



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:54 PM UTC

PDB ID : 4ATZ / pdb_00004atz
Title : Ad5 knob in complex with a designed ankyrin repeat protein
Authors : Mittl, P.R.E.; Hess, C.; Dreier, B.
Deposited on : 2012-05-11
Resolution : 1.95 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

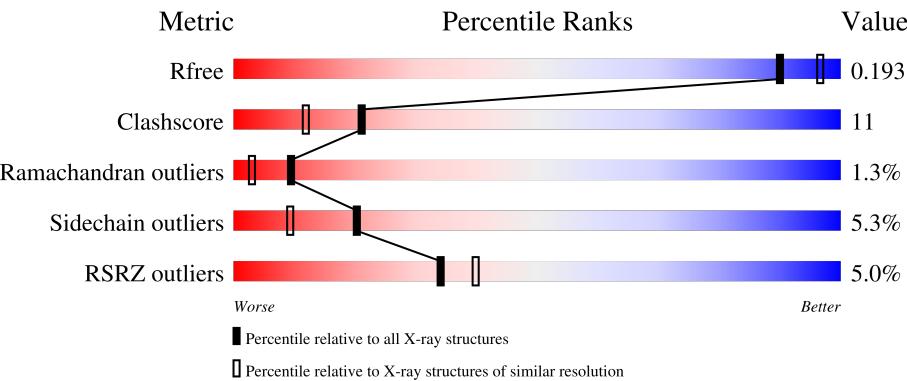
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	201	3% 69% 17% •• 9%
1	B	201	4% 61% 22% • 15%
1	C	201	4% 71% 12% •• 12%
2	D	154	% 75% 18% 7%
2	E	154	4% 77% 19% •

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Mol	Chain	Length	Quality of chain
2	F	154	12% 73% 21% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8492 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 Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	14	0
			1499	949	250	296	4			
1	B	171	Total	C	N	O	S	0	11	0
			1402	892	233	273	4			
1	C	176	Total	C	N	O	S	0	3	0
			1374	873	226	271	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	MET	-	initiating methionine	UNP P11818
A	382	ALA	-	expression tag	UNP P11818
A	383	HIS	-	expression tag	UNP P11818
A	384	HIS	-	expression tag	UNP P11818
A	385	HIS	-	expression tag	UNP P11818
A	386	HIS	-	expression tag	UNP P11818
A	387	HIS	-	expression tag	UNP P11818
A	388	HIS	-	expression tag	UNP P11818
A	389	GLY	-	expression tag	UNP P11818
A	390	SER	-	expression tag	UNP P11818
A	?	-	THR	deletion	UNP P11818
A	?	-	ALA	deletion	UNP P11818
A	?	-	TYR	deletion	UNP P11818
A	?	-	THR	deletion	UNP P11818
B	377	MET	-	initiating methionine	UNP P11818
B	378	ALA	-	expression tag	UNP P11818
B	379	HIS	-	expression tag	UNP P11818
B	380	HIS	-	expression tag	UNP P11818
B	381	HIS	-	expression tag	UNP P11818
B	382	HIS	-	expression tag	UNP P11818
B	383	HIS	-	expression tag	UNP P11818
B	384	HIS	-	expression tag	UNP P11818
B	385	GLY	-	expression tag	UNP P11818

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Chain	Residue	Modelled	Actual	Comment	Reference
B	386	SER	-	expression tag	UNP P11818
B	?	-	THR	deletion	UNP P11818
B	?	-	ALA	deletion	UNP P11818
B	?	-	TYR	deletion	UNP P11818
B	?	-	THR	deletion	UNP P11818
C	377	MET	-	initiating methionine	UNP P11818
C	378	ALA	-	expression tag	UNP P11818
C	379	HIS	-	expression tag	UNP P11818
C	380	HIS	-	expression tag	UNP P11818
C	381	HIS	-	expression tag	UNP P11818
C	382	HIS	-	expression tag	UNP P11818
C	383	HIS	-	expression tag	UNP P11818
C	384	HIS	-	expression tag	UNP P11818
C	385	GLY	-	expression tag	UNP P11818
C	386	SER	-	expression tag	UNP P11818
C	?	-	THR	deletion	UNP P11818
C	?	-	ALA	deletion	UNP P11818
C	?	-	TYR	deletion	UNP P11818
C	?	-	THR	deletion	UNP P11818

- Molecule 2 is a protein called DESIGNED ANKYRIN REPEAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	154	Total	C	N	O	S	0	2	0
			1172	742	200	228	2			
2	E	154	Total	C	N	O	S	0	1	0
			1167	739	199	227	2			
2	F	152	Total	C	N	O	S	0	0	0
			1143	721	197	223	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total	O	0	0
			201	201		
3	B	178	Total	O	0	0
			178	178		
3	C	132	Total	O	0	0
			132	132		
3	D	102	Total	O	0	0
			102	102		
3	E	74	Total	O	0	0
			74	74		

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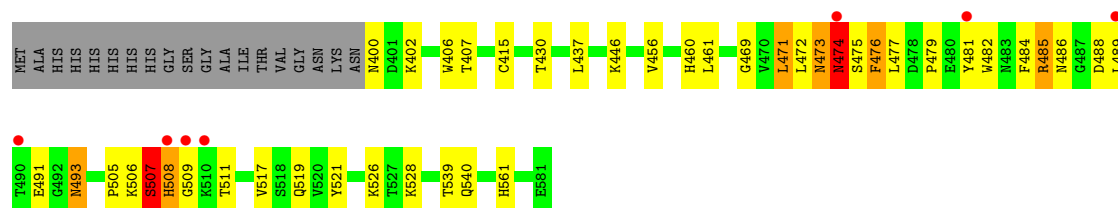
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	48	Total	O	0	0
			48	48		

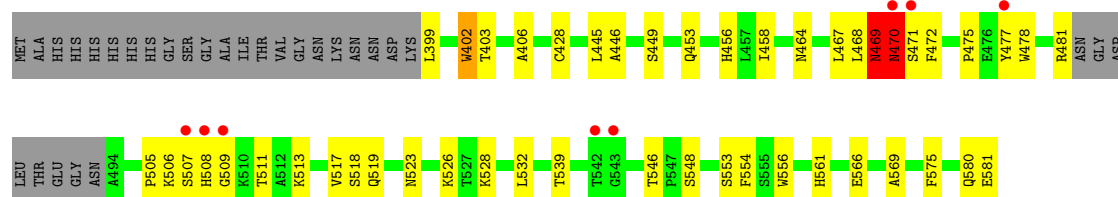
3 Residue-property plots [i](#)

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.

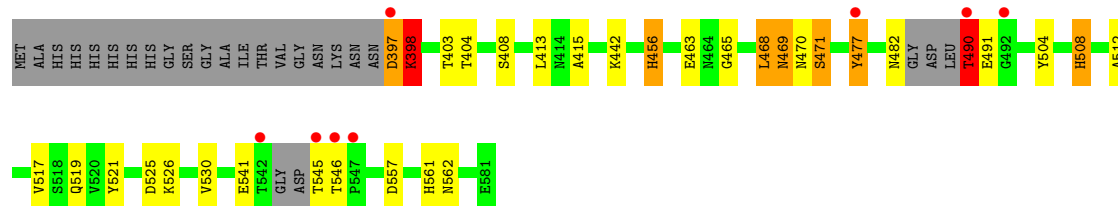
- Molecule 1: Fiber protein



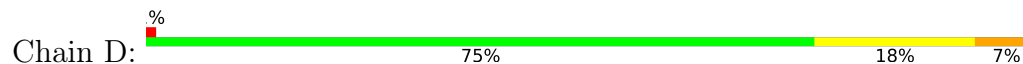
- Molecule 1: Fiber protein

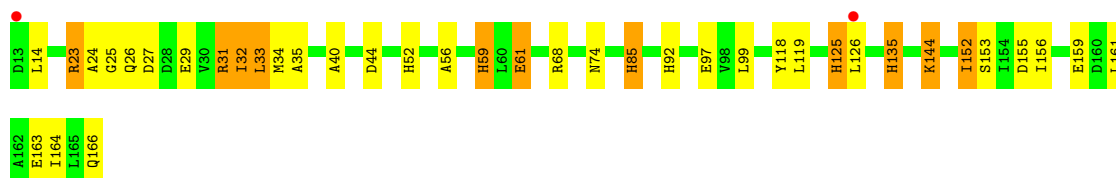


- Molecule 1: Fiber protein

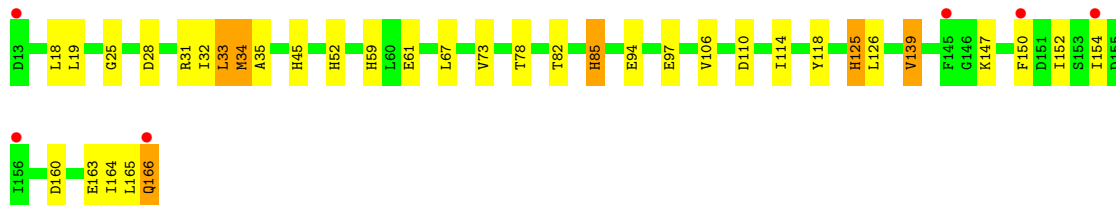
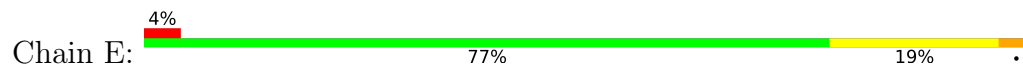


- Molecule 2: DESIGNED ANKYRIN REPEAT PROTEIN

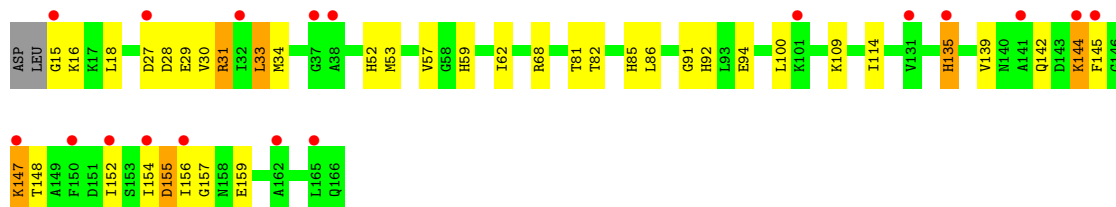




● Molecule 2: DESIGNED ANKYRIN REPEAT PROTEIN



● Molecule 2: DESIGNED ANKYRIN REPEAT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.60Å 112.10Å 129.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 1.95 46.57 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.57-1.95) 100.0 (46.57-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.161 , 0.193 (Not available) , 0.193	Depositor DCC
R_{free} test set	5802 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8492	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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	1.78	13/1540 (0.8%)	1.51	5/2096 (0.2%)
1	B	1.75	21/1439 (1.5%)	1.42	5/1959 (0.3%)
1	C	1.64	10/1411 (0.7%)	1.45	10/1922 (0.5%)
2	D	1.71	11/1193 (0.9%)	1.33	4/1623 (0.2%)
2	E	1.55	10/1189 (0.8%)	1.29	4/1617 (0.2%)
2	F	1.37	7/1161 (0.6%)	1.17	0/1579
All	All	1.65	72/7933 (0.9%)	1.38	28/10796 (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	A	0	3
1	B	0	1
1	C	0	2
All	All	0	6

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	85	HIS	ND1-CE1	9.05	1.41	1.32
1	C	561	HIS	ND1-CE1	7.98	1.40	1.32
1	A	493	ASN	C-O	7.76	1.32	1.24
1	B	554	PHE	C-O	7.44	1.32	1.24
1	B	528	LYS	N-CA	7.25	1.54	1.46
1	A	484	PHE	CA-C	-7.20	1.43	1.53
1	B	561	HIS	ND1-CE1	7.16	1.39	1.32
2	D	92	HIS	ND1-CE1	6.92	1.39	1.32
1	C	456	HIS	ND1-CE1	6.67	1.39	1.32
1	B	449	SER	C-O	6.65	1.32	1.23
2	D	135	HIS	ND1-CE1	6.64	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	LYS	N-CA	6.63	1.53	1.46
1	A	485	ARG	CZ-NH1	6.59	1.42	1.32
1	A	460	HIS	ND1-CE1	6.56	1.39	1.32
1	A	528	LYS	N-CA	6.52	1.53	1.46
2	D	125	HIS	ND1-CE1	6.51	1.39	1.32
1	B	539	THR	N-CA	6.48	1.53	1.45
1	A	471	LEU	CA-C	-6.38	1.45	1.52
1	A	456	VAL	CA-C	6.34	1.60	1.52
2	F	52	HIS	ND1-CE1	6.19	1.38	1.32
1	B	569	ALA	N-CA	6.08	1.53	1.46
1	A	406	TRP	C-O	5.98	1.31	1.23
1	C	442	LYS	N-CA	5.94	1.53	1.46
2	D	119	LEU	N-CA	5.93	1.53	1.46
2	F	135	HIS	CE1-NE2	5.88	1.38	1.32
2	D	85	HIS	CE1-NE2	5.87	1.38	1.32
2	E	45	HIS	CG-CD2	5.79	1.42	1.35
2	D	125	HIS	CG-CD2	5.78	1.42	1.35
1	B	561	HIS	CE1-NE2	5.78	1.38	1.32
2	E	97	GLU	N-CA	5.76	1.53	1.46
2	D	74	ASN	CA-CB	5.68	1.61	1.53
2	E	125	HIS	CE1-NE2	5.67	1.38	1.32
2	D	99	LEU	CA-C	5.63	1.60	1.52
1	B	478	TRP	CA-C	-5.62	1.47	1.53
1	B	402	TRP	CD2-CE2	5.58	1.50	1.41
1	B	446	ALA	N-CA	-5.58	1.41	1.46
1	B	532	LEU	CA-C	5.56	1.59	1.52
1	A	561	HIS	ND1-CE1	5.55	1.38	1.32
1	A	482	TRP	CA-C	-5.54	1.47	1.53
1	B	456	HIS	ND1-CE1	5.51	1.38	1.32
1	A	461	LEU	C-O	5.50	1.30	1.23
2	E	19	LEU	N-CA	5.50	1.52	1.46
2	E	73	VAL	CA-C	5.49	1.60	1.52
2	E	52	HIS	ND1-CE1	5.49	1.38	1.32
2	F	81	THR	CA-CB	5.46	1.61	1.53
2	F	52	HIS	CG-CD2	5.46	1.41	1.35
2	F	81	THR	N-CA	5.40	1.52	1.46
2	E	118	TYR	N-CA	5.38	1.52	1.46
2	E	67	LEU	CA-C	5.36	1.59	1.52
2	E	110	ASP	CA-CB	5.30	1.60	1.53
1	B	453	GLN	N-CA	5.29	1.51	1.46
1	B	513	LYS	CA-C	5.29	1.60	1.52
1	B	511	THR	N-CA	5.28	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	415	ALA	N-CA	5.28	1.52	1.45
1	C	471	SER	N-CA	5.28	1.53	1.46
1	C	517	VAL	C-O	5.22	1.29	1.24
1	B	575	PHE	C-O	5.21	1.30	1.23
1	C	508	HIS	CG-CD2	5.21	1.41	1.35
1	C	525	ASP	N-CA	5.20	1.52	1.46
1	B	464	ASN	CA-CB	5.20	1.61	1.53
1	A	484	PHE	N-CA	5.20	1.52	1.45
2	F	86	LEU	N-CA	5.20	1.52	1.46
1	B	518	SER	CB-OG	5.17	1.52	1.42
1	B	556	TRP	C-O	5.16	1.30	1.23
1	B	566	GLU	N-CA	5.15	1.52	1.45
2	F	135	HIS	CG-CD2	5.14	1.41	1.35
2	D	59	HIS	CG-CD2	5.11	1.41	1.35
2	D	52	HIS	ND1-CE1	5.10	1.37	1.32
1	C	465	GLY	N-CA	5.08	1.52	1.45
1	C	456	HIS	CG-CD2	5.03	1.41	1.35
1	B	580	GLN	C-O	5.03	1.30	1.24
2	D	56	ALA	N-CA	5.01	1.52	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	THR	CA-C-N	-6.69	113.76	120.31
1	B	546	THR	C-N-CA	-6.69	113.76	120.31
2	E	34	MET	N-CA-C	-6.61	103.99	111.07
2	E	139	VAL	CB-CA-C	-6.33	99.71	111.79
2	E	94	GLU	N-CA-C	-6.25	104.35	112.23
2	D	97	GLU	CA-CB-CG	-6.10	101.89	114.10
1	C	477	TYR	CA-C-N	-5.76	113.83	122.47
1	C	477	TYR	C-N-CA	-5.76	113.83	122.47
2	D	24	ALA	N-CA-C	-5.59	106.31	113.02
1	C	404	THR	N-CA-CB	5.57	120.29	110.37
1	C	398	LYS	N-CA-C	-5.53	106.39	113.02
2	E	126	LEU	N-CA-C	5.52	117.29	111.28
1	A	437	LEU	N-CA-C	-5.51	100.20	109.07
1	C	504	TYR	CA-C-N	-5.33	114.47	119.85
1	C	504	TYR	C-N-CA	-5.33	114.47	119.85
1	B	406	ALA	CA-C-N	-5.32	114.76	120.03
1	B	406	ALA	C-N-CA	-5.32	114.76	120.03
2	D	44	ASP	CA-C-N	-5.29	111.35	121.94
2	D	44	ASP	C-N-CA	-5.29	111.35	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	530	VAL	N-CA-C	-5.24	100.52	108.17
1	B	467	LEU	CB-CA-C	-5.20	101.09	109.72
1	A	485	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	C	413	LEU	N-CA-C	-5.08	106.77	113.12
1	A	469	GLY	N-CA-C	-5.08	108.24	115.30
1	A	486	ASN	CA-C-N	-5.07	117.56	121.82
1	A	486	ASN	C-N-CA	-5.07	117.56	121.82
1	C	408	SER	CA-C-N	-5.02	114.41	119.83
1	C	408	SER	C-N-CA	-5.02	114.41	119.83

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472[B]	LEU	Peptide
1	A	474[B]	ASN	Peptide
1	A	507[B]	SER	Peptide
1	B	469[B]	ASN	Peptide
1	C	397	ASP	Peptide
1	C	490	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1499	0	1467	38	0
1	B	1402	0	1373	29	0
1	C	1374	0	1348	20	0
2	D	1172	0	1166	40	0
2	E	1167	0	1154	17	0
2	F	1143	0	1130	31	0
3	A	201	0	0	10	1
3	B	178	0	0	13	1
3	C	132	0	0	6	0
3	D	102	0	0	8	1
3	E	74	0	0	1	1
3	F	48	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8492	0	7638	170	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (170) 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)
2:D:166:GLN:HG3	3:D:2091:HOH:O	1.40	1.19
1:B:481:ARG:C	3:B:2079:HOH:O	1.84	1.18
2:D:126[B]:LEU:HD13	2:D:164:ILE:CD1	1.80	1.12
1:A:473[B]:ASN:HB3	3:A:2082:HOH:O	1.49	1.09
1:A:474[B]:ASN:OD1	1:A:475[B]:SER:O	1.71	1.08
1:B:581:GLU:CD	3:B:2178:HOH:O	1.95	1.06
1:A:519:GLN:HG2	3:A:2119:HOH:O	1.58	1.02
1:B:581:GLU:OE1	3:B:2178:HOH:O	1.84	0.94
3:B:2041:HOH:O	2:E:78:THR:HG23	1.67	0.93
2:F:31:ARG:HH12	2:F:68:ARG:HH22	1.15	0.93
1:B:481:ARG:NH2	3:B:2081:HOH:O	1.92	0.91
2:D:31:ARG:HB2	2:D:31:ARG:HH11	1.36	0.91
1:B:519[B]:GLN:NE2	3:B:2115:HOH:O	2.06	0.89
2:E:34:MET:HA	2:E:34:MET:HE2	1.53	0.89
2:D:126[B]:LEU:CD1	2:D:164:ILE:CD1	2.51	0.88
2:D:61:GLU:HB3	3:D:2020:HOH:O	1.74	0.88
2:D:31:ARG:HB2	2:D:31:ARG:NH1	1.89	0.86
1:B:399:LEU:N	3:B:2001:HOH:O	2.08	0.85
1:A:506[B]:LYS:O	1:A:507[B]:SER:CB	2.25	0.84
1:A:506[B]:LYS:O	1:A:507[B]:SER:HB2	1.76	0.84
2:F:34:MET:HE2	2:F:34:MET:HA	1.63	0.81
1:A:511:THR:HG21	3:A:2099:HOH:O	1.81	0.80
1:A:474[B]:ASN:CG	1:A:475[B]:SER:O	2.25	0.79
2:D:126[B]:LEU:CD1	2:D:164:ILE:HD13	2.12	0.79
2:F:18:LEU:HD22	2:F:34:MET:HE1	1.63	0.79
1:B:519[B]:GLN:CD	3:B:2115:HOH:O	2.26	0.78
2:D:68:ARG:NH2	3:D:2022:HOH:O	2.16	0.78
1:C:398:LYS:HD3	1:C:398:LYS:H	1.50	0.77
1:C:482:ASN:C	1:C:490:THR:HG23	2.10	0.76
2:D:126[B]:LEU:HD13	2:D:164:ILE:HD13	1.67	0.75
1:C:519:GLN:HG2	3:C:2084:HOH:O	1.87	0.75
1:B:506[A]:LYS:HE2	1:B:548:SER:O	1.88	0.74
2:F:135:HIS:HD2	3:F:2027:HOH:O	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507[B]:SER:OG	1:A:540:GLN:HB2	1.88	0.73
2:D:126[B]:LEU:HD13	2:D:164:ILE:HD11	1.68	0.73
1:C:508:HIS:HD2	3:C:2075:HOH:O	1.71	0.73
2:D:126[B]:LEU:O	2:D:126[B]:LEU:HD12	1.89	0.72
1:A:505:PRO:O	1:A:508[B]:HIS:HB2	1.89	0.72
2:F:29:GLU:O	2:F:33:LEU:HD23	1.89	0.72
1:A:473[A]:ASN:OD1	3:A:2081:HOH:O	2.06	0.72
2:D:23:ARG:O	2:D:23:ARG:HG2	1.89	0.71
1:B:519[A]:GLN:NE2	3:B:2112:HOH:O	2.15	0.71
1:A:475[B]:SER:C	1:A:477:LEU:N	2.49	0.70
2:F:31:ARG:NH1	2:F:68:ARG:HH22	1.88	0.70
2:F:144:LYS:HG3	2:F:145:PHE:H	1.55	0.70
1:A:471:LEU:HD22	1:A:475[B]:SER:HB2	1.76	0.68
2:F:142:GLN:HG2	2:F:148:THR:HG22	1.76	0.66
2:F:91:GLY:O	3:F:2021:HOH:O	2.14	0.66
3:B:2043:HOH:O	2:E:78:THR:HG21	1.97	0.65
1:B:468:LEU:O	1:B:469[B]:ASN:HB3	1.97	0.64
1:B:470[A]:ASN:HA	1:B:475:PRO:HD3	1.77	0.64
2:E:34:MET:HE2	2:E:34:MET:CA	2.27	0.64
1:A:511:THR:CG2	3:A:2099:HOH:O	2.41	0.64
1:A:493:ASN:ND2	3:A:2074:HOH:O	2.31	0.63
2:E:25:GLY:HA3	2:E:59:HIS:CE1	2.34	0.63
1:B:470[A]:ASN:C	1:B:470[A]:ASN:HD22	2.06	0.63
2:D:126[B]:LEU:CD1	2:D:164:ILE:HD11	2.26	0.63
2:D:144:LYS:CB	2:D:144:LYS:NZ	2.61	0.62
2:E:82:THR:H	2:E:85:HIS:HD2	1.47	0.62
2:F:59:HIS:CD2	3:F:2011:HOH:O	2.51	0.62
2:E:165:LEU:O	2:E:166:GLN:NE2	2.33	0.62
2:D:126[B]:LEU:HD12	2:D:126[B]:LEU:C	2.25	0.61
1:A:507[B]:SER:C	1:A:509[B]:GLY:H	2.08	0.61
2:F:59:HIS:HD2	3:F:2011:HOH:O	1.82	0.61
1:A:474[A]:ASN:HA	1:A:479:PRO:HD3	1.81	0.61
1:A:473[A]:ASN:CG	1:A:474[A]:ASN:H	2.10	0.60
2:D:166:GLN:C	3:D:2088:HOH:O	2.45	0.60
1:A:473[B]:ASN:CB	3:A:2082:HOH:O	2.23	0.59
1:B:468:LEU:O	1:B:469[A]:ASN:HB3	2.03	0.59
2:D:135:HIS:HE1	3:D:2041:HOH:O	1.85	0.59
2:E:82:THR:H	2:E:85:HIS:CD2	2.21	0.58
2:F:53:MET:O	2:F:57:VAL:HG23	2.04	0.57
1:A:473[A]:ASN:CG	1:A:474[A]:ASN:N	2.63	0.57
2:E:165:LEU:O	2:E:166:GLN:CD	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LYS:HD3	1:C:398:LYS:N	2.19	0.56
2:D:29:GLU:HG3	2:D:33:LEU:HD22	1.87	0.56
2:D:118:TYR:OH	2:D:152:ILE:HD11	2.04	0.56
2:F:92:HIS:HD2	3:F:2023:HOH:O	1.89	0.56
1:C:469:ASN:HA	3:C:2056:HOH:O	2.05	0.56
1:C:463:GLU:H	1:C:463:GLU:CD	2.15	0.55
1:B:526:LYS:HE3	1:C:557:ASP:CG	2.31	0.55
2:D:25:GLY:HA3	2:D:59:HIS:CE1	2.42	0.54
1:C:468:LEU:O	1:C:471:SER:HB2	2.07	0.54
1:C:482:ASN:HB2	1:C:490:THR:CG2	2.38	0.53
1:B:458:ILE:HG12	1:B:553[A]:SER:HB2	1.89	0.53
2:E:85:HIS:HE1	2:E:114:ILE:O	1.92	0.53
2:D:118:TYR:CZ	2:D:152:ILE:HD12	2.44	0.52
1:C:469:ASN:O	1:C:470:ASN:HB2	2.09	0.52
2:F:18:LEU:HD22	2:F:34:MET:CE	2.35	0.52
2:F:85:HIS:HE1	2:F:114:ILE:O	1.93	0.52
1:B:506[A]:LYS:O	1:B:507[A]:SER:HB2	2.09	0.52
2:F:29:GLU:HG3	2:F:33:LEU:HD21	1.92	0.52
1:C:403:THR:HA	1:C:477:TYR:O	2.08	0.52
1:B:468:LEU:O	1:B:469[B]:ASN:CB	2.58	0.51
1:A:526[B]:LYS:CE	3:A:2127:HOH:O	2.58	0.51
2:D:118:TYR:CZ	2:D:152:ILE:CD1	2.94	0.51
2:D:32:ILE:O	2:D:35:ALA:HB3	2.11	0.50
2:F:82:THR:H	2:F:85:HIS:CD2	2.30	0.50
2:E:32:ILE:O	2:E:35:ALA:HB3	2.11	0.50
1:A:506[B]:LYS:O	1:A:507[B]:SER:OG	2.30	0.50
2:F:144:LYS:HG3	2:F:145:PHE:N	2.27	0.49
1:B:469[B]:ASN:C	1:B:471[B]:SER:N	2.70	0.49
2:D:144:LYS:NZ	2:D:144:LYS:HB3	2.26	0.49
2:F:27:ASP:OD1	2:F:62:ILE:HG13	2.12	0.49
2:D:144:LYS:HB3	2:D:144:LYS:HZ3	1.77	0.49
1:A:507[B]:SER:C	1:A:509[B]:GLY:N	2.70	0.49
1:A:473[A]:ASN:OD1	1:A:475[A]:SER:HB2	2.12	0.49
2:F:29:GLU:HG3	2:F:33:LEU:CD2	2.43	0.48
2:F:15:GLY:N	3:F:2001:HOH:O	2.46	0.48
1:B:523:ASN:HA	1:C:512:ALA:HB2	1.95	0.48
2:D:26:GLN:O	2:D:27:ASP:C	2.54	0.48
2:D:125:HIS:HD2	3:D:2098:HOH:O	1.95	0.48
1:B:469[B]:ASN:C	1:B:471[B]:SER:H	2.21	0.48
2:D:126[B]:LEU:HD13	2:D:164:ILE:HD12	1.86	0.48
1:A:473[A]:ASN:ND2	1:A:474[A]:ASN:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:ASN:C	1:C:471:SER:H	2.21	0.47
2:F:142:GLN:HA	2:F:147:LYS:O	2.15	0.47
2:F:82:THR:H	2:F:85:HIS:HD2	1.61	0.47
2:D:144:LYS:NZ	2:D:144:LYS:HB2	2.29	0.47
2:F:145:PHE:HB2	2:F:147:LYS:HE2	1.96	0.47
2:F:34:MET:HE2	2:F:34:MET:CA	2.41	0.46
2:E:18:LEU:HA	2:E:33:LEU:HD23	1.98	0.46
1:B:403:THR:HA	1:B:477:TYR:O	2.16	0.46
2:D:118:TYR:CE2	2:D:152:ILE:HD12	2.50	0.46
2:F:155:ASP:C	2:F:157:GLY:H	2.24	0.46
1:A:415:CYS:HA	1:A:476[B]:PHE:O	2.15	0.46
2:F:18:LEU:CD2	2:F:34:MET:HE1	2.42	0.45
2:D:159:GLU:O	2:D:163:GLU:HG3	2.16	0.45
1:B:445:LEU:HB2	3:B:2040:HOH:O	2.15	0.45
3:B:2041:HOH:O	2:E:78:THR:CG2	2.43	0.45
1:C:456:HIS:HE1	3:C:2099:HOH:O	1.98	0.45
1:C:541:GLU:HG2	1:C:546:THR:O	2.17	0.45
1:C:482:ASN:HB2	1:C:490:THR:HG21	1.98	0.45
2:D:153:SER:OG	2:D:161:LEU:CD2	2.64	0.45
2:D:153:SER:OG	2:D:161:LEU:HD23	2.17	0.45
1:B:505:PRO:O	1:B:508[A]:HIS:HB2	2.17	0.45
2:D:29:GLU:N	3:D:2004:HOH:O	2.41	0.45
2:E:125:HIS:HD2	3:E:2055:HOH:O	2.00	0.44
1:A:517:VAL:HB	1:C:521:TYR:CD2	2.53	0.44
1:A:474[A]:ASN:OD1	1:A:474[A]:ASN:C	2.60	0.44
1:C:526:LYS:HE2	3:C:2089:HOH:O	2.18	0.44
2:F:100:LEU:HD13	2:F:135:HIS:CG	2.53	0.44
1:B:470[A]:ASN:C	1:B:470[A]:ASN:ND2	2.71	0.43
2:E:34:MET:O	2:E:35:ALA:C	2.61	0.43
2:F:94:GLU:HG3	3:F:2025:HOH:O	2.18	0.43
2:F:144:LYS:CG	2:F:145:PHE:H	2.28	0.43
2:E:160:ASP:O	2:E:164:ILE:HG13	2.19	0.43
1:A:407:THR:HA	1:A:481:TYR:O	2.19	0.43
1:B:402:TRP:CZ2	1:B:481:ARG:HG3	2.54	0.43
1:A:430:THR:HG21	1:B:428:CYS:O	2.19	0.43
2:D:166:GLN:CG	3:D:2091:HOH:O	2.22	0.42
1:B:509[A]:GLY:N	3:B:2100:HOH:O	2.37	0.42
1:A:485:ARG:NH1	3:A:2087:HOH:O	2.52	0.42
2:E:150[A]:PHE:CE1	2:E:165:LEU:HB3	2.55	0.42
1:A:521:TYR:CD1	1:B:517:VAL:HB	2.54	0.42
1:A:476[B]:PHE:N	1:A:476[B]:PHE:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476[B]:PHE:N	1:A:476[B]:PHE:HD1	2.18	0.41
2:D:144:LYS:HB2	2:D:144:LYS:HZ2	1.85	0.41
1:A:526[B]:LYS:NZ	3:A:2127:HOH:O	2.49	0.41
2:D:34:MET:HE1	2:D:40:ALA:HB2	2.01	0.41
1:A:506[B]:LYS:HE3	1:A:539:THR:O	2.21	0.41
2:D:126[A]:LEU:HD22	2:D:161:LEU:HD13	2.03	0.41
1:A:505:PRO:O	1:A:506[B]:LYS:C	2.64	0.40
1:A:474[B]:ASN:C	1:A:475[B]:SER:O	2.62	0.40
1:B:526:LYS:HD2	3:C:2096:HOH:O	2.20	0.40
1:C:562:ASN:C	1:C:562:ASN:HD22	2.28	0.40
2:F:30:VAL:O	2:F:34:MET:HG2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2170:HOH:O	3:E:2038:HOH:O[3_555]	2.14	0.06
3:A:2183:HOH:O	3:D:2078:HOH:O[4_555]	2.17	0.03

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	194/201 (96%)	175 (90%)	9 (5%)	10 (5%)	1	0
1	B	178/201 (89%)	164 (92%)	8 (4%)	6 (3%)	3	0
1	C	173/201 (86%)	162 (94%)	11 (6%)	0	100	100
2	D	154/154 (100%)	151 (98%)	1 (1%)	2 (1%)	9	3
2	E	153/154 (99%)	152 (99%)	1 (1%)	0	100	100
2	F	150/154 (97%)	138 (92%)	9 (6%)	3 (2%)	6	1
All	All	1002/1065 (94%)	942 (94%)	39 (4%)	21 (2%)	9	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474[A]	ASN
1	A	474[B]	ASN
1	A	476[A]	PHE
1	A	476[B]	PHE
1	A	507[A]	SER
1	A	507[B]	SER
1	A	508[A]	HIS
1	A	508[B]	HIS
1	B	470[A]	ASN
1	B	470[B]	ASN
1	B	472[A]	PHE
1	B	472[B]	PHE
1	A	473[A]	ASN
1	A	473[B]	ASN
2	D	155	ASP
2	D	156	ILE
2	F	144	LYS
2	F	155	ASP
1	B	469[A]	ASN
1	B	469[B]	ASN
2	F	156	ILE

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	169/171 (99%)	164 (97%)	5 (3%)	36	27
1	B	158/171 (92%)	154 (98%)	4 (2%)	42	34
1	C	156/171 (91%)	149 (96%)	7 (4%)	24	14
2	D	119/117 (102%)	111 (93%)	8 (7%)	15	5
2	E	118/117 (101%)	107 (91%)	11 (9%)	8	2
2	F	115/117 (98%)	105 (91%)	10 (9%)	9	2
All	All	835/864 (97%)	790 (95%)	45 (5%)	20	9

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	A	402	LYS
1	A	488	ASP
1	A	489	LEU
1	A	491	GLU
1	B	469[A]	ASN
1	B	469[B]	ASN
1	B	470[A]	ASN
1	B	470[B]	ASN
1	C	397	ASP
1	C	398	LYS
1	C	468	LEU
1	C	469	ASN
1	C	490	THR
1	C	491	GLU
1	C	545	THR
2	D	14	LEU
2	D	23	ARG
2	D	31	ARG
2	D	32	ILE
2	D	33	LEU
2	D	61	GLU
2	D	144	LYS
2	D	152	ILE
2	E	28	ASP
2	E	31	ARG
2	E	33	LEU
2	E	61	GLU
2	E	106	VAL
2	E	139	VAL
2	E	147	LYS
2	E	152	ILE
2	E	154	ILE
2	E	163	GLU
2	E	166	GLN
2	F	16	LYS
2	F	28	ASP
2	F	31	ARG
2	F	33	LEU
2	F	109	LYS
2	F	139	VAL
2	F	147	LYS

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Mol	Chain	Res	Type
2	F	152	ILE
2	F	154	ILE
2	F	159	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	GLN
1	A	460	HIS
1	A	486	ASN
1	A	493	ASN
1	A	562	ASN
1	B	414	ASN
1	B	562	ASN
1	B	565	ASN
1	C	456	HIS
1	C	470	ASN
1	C	493	ASN
1	C	508	HIS
1	C	562	ASN
2	D	26	GLN
2	D	59	HIS
2	D	85	HIS
2	D	125	HIS
2	E	45	HIS
2	E	59	HIS
2	E	85	HIS
2	E	125	HIS
2	E	166	GLN
2	F	59	HIS
2	F	85	HIS
2	F	125	HIS
2	F	142	GLN

5.3.3 RNA ⓘ

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	182/201 (90%)	-0.34	7 (3%)	44	50	11, 27, 57, 94	14 (7%)
1	B	171/201 (85%)	-0.34	8 (4%)	36	42	12, 29, 60, 75	11 (6%)
1	C	176/201 (87%)	-0.18	8 (4%)	38	44	15, 35, 89, 116	3 (1%)
2	D	154/154 (100%)	0.00	2 (1%)	75	81	16, 39, 76, 99	2 (1%)
2	E	154/154 (100%)	0.21	6 (3%)	43	50	28, 46, 82, 104	1 (0%)
2	F	152/154 (98%)	0.79	18 (11%)	9	10	37, 59, 110, 122	0
All	All	989/1065 (92%)	0.00	49 (4%)	34	40	11, 37, 89, 122	31 (3%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509[A]	GLY	10.3
1	A	508[A]	HIS	7.3
2	F	154	ILE	5.5
2	F	145	PHE	4.8
1	C	490	THR	4.2
2	F	156	ILE	4.1
1	A	489	LEU	4.0
1	B	508[A]	HIS	3.9
1	B	470[A]	ASN	3.7
1	C	542	THR	3.5
2	F	150	PHE	3.5
1	A	481	TYR	3.4
2	F	165	LEU	3.4
2	E	150[A]	PHE	3.4
2	E	154	ILE	3.3
1	C	547	PRO	3.3
1	C	545	THR	3.2
1	C	477	TYR	3.2
1	B	471[A]	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	474[A]	ASN	3.1
1	C	546	THR	3.0
1	B	509[A]	GLY	3.0
2	D	126[A]	LEU	2.9
2	F	27	ASP	2.9
1	C	397	ASP	2.9
2	F	144	LYS	2.8
2	D	13	ASP	2.7
2	F	32	ILE	2.7
2	E	156	ILE	2.6
2	F	38	ALA	2.6
2	F	162	ALA	2.5
1	B	477	TYR	2.5
2	F	15	GLY	2.5
1	A	510[A]	LYS	2.4
1	B	543	GLY	2.4
1	B	542	THR	2.3
2	F	101	LYS	2.3
1	A	490	THR	2.3
2	F	147	LYS	2.2
2	F	152	ILE	2.2
2	E	145	PHE	2.2
2	F	131	VAL	2.2
2	E	13	ASP	2.1
2	F	37	GLY	2.1
2	F	135	HIS	2.1
1	C	492	GLY	2.0
2	E	166	GLN	2.0
2	F	141	ALA	2.0
1	B	507[A]	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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.