.25	0.40
1:C:390:VAL:HG23	1:C:403:PRO:O	2.21	0.40
1:D:337:THR:HG23	1:D:344:SER:HA	2.02	0.40
1:A:217:SER:HB3	4:A:538:HOH:O	2.21	0.40
1:B:301:THR:HG21	1:B:306:ASP:OD2	2.22	0.40
1:C:460:CYS:HB3	1:C:462:GLN:NE2	2.37	0.40
1:C:475:HIS:HA	4:C:512:HOH:O	2.20	0.40
1:H:255:HIS:ND1	1:H:403:PRO:HD2	2.37	0.40
1:H:367:PHE:HB3	1:H:412:ILE:HG13	2.03	0.40
1:C:417:ASP:C	1:C:419:GLY:H	2.28	0.40
1:D:246:MET:HE3	1:D:316:PHE:CZ	2.56	0.40
1:F:240:ARG:HB2	4:F:516:HOH:O	2.20	0.40
1:A:392:ALA:HB2	4:A:557:HOH:O	2.21	0.40
1:B:279:PRO:HG3	1:B:292:PHE:HD1	1.86	0.40
1:C:229:LYS:H	1:C:229:LYS:HG2	1.64	0.40
1:C:459:HIS:O	1:C:461:PRO:HD3	2.21	0.40
1:D:284:SER:HB2	1:D:287:GLN:HB2	2.02	0.40
1:D:287:GLN:HG3	4:D:552:HOH:O	2.21	0.40
1:D:387:SER:O	1:D:396:ALA:HB3	2.22	0.40
1:D:463:LEU:CD1	1:G:463:LEU:HD21	2.50	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	286/316 (90%)	258 (90%)	26 (9%)	2 (1%)	18	47
1	B	283/316 (90%)	259 (92%)	24 (8%)	0	100	100
1	C	285/316 (90%)	262 (92%)	23 (8%)	0	100	100
1	D	283/316 (90%)	255 (90%)	25 (9%)	3 (1%)	11	36
1	E	276/316 (87%)	255 (92%)	19 (7%)	2 (1%)	18	47
1	F	291/316 (92%)	259 (89%)	31 (11%)	1 (0%)	36	66
1	G	287/316 (91%)	269 (94%)	16 (6%)	2 (1%)	18	47
1	H	275/316 (87%)	255 (93%)	18 (6%)	2 (1%)	18	47
All	All	2266/2528 (90%)	2072 (91%)	182 (8%)	12 (0%)	24	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	351	ASP
1	A	304	ASP
1	E	467	CYS
1	H	395	MET
1	A	467	CYS
1	D	221	GLU
1	D	320	ASP
1	D	497	PRO
1	H	256	PRO
1	F	460	CYS
1	G	460	CYS
1	G	283	PRO

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	238/261 (91%)	228 (96%)	10 (4%)	26	61
1	B	236/261 (90%)	227 (96%)	9 (4%)	29	64
1	C	237/261 (91%)	227 (96%)	10 (4%)	26	61
1	D	236/261 (90%)	226 (96%)	10 (4%)	26	61
1	E	232/261 (89%)	218 (94%)	14 (6%)	17	47
1	F	239/261 (92%)	224 (94%)	15 (6%)	16	45
1	G	238/261 (91%)	233 (98%)	5 (2%)	47	79
1	H	231/261 (88%)	221 (96%)	10 (4%)	26	60
All	All	1887/2088 (90%)	1804 (96%)	83 (4%)	25	59

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
1	A	243	LEU
1	A	265	VAL
1	A	277	GLU
1	A	280	GLN
1	A	293	CYS
1	A	314	ILE
1	A	338	VAL
1	A	397	HIS
1	A	457	SER
1	B	216	LEU
1	B	263	SER
1	B	269	LEU
1	B	293	CYS
1	B	314	ILE
1	B	329	THR
1	B	330	LEU
1	B	394	VAL
1	B	499	GLN
1	C	222	THR
1	C	265	VAL
1	C	269	LEU
1	C	272	LEU

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Mol	Chain	Res	Type
1	C	288	THR
1	C	293	CYS
1	C	329	THR
1	C	338	VAL
1	C	353	LEU
1	C	481	MET
1	D	268	ARG
1	D	270	VAL
1	D	272	LEU
1	D	293	CYS
1	D	314	ILE
1	D	387	SER
1	D	405	SER
1	D	424	LEU
1	D	451	LEU
1	D	473	SER
1	E	225	VAL
1	E	227	ASP
1	E	228	ASP
1	E	243	LEU
1	E	244	THR
1	E	288	THR
1	E	293	CYS
1	E	306	ASP
1	E	321	LEU
1	E	338	VAL
1	E	456	ASP
1	E	463	LEU
1	E	495	CYS
1	E	499	GLN
1	F	216	LEU
1	F	227	ASP
1	F	243	LEU
1	F	245	VAL
1	F	264	LEU
1	F	265	VAL
1	F	270	VAL
1	F	281	VAL
1	F	289	LEU
1	F	293	CYS
1	F	296	GLN
1	F	325	SER

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Mol	Chain	Res	Type
1	F	329	THR
1	F	380	LEU
1	F	491	ASP
1	G	243	LEU
1	G	264	LEU
1	G	296	GLN
1	G	314	ILE
1	G	335	VAL
1	H	225	VAL
1	H	293	CYS
1	H	321	LEU
1	H	338	VAL
1	H	353	LEU
1	H	378	ILE
1	H	411	PHE
1	H	424	LEU
1	H	462	GLN
1	H	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	368	ASN
1	A	475	HIS
1	B	260	ASN
1	B	319	GLN
1	B	368	ASN
1	B	450	GLN
1	C	418	ASN
1	E	483	GLN
1	E	499	GLN
1	F	255	HIS
1	G	234	HIS
1	H	234	HIS
1	H	362	GLN
1	H	381	ASN
1	H	477	ASN
1	H	508	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](#)

Of 24 ligands modelled in this entry, 24 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 [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

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.