



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 1AEI / pdb_00001aei
Title : CRYSTAL STRUCTURE OF THE ANNEXIN XII HEXAMER
Authors : Luecke, H.; Chang, B.T.; Mailliard, W.S.; Schlaepfer, D.D.; Haigler, H.T.
Deposited on : 1995-09-23
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

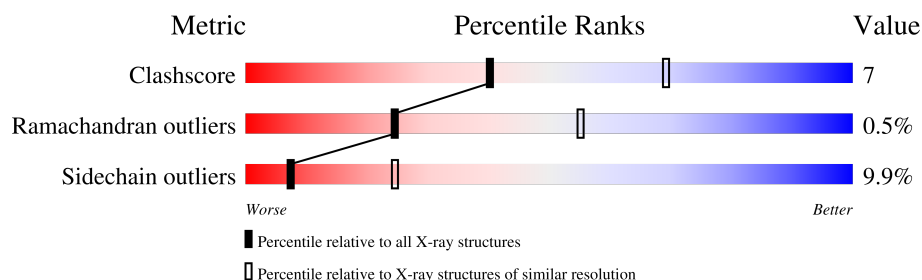
1 Overall quality at a glance

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	315	
1	B	315	
1	C	315	
1	D	315	
1	E	315	
1	F	315	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18252 atoms, of which 3456 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 ANNEXIN XII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	315	Total	C	H	N	O	S	0	0	0
			3038	1543	576	428	484	7			
1	B	315	Total	C	H	N	O	S	0	0	0
			3038	1543	576	428	484	7			
1	C	315	Total	C	H	N	O	S	0	0	0
			3038	1543	576	428	484	7			
1	D	315	Total	C	H	N	O	S	0	0	0
			3038	1543	576	428	484	7			
1	E	315	Total	C	H	N	O	S	0	0	0
			3038	1543	576	428	484	7			
1	F	315	Total	C	H	N	O	S	0	0	0
			3038	1543	576	428	484	7			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

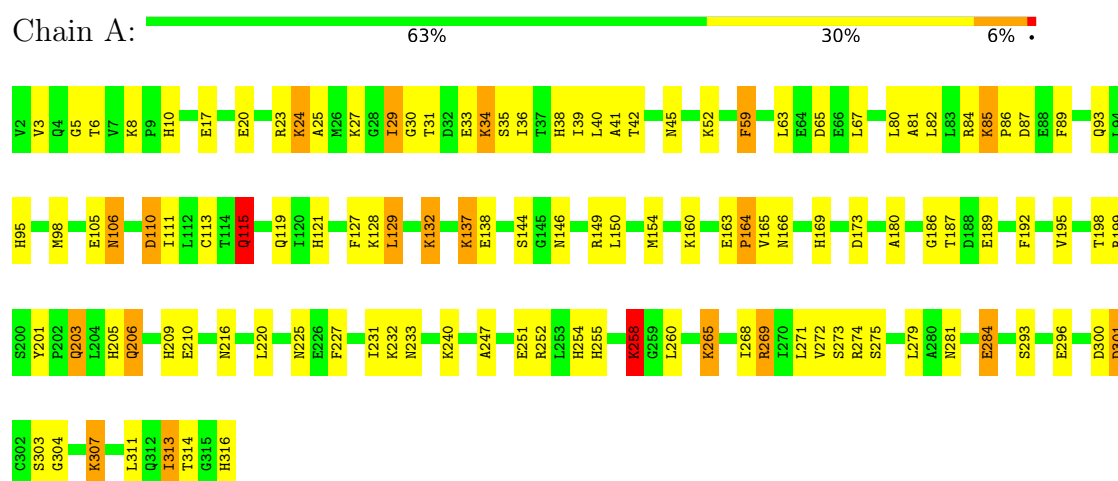
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		
2	B	4	Total	Ca	0	0
			4	4		
2	C	4	Total	Ca	0	0
			4	4		
2	D	4	Total	Ca	0	0
			4	4		
2	E	4	Total	Ca	0	0
			4	4		
2	F	4	Total	Ca	0	0
			4	4		

3 Residue-property plots

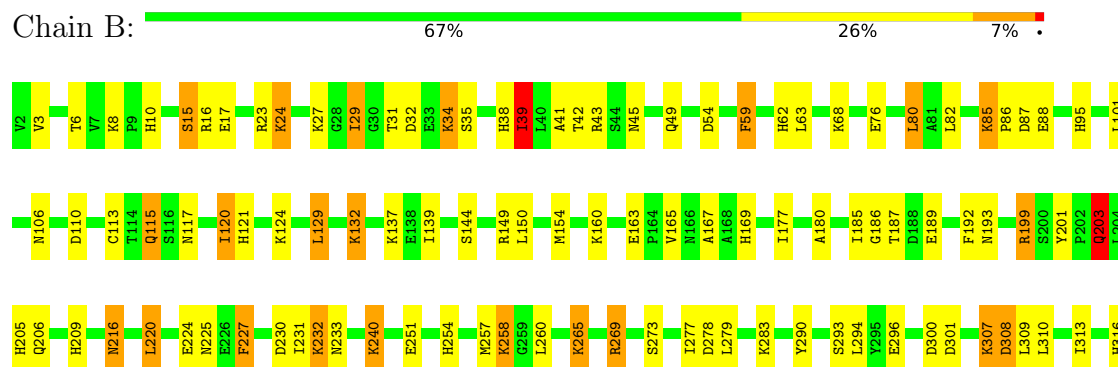
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

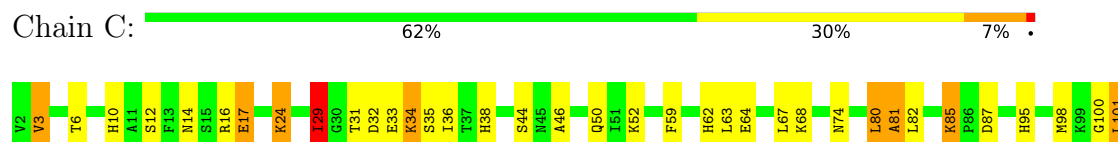
• Molecule 1: ANNEXIN XII

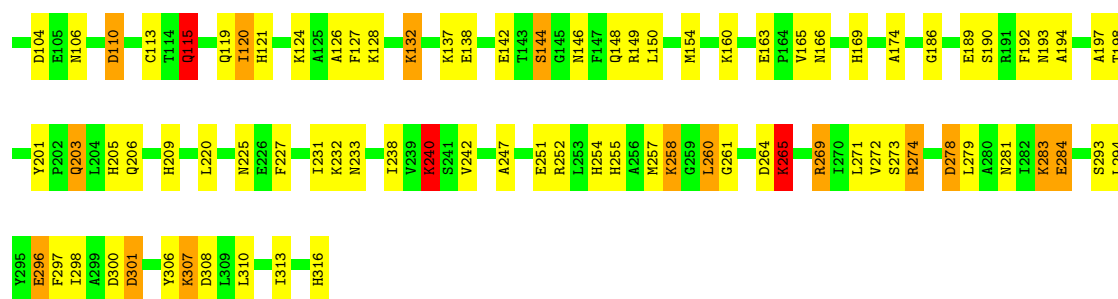


• Molecule 1: ANNEXIN XII



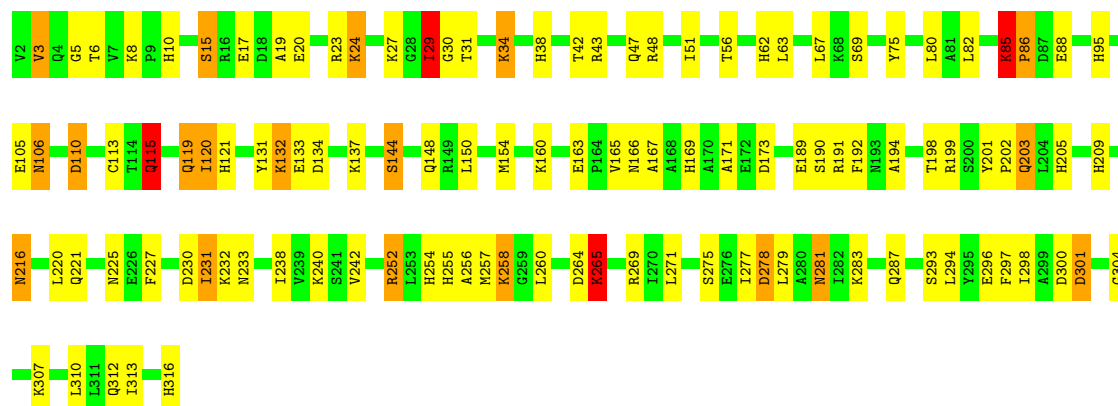
• Molecule 1: ANNEXIN XII





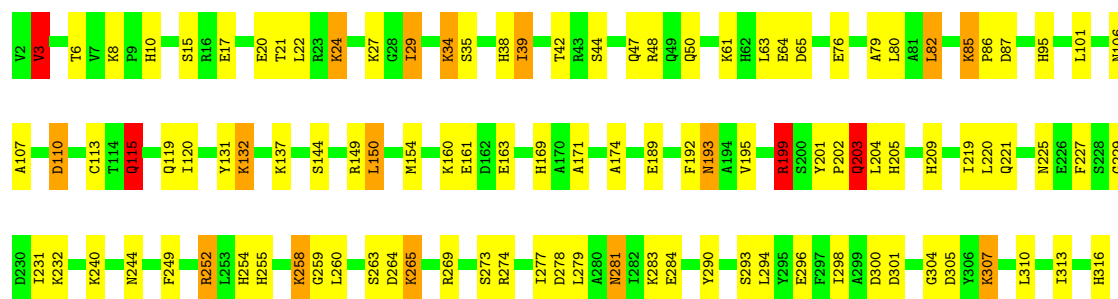
• Molecule 1: ANNEXIN XII

Chain D: 64% 29% 6% •



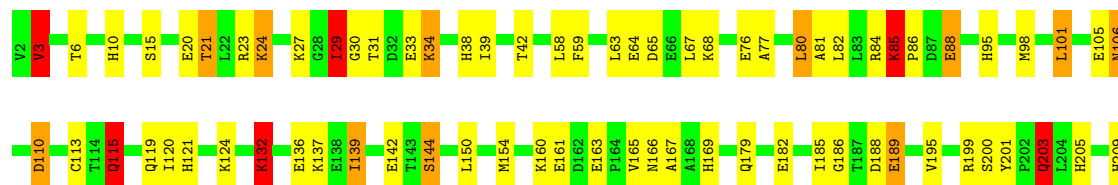
• Molecule 1: ANNEXIN XII

Chain E: 66% 28% 5% •



• Molecule 1: ANNEXIN XII

Chain F: 64% 29% 5% •





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	71.20Å 179.20Å 100.70Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18252	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: 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	1.38	10/2498 (0.4%)	1.97	76/3361 (2.3%)
1	B	1.37	18/2498 (0.7%)	2.01	69/3361 (2.1%)
1	C	1.44	19/2498 (0.8%)	2.09	100/3361 (3.0%)
1	D	1.36	16/2498 (0.6%)	2.02	79/3361 (2.4%)
1	E	1.36	14/2498 (0.6%)	2.03	88/3361 (2.6%)
1	F	1.41	15/2498 (0.6%)	2.05	74/3361 (2.2%)
All	All	1.39	92/14988 (0.6%)	2.03	486/20166 (2.4%)

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

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

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	254	HIS	CD2-NE2	-8.08	1.28	1.37
1	D	62	HIS	CD2-NE2	-7.66	1.29	1.37
1	E	95	HIS	CD2-NE2	-7.48	1.29	1.37
1	D	169	HIS	CD2-NE2	-7.37	1.29	1.37
1	A	164	PRO	CA-CB	-7.37	1.45	1.54
1	F	88	GLU	CA-CB	-7.24	1.41	1.53
1	D	10	HIS	CD2-NE2	-7.06	1.30	1.37
1	B	209	HIS	CD2-NE2	-7.02	1.30	1.37
1	B	254	HIS	CD2-NE2	-7.01	1.30	1.37
1	D	95	HIS	CD2-NE2	-6.94	1.30	1.37
1	E	10	HIS	CD2-NE2	-6.93	1.30	1.37
1	B	88	GLU	CA-CB	-6.90	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	42	THR	CA-CB	6.89	1.62	1.53
1	A	169	HIS	CD2-NE2	-6.82	1.30	1.37
1	F	10	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	95	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	38	HIS	CD2-NE2	-6.58	1.30	1.37
1	E	254	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	205	HIS	CD2-NE2	-6.49	1.30	1.37
1	C	38	HIS	CG-ND1	-6.47	1.31	1.38
1	B	129	LEU	CA-CB	-6.46	1.43	1.53
1	C	209	HIS	CD2-NE2	-6.44	1.30	1.37
1	C	95	HIS	CD2-NE2	-6.43	1.30	1.37
1	F	169	HIS	CD2-NE2	-6.38	1.30	1.37
1	C	121	HIS	CD2-NE2	-6.37	1.30	1.37
1	C	38	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	316	HIS	CD2-NE2	-6.35	1.30	1.37
1	D	121	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	10	HIS	CD2-NE2	-6.31	1.30	1.37
1	B	42	THR	CA-CB	6.26	1.63	1.53
1	A	254	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	10	HIS	CD2-NE2	-6.23	1.30	1.37
1	D	209	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	38	HIS	CD2-NE2	-6.18	1.31	1.37
1	D	38	HIS	CD2-NE2	-6.14	1.31	1.37
1	E	209	HIS	CD2-NE2	-6.11	1.31	1.37
1	F	209	HIS	CD2-NE2	-6.09	1.31	1.37
1	F	316	HIS	CD2-NE2	-6.07	1.31	1.37
1	F	64	GLU	CA-CB	-6.02	1.44	1.53
1	F	205	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	10	HIS	CD2-NE2	-5.99	1.31	1.37
1	E	316	HIS	CD2-NE2	-5.99	1.31	1.37
1	D	254	HIS	CD2-NE2	-5.95	1.31	1.37
1	B	251	GLU	CA-CB	-5.92	1.44	1.53
1	F	95	HIS	CD2-NE2	-5.92	1.31	1.37
1	C	62	HIS	CG-ND1	-5.90	1.31	1.38
1	E	38	HIS	CD2-NE2	-5.87	1.31	1.37
1	F	77	ALA	CA-C	-5.87	1.45	1.52
1	B	15	SER	CA-CB	-5.85	1.44	1.53
1	D	88	GLU	CA-CB	-5.82	1.43	1.53
1	E	205	HIS	CD2-NE2	-5.79	1.31	1.37
1	C	298	ILE	CA-CB	5.78	1.61	1.54
1	A	255	HIS	CD2-NE2	-5.71	1.31	1.37
1	C	62	HIS	CD2-NE2	-5.71	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	17	GLU	CA-CB	-5.68	1.44	1.53
1	C	169	HIS	CD2-NE2	-5.67	1.31	1.37
1	C	35	SER	CA-CB	-5.66	1.44	1.53
1	B	62	HIS	CD2-NE2	-5.65	1.31	1.37
1	D	23	ARG	NE-CZ	5.63	1.39	1.33
1	C	316	HIS	CD2-NE2	-5.63	1.31	1.37
1	E	255	HIS	CD2-NE2	-5.61	1.31	1.37
1	E	64	GLU	CA-CB	-5.57	1.44	1.53
1	A	316	HIS	CD2-NE2	-5.50	1.31	1.37
1	D	316	HIS	CD2-NE2	-5.48	1.31	1.37
1	D	255	HIS	CB-CG	5.47	1.57	1.50
1	B	169	HIS	CD2-NE2	-5.46	1.31	1.37
1	C	255	HIS	CD2-NE2	-5.46	1.31	1.37
1	F	38	HIS	CD2-NE2	-5.45	1.31	1.37
1	E	169	HIS	CD2-NE2	-5.40	1.31	1.37
1	B	209	HIS	CG-ND1	-5.38	1.32	1.38
1	B	121	HIS	CD2-NE2	-5.32	1.31	1.37
1	E	254	HIS	CG-ND1	-5.27	1.32	1.38
1	C	166	ASN	CA-CB	-5.25	1.45	1.53
1	F	121	HIS	CD2-NE2	-5.24	1.32	1.37
1	C	254	HIS	CD2-NE2	-5.23	1.32	1.37
1	C	247	ALA	CA-CB	-5.22	1.44	1.53
1	C	10	HIS	CG-ND1	-5.21	1.32	1.38
1	C	64	GLU	CA-CB	-5.21	1.45	1.53
1	D	255	HIS	CG-CD2	5.21	1.41	1.35
1	A	129	LEU	CA-CB	-5.20	1.45	1.53
1	D	119	GLN	CA-CB	-5.20	1.45	1.53
1	F	254	HIS	CG-ND1	-5.18	1.32	1.38
1	F	255	HIS	CD2-NE2	-5.16	1.32	1.37
1	B	10	HIS	CG-ND1	-5.14	1.32	1.38
1	C	46	ALA	CA-CB	-5.14	1.44	1.53
1	D	121	HIS	CG-ND1	-5.09	1.32	1.38
1	E	10	HIS	CG-ND1	-5.08	1.32	1.38
1	A	121	HIS	CD2-NE2	-5.04	1.32	1.37
1	E	219	ILE	CA-CB	5.03	1.60	1.54
1	F	205	HIS	CG-ND1	-5.00	1.32	1.38
1	D	192	PHE	CA-CB	-5.00	1.45	1.53

All (486) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	203	GLN	OE1-CD-NE2	-14.70	107.90	122.60
1	B	203	GLN	OE1-CD-NE2	-12.63	109.97	122.60
1	D	203	GLN	OE1-CD-NE2	-10.77	111.83	122.60
1	F	304	GLY	O-C-N	10.68	134.03	122.60
1	C	106	ASN	OD1-CG-ND2	-10.39	112.21	122.60
1	F	106	ASN	CB-CG-ND2	10.17	131.65	116.40
1	E	193	ASN	CA-CB-CG	10.16	122.76	112.60
1	C	106	ASN	CB-CG-ND2	10.15	131.62	116.40
1	D	277	ILE	CA-C-O	-9.95	112.25	120.70
1	B	300	ASP	CA-CB-CG	9.72	122.32	112.60
1	D	106	ASN	OD1-CG-ND2	-9.68	112.92	122.60
1	D	106	ASN	CB-CG-ND2	9.26	130.28	116.40
1	E	203	GLN	OE1-CD-NE2	-9.11	113.50	122.60
1	D	300	ASP	CA-CB-CG	9.04	121.64	112.60
1	A	313	ILE	CB-CG1-CD1	-8.97	94.97	113.80
1	E	300	ASP	CA-CB-CG	8.96	121.56	112.60
1	C	205	HIS	CB-CG-CD2	-8.65	119.95	131.20
1	E	106	ASN	CB-CG-ND2	8.61	129.32	116.40
1	F	203	GLN	CG-CD-NE2	8.47	129.10	116.40
1	A	106	ASN	CB-CG-ND2	8.45	129.08	116.40
1	B	201	TYR	CA-C-N	8.21	127.78	119.24
1	B	201	TYR	C-N-CA	8.21	127.78	119.24
1	B	203	GLN	CG-CD-NE2	8.15	128.63	116.40
1	D	312	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	C	265	LYS	N-CA-C	-8.12	102.51	111.36
1	E	203	GLN	CG-CD-NE2	8.08	128.52	116.40
1	E	281	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	A	203	GLN	OE1-CD-NE2	-7.92	114.67	122.60
1	E	174	ALA	N-CA-C	-7.92	102.64	111.28
1	B	233	ASN	OD1-CG-ND2	-7.92	114.68	122.60
1	D	173	ASP	CA-CB-CG	7.91	120.51	112.60
1	E	106	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	E	201	TYR	CA-C-N	7.68	128.08	119.32
1	E	201	TYR	C-N-CA	7.68	128.08	119.32
1	C	225	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	B	193	ASN	CA-CB-CG	7.61	120.21	112.60
1	B	313	ILE	CB-CG1-CD1	-7.59	97.86	113.80
1	F	273	SER	N-CA-C	7.56	120.40	111.71
1	A	300	ASP	CA-CB-CG	7.54	120.14	112.60
1	E	225	ASN	CA-CB-CG	7.53	120.13	112.60
1	B	110	ASP	CA-CB-CG	7.52	120.12	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	TYR	CA-C-N	7.51	127.38	119.05
1	D	201	TYR	C-N-CA	7.51	127.38	119.05
1	C	110	ASP	CA-CB-CG	7.43	120.03	112.60
1	F	167	ALA	CA-C-O	-7.41	112.70	120.55
1	C	197	ALA	N-CA-C	7.41	121.56	112.23
1	E	269	ARG	CA-C-O	-7.38	113.00	120.90
1	C	205	HIS	CA-CB-CG	-7.35	106.45	113.80
1	F	203	GLN	CA-C-O	-7.35	112.76	120.55
1	A	110	ASP	CA-CB-CG	7.33	119.93	112.60
1	C	300	ASP	CA-CB-CG	7.31	119.91	112.60
1	B	278	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	198	THR	N-CA-C	7.27	122.44	113.50
1	E	115	GLN	N-CA-C	7.24	121.83	110.17
1	A	138	GLU	CA-C-O	-7.21	112.24	120.24
1	D	205	HIS	CB-CG-CD2	-7.20	121.84	131.20
1	C	190	SER	CA-CB-OG	7.17	125.43	111.10
1	C	193	ASN	CA-CB-CG	7.12	119.72	112.60
1	A	201	TYR	CA-C-N	7.12	126.38	118.97
1	A	201	TYR	C-N-CA	7.12	126.38	118.97
1	D	203	GLN	CG-CD-NE2	7.12	127.08	116.40
1	F	30	GLY	O-C-N	7.08	129.64	122.91
1	C	225	ASN	CB-CG-ND2	7.06	127.00	116.40
1	E	87	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	106	ASN	CB-CG-ND2	7.05	126.97	116.40
1	D	190	SER	CA-CB-OG	7.03	125.17	111.10
1	A	30	GLY	O-C-N	7.00	129.42	122.77
1	D	42	THR	N-CA-C	7.00	121.53	112.92
1	E	205	HIS	CA-CB-CG	-7.00	106.80	113.80
1	C	87	ASP	CA-C-N	6.98	130.20	120.29
1	C	87	ASP	C-N-CA	6.98	130.20	120.29
1	A	42	THR	N-CA-C	6.98	121.50	112.92
1	F	272	VAL	CA-C-O	-6.98	113.30	121.05
1	A	40	LEU	N-CA-C	6.96	118.52	111.07
1	A	8	LYS	CA-C-N	6.94	126.98	119.90
1	A	8	LYS	C-N-CA	6.94	126.98	119.90
1	C	10	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	F	10	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	A	98	MET	N-CA-C	6.93	119.86	111.40
1	C	233	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	A	265	LYS	N-CA-C	-6.92	103.82	111.36
1	C	52	LYS	N-CA-C	6.89	119.63	111.71
1	E	281	ASN	O-C-N	-6.86	114.96	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	79	ALA	O-C-N	-6.85	114.34	122.15
1	C	274	ARG	NE-CZ-NH2	6.85	125.37	119.20
1	F	85	LYS	N-CA-C	-6.85	100.63	110.08
1	C	87	ASP	O-C-N	-6.82	114.89	122.12
1	D	8	LYS	CA-C-N	6.82	126.86	119.90
1	D	8	LYS	C-N-CA	6.82	126.86	119.90
1	F	110	ASP	CA-CB-CG	6.82	119.42	112.60
1	F	205	HIS	CB-CG-CD2	-6.81	122.34	131.20
1	D	233	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	F	201	TYR	CA-C-N	6.77	126.02	118.97
1	F	201	TYR	C-N-CA	6.77	126.02	118.97
1	C	98	MET	N-CA-C	6.76	119.65	111.40
1	C	194	ALA	CA-C-O	-6.75	113.68	120.90
1	D	271	LEU	O-C-N	6.74	129.01	122.07
1	B	205	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	E	86	PRO	CA-C-N	6.70	129.80	120.29
1	E	86	PRO	C-N-CA	6.70	129.80	120.29
1	D	256	ALA	CA-C-O	6.69	127.64	120.55
1	D	216	ASN	CA-CB-CG	6.68	119.28	112.60
1	F	250	ALA	CA-C-O	6.67	127.64	120.10
1	A	86	PRO	CA-C-N	6.64	129.17	120.28
1	A	86	PRO	C-N-CA	6.64	129.17	120.28
1	A	316	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	117	ASN	OD1-CG-ND2	-6.62	115.97	122.60
1	E	265	LYS	N-CA-C	-6.62	103.99	111.14
1	C	169	HIS	CA-C-O	-6.58	113.92	120.70
1	C	233	ASN	CA-C-N	6.58	127.24	119.94
1	C	233	ASN	C-N-CA	6.58	127.24	119.94
1	F	144	SER	CA-CB-OG	6.56	124.23	111.10
1	D	106	ASN	CA-C-O	-6.55	113.47	120.42
1	D	205	HIS	CA-CB-CG	-6.55	107.25	113.80
1	B	54	ASP	CA-CB-CG	-6.54	106.06	112.60
1	D	144	SER	CA-CB-OG	6.53	124.17	111.10
1	D	313	ILE	CB-CG1-CD1	-6.53	100.10	113.80
1	D	298	ILE	N-CA-C	-6.49	104.43	110.53
1	F	244	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	C	203	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	B	59	PHE	N-CA-C	6.46	121.33	113.38
1	F	188	ASP	N-CA-C	-6.46	98.01	108.41
1	F	110	ASP	CB-CA-C	-6.46	99.70	110.68
1	F	313	ILE	CB-CG1-CD1	-6.46	100.24	113.80
1	F	257	MET	O-C-N	-6.44	114.29	122.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	273	SER	N-CA-C	6.40	119.07	111.71
1	E	161	GLU	N-CA-C	6.38	120.17	112.38
1	C	201	TYR	CA-C-N	6.37	126.12	119.05
1	C	201	TYR	C-N-CA	6.37	126.12	119.05
1	D	56	THR	O-C-N	-6.37	114.94	122.20
1	F	95	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	A	216	ASN	CA-CB-CG	6.35	118.95	112.60
1	E	38	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	C	67	LEU	O-C-N	-6.33	115.41	122.12
1	B	95	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	C	95	HIS	CB-CG-CD2	-6.32	122.98	131.20
1	D	231	ILE	CA-C-O	-6.32	114.15	120.85
1	F	195	VAL	O-C-N	-6.31	115.33	121.83
1	D	277	ILE	CB-CA-C	-6.30	106.35	111.71
1	D	304	GLY	O-C-N	6.30	129.35	122.60
1	B	192	PHE	CA-C-N	6.30	128.63	120.44
1	B	192	PHE	C-N-CA	6.30	128.63	120.44
1	B	232	LYS	N-CA-C	-6.30	103.94	111.69
1	B	225	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	D	265	LYS	N-CA-C	-6.26	104.37	111.07
1	A	169	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	C	149	ARG	CA-CB-CG	-6.24	101.61	114.10
1	F	67	LEU	O-C-N	-6.24	115.50	122.12
1	F	316	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	D	194	ALA	CA-C-O	-6.22	114.29	120.82
1	C	273	SER	N-CA-C	6.20	118.84	111.71
1	A	274	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	A	203	GLN	CG-CD-NE2	6.19	125.69	116.40
1	F	84	ARG	CB-CG-CD	-6.18	97.08	111.30
1	B	149	ARG	CA-CB-CG	-6.18	101.74	114.10
1	F	161	GLU	N-CA-C	6.17	120.37	112.34
1	B	87	ASP	CA-CB-CG	6.17	118.77	112.60
1	D	171	ALA	N-CA-C	6.17	118.08	111.36
1	E	110	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	198	THR	N-CA-C	6.16	121.07	113.50
1	E	15	SER	N-CA-C	6.15	118.79	111.71
1	E	290	TYR	N-CA-C	6.15	121.72	113.72
1	C	269	ARG	CA-C-O	-6.15	114.32	120.90
1	C	272	VAL	N-CA-C	-6.15	104.75	110.53
1	D	115	GLN	N-CA-C	6.15	120.09	110.32
1	A	52	LYS	N-CA-C	6.12	118.46	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	LYS	CB-CG-CD	-6.11	97.24	111.30
1	B	225	ASN	CA-CB-CG	6.11	118.71	112.60
1	C	190	SER	CB-CA-C	-6.11	101.03	110.81
1	A	115	GLN	N-CA-C	6.09	119.97	110.17
1	A	205	HIS	CB-CG-CD2	-6.09	123.29	131.20
1	C	272	VAL	CA-C-O	-6.08	114.30	121.05
1	A	205	HIS	CA-CB-CG	-6.06	107.74	113.80
1	B	8	LYS	CA-C-N	6.06	126.41	119.93
1	B	8	LYS	C-N-CA	6.06	126.41	119.93
1	B	85	LYS	N-CA-C	-6.06	101.95	109.64
1	A	17	GLU	CA-CB-CG	6.05	126.20	114.10
1	A	225	ASN	CB-CG-ND2	6.04	125.46	116.40
1	A	269	ARG	CD-NE-CZ	-6.04	115.95	124.40
1	E	65	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	105	GLU	CA-C-O	6.03	126.94	120.55
1	E	24	LYS	CG-CD-CE	6.03	125.17	111.30
1	A	95	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	E	273	SER	N-CA-C	6.02	118.80	111.82
1	D	191	ARG	N-CA-C	6.01	117.83	111.28
1	C	50	GLN	CA-C-O	-5.98	114.08	120.42
1	F	65	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	121	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	137	LYS	N-CA-C	-5.96	104.86	111.36
1	B	86	PRO	CA-C-N	5.96	128.26	120.28
1	B	86	PRO	C-N-CA	5.96	128.26	120.28
1	E	316	HIS	CB-CG-CD2	-5.96	123.46	131.20
1	F	139	ILE	N-CA-C	-5.96	104.71	110.72
1	A	192	PHE	CA-C-N	5.94	128.16	120.44
1	A	192	PHE	C-N-CA	5.94	128.16	120.44
1	C	110	ASP	CB-CA-C	-5.92	101.33	110.81
1	D	169	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	F	225	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	B	273	SER	N-CA-C	5.89	118.65	111.82
1	E	29	ILE	N-CA-C	-5.89	101.43	109.55
1	A	20	GLU	CB-CG-CD	5.88	122.60	112.60
1	D	316	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	A	25	ALA	O-C-N	-5.87	115.35	122.22
1	C	283	LYS	CA-C-O	-5.86	114.34	120.55
1	C	81	ALA	CA-C-O	5.86	126.95	120.63
1	F	179	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	C	278	ASP	CA-CB-CG	5.84	118.44	112.60
1	F	98	MET	N-CA-C	5.83	120.44	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	205	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	E	85	LYS	N-CA-C	-5.83	102.24	109.64
1	C	85	LYS	CA-C-N	5.83	125.52	119.05
1	C	85	LYS	C-N-CA	5.83	125.52	119.05
1	E	61	LYS	O-C-N	-5.83	116.51	123.27
1	C	201	TYR	O-C-N	-5.82	114.63	121.32
1	F	300	ASP	CB-CA-C	-5.81	101.02	110.79
1	A	146	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	F	256	ALA	CA-C-O	5.80	126.64	119.97
1	B	290	TYR	N-CA-C	5.79	121.24	113.72
1	D	10	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	106	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	C	10	HIS	CB-CG-ND1	5.77	131.35	122.70
1	E	277	ILE	CB-CA-C	-5.77	106.81	111.71
1	C	126	ALA	CA-C-O	-5.76	114.40	120.63
1	C	203	GLN	CG-CD-NE2	5.76	125.05	116.40
1	B	32	ASP	CA-C-O	5.76	127.27	120.70
1	C	32	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	268	ILE	N-CA-C	-5.75	105.12	110.53
1	B	309	LEU	CA-C-O	-5.75	114.75	121.07
1	D	24	LYS	CG-CD-CE	5.75	124.52	111.30
1	A	27	LYS	CB-CG-CD	5.74	124.51	111.30
1	F	279	LEU	N-CA-C	-5.74	105.54	112.54
1	F	29	ILE	N-CA-C	-5.74	101.63	109.55
1	C	29	ILE	N-CA-C	-5.73	101.64	109.55
1	F	225	ASN	CA-CB-CG	5.73	118.33	112.60
1	B	308	ASP	N-CA-C	5.73	117.33	111.14
1	B	209	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	C	169	HIS	CB-CG-CD2	-5.72	123.77	131.20
1	E	249	PHE	CA-CB-CG	-5.71	108.09	113.80
1	B	117	ASN	O-C-N	5.71	128.26	122.09
1	D	15	SER	CA-CB-OG	5.70	122.50	111.10
1	E	195	VAL	O-C-N	-5.70	115.97	121.90
1	C	271	LEU	O-C-N	5.70	128.16	122.12
1	D	252	ARG	CG-CD-NE	5.70	124.53	112.00
1	A	314	THR	N-CA-C	5.69	117.56	111.36
1	E	82	LEU	N-CA-CB	-5.68	101.48	110.28
1	F	132	LYS	O-C-N	-5.68	115.04	122.59
1	C	148	GLN	N-CA-C	-5.67	105.10	111.28
1	E	171	ALA	N-CA-C	5.67	117.14	111.07
1	D	20	GLU	CB-CG-CD	5.67	122.24	112.60
1	F	185	ILE	CA-C-O	-5.67	113.69	120.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	LYS	CB-CG-CD	5.66	124.32	111.30
1	D	110	ASP	CB-CA-C	-5.66	101.39	110.79
1	D	225	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	B	27	LYS	CB-CG-CD	5.66	124.31	111.30
1	E	50	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	C	121	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	C	115	GLN	N-CA-C	5.65	119.27	110.17
1	E	85	LYS	CA-C-N	5.65	125.50	119.28
1	E	85	LYS	C-N-CA	5.65	125.50	119.28
1	F	259	GLY	O-C-N	5.64	129.84	122.96
1	D	301	ASP	OD1-CG-OD2	-5.64	109.37	122.90
1	D	225	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	225	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	87	ASP	CA-CB-CG	5.62	118.22	112.60
1	E	169	HIS	CB-CG-CD2	-5.62	123.90	131.20
1	B	169	HIS	CA-C-O	-5.61	114.02	120.24
1	A	85	LYS	O-C-N	-5.60	115.53	121.30
1	C	316	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	D	269	ARG	CA-C-O	-5.60	114.91	120.90
1	E	313	ILE	CB-CG1-CD1	-5.60	102.04	113.80
1	E	304	GLY	O-C-N	5.59	128.58	122.60
1	E	229	GLY	O-C-N	5.59	128.82	122.62
1	B	24	LYS	CG-CD-CE	5.58	124.13	111.30
1	E	307	LYS	CA-C-O	-5.57	114.94	120.90
1	C	148	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	124	LYS	N-CA-C	5.57	117.03	111.07
1	A	303	SER	N-CA-C	5.56	115.63	108.34
1	E	17	GLU	CA-CB-CG	5.55	125.19	114.10
1	D	19	ALA	N-CA-C	-5.54	105.32	111.36
1	D	264	ASP	CA-C-N	5.54	127.64	120.44
1	D	264	ASP	C-N-CA	5.54	127.64	120.44
1	D	67	LEU	CA-C-O	-5.53	114.55	120.42
1	C	174	ALA	CA-C-O	5.53	126.41	120.55
1	D	29	ILE	N-CA-C	-5.53	101.92	109.55
1	D	167	ALA	N-CA-C	5.52	116.97	111.07
1	C	104	ASP	N-CA-C	-5.51	96.87	107.57
1	F	105	GLU	CA-C-O	5.51	126.58	120.63
1	F	136	GLU	N-CA-C	-5.50	105.36	111.36
1	F	205	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	205	HIS	CA-CB-CG	-5.50	108.30	113.80
1	A	271	LEU	O-C-N	5.49	128.02	122.09
1	F	106	ASN	N-CA-C	5.49	118.18	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	LYS	CG-CD-CE	5.48	123.90	111.30
1	A	173	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	254	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	E	27	LYS	CB-CG-CD	5.48	123.90	111.30
1	C	144	SER	CA-CB-OG	5.47	122.05	111.10
1	E	252	ARG	CG-CD-NE	5.47	124.03	112.00
1	B	316	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	A	10	HIS	CB-CG-CD2	-5.46	124.09	131.20
1	D	17	GLU	N-CA-CB	-5.46	102.07	110.16
1	D	86	PRO	CA-C-N	5.46	128.05	120.29
1	D	86	PRO	C-N-CA	5.46	128.05	120.29
1	E	48	ARG	N-CA-C	-5.45	105.34	111.28
1	E	3	VAL	N-CA-C	-5.45	100.54	108.17
1	A	304	GLY	O-C-N	5.43	128.25	122.60
1	B	39	ILE	N-CA-C	5.42	115.63	110.53
1	A	65	ASP	CA-CB-CG	5.42	118.02	112.60
1	E	199	ARG	CA-C-O	-5.42	115.24	121.47
1	B	240	LYS	CA-C-O	-5.41	114.78	120.63
1	C	87	ASP	CA-C-O	5.41	126.29	120.55
1	D	85	LYS	O-C-N	-5.41	115.73	121.30
1	F	115	GLN	N-CA-C	5.41	118.53	110.52
1	E	254	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	C	255	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	E	209	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	D	281	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	F	221	GLN	CA-C-O	-5.40	115.15	120.82
1	E	8	LYS	CA-C-N	5.40	125.70	119.93
1	E	8	LYS	C-N-CA	5.40	125.70	119.93
1	D	198	THR	N-CA-C	5.39	119.99	113.41
1	D	287	GLN	OE1-CD-NE2	-5.39	117.20	122.60
1	E	244	ASN	CA-C-O	5.39	125.54	120.09
1	A	84	ARG	NE-CZ-NH2	-5.38	114.35	119.20
1	E	64	GLU	N-CA-C	5.38	116.83	111.07
1	B	167	ALA	N-CA-C	5.38	117.15	111.28
1	E	149	ARG	CA-CB-CG	-5.38	103.33	114.10
1	F	189	GLU	CA-C-O	-5.38	114.72	120.42
1	A	29	ILE	N-CA-C	-5.38	102.13	109.55
1	F	252	ARG	CA-C-N	5.38	127.48	120.28
1	F	252	ARG	C-N-CA	5.38	127.48	120.28
1	D	202	PRO	CA-N-CD	-5.37	104.48	112.00
1	F	286	PHE	CA-C-N	5.37	127.79	120.54
1	F	286	PHE	C-N-CA	5.37	127.79	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	225	ASN	CB-CG-ND2	5.37	124.45	116.40
1	B	265	LYS	N-CA-C	-5.36	105.33	111.07
1	B	42	THR	N-CA-C	5.36	119.79	112.88
1	E	263	SER	CA-C-N	5.36	127.99	120.28
1	E	263	SER	C-N-CA	5.36	127.99	120.28
1	B	139	ILE	N-CA-C	-5.35	105.50	110.53
1	C	257	MET	O-C-N	-5.35	115.65	122.34
1	C	16	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	D	233	ASN	CB-CG-ND2	5.35	124.42	116.40
1	C	233	ASN	CB-CG-ND2	5.34	124.41	116.40
1	C	260	LEU	CD1-CG-CD2	-5.34	99.05	110.80
1	B	206	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	B	227	PHE	N-CA-C	5.33	118.43	109.95
1	D	297	PHE	N-CA-C	5.33	116.77	111.07
1	D	225	ASN	CB-CG-ND2	5.33	124.39	116.40
1	C	44	SER	N-CA-C	-5.33	103.66	110.53
1	D	257	MET	CA-CB-CG	-5.33	103.44	114.10
1	D	192	PHE	CA-C-N	5.33	128.19	120.79
1	D	192	PHE	C-N-CA	5.33	128.19	120.79
1	A	59	PHE	N-CA-C	5.33	120.79	113.97
1	C	205	HIS	CB-CG-ND1	5.32	130.68	122.70
1	C	296	GLU	CA-CB-CG	5.32	124.74	114.10
1	A	225	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	E	259	GLY	O-C-N	5.32	128.29	122.60
1	F	115	GLN	N-CA-CB	-5.32	101.96	110.46
1	F	290	TYR	N-CA-C	5.31	120.62	113.72
1	A	110	ASP	CB-CA-C	-5.31	99.86	110.42
1	C	264	ASP	CA-C-N	5.30	127.82	120.29
1	C	264	ASP	C-N-CA	5.30	127.82	120.29
1	E	131	TYR	CA-C-O	-5.30	112.92	119.18
1	B	225	ASN	CB-CG-ND2	5.29	124.34	116.40
1	F	77	ALA	CA-C-O	-5.29	115.25	120.70
1	C	261	GLY	O-C-N	5.29	128.50	123.05
1	A	284	GLU	CB-CG-CD	5.29	121.59	112.60
1	F	58	LEU	O-C-N	-5.29	116.62	122.07
1	F	214	ILE	O-C-N	-5.29	117.05	122.23
1	C	240	LYS	CA-C-O	-5.29	114.95	120.55
1	C	313	ILE	CB-CG1-CD1	-5.28	102.71	113.80
1	D	105	GLU	CA-C-O	5.28	126.33	120.63
1	E	76	GLU	CA-C-N	5.28	127.62	120.44
1	E	76	GLU	C-N-CA	5.28	127.62	120.44
1	B	38	HIS	CA-C-O	-5.27	114.83	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	GLN	CA-C-O	-5.26	115.27	120.90
1	D	278	ASP	CA-CB-CG	5.26	117.86	112.60
1	F	264	ASP	CA-C-N	5.26	127.59	120.44
1	F	264	ASP	C-N-CA	5.26	127.59	120.44
1	F	21	THR	O-C-N	-5.25	116.55	122.12
1	B	216	ASN	CA-CB-CG	5.25	117.85	112.60
1	F	269	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	D	221	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	128	LYS	CA-CB-CG	5.24	124.58	114.10
1	A	272	VAL	O-C-N	-5.24	116.45	121.90
1	C	301	ASP	OD1-CG-OD2	-5.23	110.34	122.90
1	E	22	LEU	O-C-N	-5.23	116.18	122.15
1	A	41	ALA	CA-C-O	-5.23	113.96	119.97
1	C	68	LYS	CB-CG-CD	-5.23	99.28	111.30
1	A	39	ILE	N-CA-C	5.22	115.99	110.72
1	B	85	LYS	CA-C-N	5.22	124.40	118.97
1	B	85	LYS	C-N-CA	5.22	124.40	118.97
1	A	45	ASN	CB-CG-ND2	5.22	124.23	116.40
1	E	278	ASP	CA-CB-CG	5.22	117.82	112.60
1	E	313	ILE	N-CA-C	-5.22	105.41	110.42
1	C	209	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	C	12	SER	CA-C-O	5.21	128.54	122.03
1	C	192	PHE	CA-CB-CG	-5.21	108.59	113.80
1	F	85	LYS	CA-C-N	5.20	124.82	119.05
1	F	85	LYS	C-N-CA	5.20	124.82	119.05
1	B	29	ILE	N-CA-C	-5.20	102.89	109.80
1	A	206	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	C	85	LYS	N-CA-C	-5.19	103.24	109.83
1	E	252	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	41	ALA	CA-C-O	-5.18	113.00	119.38
1	A	67	LEU	CA-C-O	-5.18	115.06	120.55
1	C	17	GLU	N-CA-CB	-5.18	102.50	110.16
1	D	205	HIS	CB-CG-ND1	5.17	130.46	122.70
1	C	146	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	F	27	LYS	CB-CG-CD	5.17	123.19	111.30
1	E	20	GLU	CB-CG-CD	5.17	121.38	112.60
1	E	35	SER	N-CA-C	5.17	116.99	111.36
1	D	312	GLN	CG-CD-NE2	5.17	124.15	116.40
1	B	169	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	C	138	GLU	CA-C-O	-5.15	114.96	120.42
1	F	142	GLU	CB-CG-CD	5.15	121.36	112.60
1	E	39	ILE	N-CA-C	5.15	115.36	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ASP	OD1-CG-OD2	-5.14	110.55	122.90
1	C	87	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	74	ASN	N-CA-C	5.14	117.78	111.82
1	E	149	ARG	N-CA-C	5.14	117.62	111.71
1	E	107	ALA	CB-CA-C	-5.13	102.12	110.85
1	E	298	ILE	N-CA-C	-5.13	105.70	110.53
1	E	44	SER	N-CA-C	-5.13	103.91	110.53
1	E	225	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	C	190	SER	N-CA-CB	5.13	117.58	109.94
1	C	284	GLU	N-CA-C	-5.13	105.60	111.14
1	C	127	PHE	CA-C-N	5.12	127.14	120.28
1	C	127	PHE	C-N-CA	5.12	127.14	120.28
1	D	75	TYR	CA-C-O	-5.12	115.12	120.55
1	A	36	ILE	N-CA-C	-5.12	105.86	110.82
1	F	106	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	C	142	GLU	CB-CG-CD	5.11	121.29	112.60
1	F	84	ARG	CA-CB-CG	5.11	124.32	114.10
1	B	277	ILE	CB-CA-C	-5.11	107.37	111.71
1	E	255	HIS	CB-CG-CD2	-5.10	124.56	131.20
1	D	134	ASP	CA-C-O	-5.10	114.87	120.43
1	F	42	THR	N-CA-C	5.10	118.81	112.59
1	B	17	GLU	N-CA-CB	-5.10	102.62	110.16
1	B	199	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	E	47	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	98	MET	CB-CA-C	-5.08	102.25	110.79
1	C	80	LEU	CA-C-N	5.08	127.34	120.38
1	C	80	LEU	C-N-CA	5.08	127.34	120.38
1	B	269	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	257	MET	CA-CB-CG	-5.08	103.94	114.10
1	A	233	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	B	185	ILE	CA-CB-CG1	-5.08	101.77	110.40
1	A	39	ILE	CA-CB-CG1	-5.08	101.77	110.40
1	B	230	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	230	ASP	N-CA-C	5.07	117.20	111.11
1	B	269	ARG	CA-C-O	-5.07	115.48	120.90
1	F	86	PRO	CA-C-N	5.07	128.01	120.31
1	F	86	PRO	C-N-CA	5.07	128.01	120.31
1	A	254	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	D	254	HIS	CB-CG-CD2	-5.06	124.63	131.20
1	E	192	PHE	CA-C-N	5.06	127.01	120.44
1	E	192	PHE	C-N-CA	5.06	127.01	120.44
1	E	264	ASP	CA-C-N	5.05	127.31	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	264	ASP	C-N-CA	5.05	127.31	120.44
1	B	310	LEU	CA-C-O	-5.05	115.49	120.90
1	E	269	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	A	127	PHE	O-C-N	-5.04	116.87	122.07
1	D	30	GLY	O-C-N	5.04	128.25	123.05
1	C	59	PHE	N-CA-C	5.04	120.06	113.30
1	D	277	ILE	O-C-N	5.04	125.68	121.85
1	D	95	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	C	306	TYR	O-C-N	5.03	127.32	122.09
1	B	233	ASN	CB-CG-ND2	5.03	123.94	116.40
1	A	85	LYS	CA-C-N	5.03	124.63	119.05
1	A	85	LYS	C-N-CA	5.03	124.63	119.05
1	E	225	ASN	CB-CG-ND2	5.02	123.93	116.40
1	E	249	PHE	CA-C-O	-5.02	115.10	120.42
1	A	149	ARG	CA-CB-CG	-5.02	104.06	114.10
1	C	36	ILE	N-CA-CB	-5.02	104.14	110.57
1	C	106	ASN	N-CA-C	5.02	117.64	111.82
1	F	68	LYS	CG-CD-CE	5.02	122.85	111.30
1	C	128	LYS	CA-C-N	5.01	127.27	120.65
1	C	128	LYS	C-N-CA	5.01	127.27	120.65
1	F	3	VAL	N-CA-C	-5.01	101.16	108.17
1	E	202	PRO	CA-N-CD	-5.00	104.99	112.00
1	A	24	LYS	CA-C-O	-5.00	115.25	120.55
1	F	106	ASN	CB-CG-OD1	-5.00	110.79	120.80
1	C	100	GLY	N-CA-C	-5.00	106.79	112.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	LYS	Mainchain

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	2462	576	2450	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2462	576	2450	28	0
1	C	2462	576	2450	37	0
1	D	2462	576	2450	32	0
1	E	2462	576	2450	26	0
1	F	2462	576	2450	39	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
All	All	14796	3456	14700	194	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 7.

All (194) 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:293:SER:HB3	1:F:296:GLU:HG3	1.67	0.76
1:D:160:LYS:HD3	1:D:163:GLU:HB2	1.69	0.73
1:B:265:LYS:HD2	1:B:265:LYS:H	1.54	0.72
1:C:160:LYS:HD3	1:C:163:GLU:HB2	1.72	0.71
1:D:165:VAL:HA	1:D:203:GLN:HE21	1.55	0.70
1:A:265:LYS:HD2	1:A:265:LYS:H	1.57	0.70
1:D:265:LYS:H	1:D:265:LYS:HD2	1.56	0.69
1:C:258:LYS:HZ3	1:C:297:PHE:HE1	1.40	0.69
1:B:160:LYS:HD3	1:B:163:GLU:HB2	1.74	0.69
1:F:265:LYS:H	1:F:265:LYS:HD2	1.58	0.68
1:B:258:LYS:HZ2	1:B:258:LYS:HA	1.58	0.67
1:D:283:LYS:HG2	1:D:294:LEU:HD23	1.78	0.66
1:D:165:VAL:HA	1:D:203:GLN:NE2	2.10	0.66
1:A:293:SER:HB3	1:A:296:GLU:HG3	1.78	0.65
1:F:160:LYS:HD3	1:F:163:GLU:HB2	1.78	0.65
1:C:238:ILE:O	1:C:242:VAL:HG23	1.97	0.64
1:F:113:CYS:HA	1:F:154:MET:HE2	1.80	0.64
1:A:160:LYS:HD3	1:A:163:GLU:HB2	1.78	0.64
1:E:160:LYS:HD3	1:E:163:GLU:HB2	1.80	0.64
1:E:3:VAL:HA	1:E:281:ASN:OD1	1.98	0.63
1:C:265:LYS:HD2	1:C:265:LYS:H	1.62	0.63
1:F:34:LYS:HD2	1:F:34:LYS:H	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:LYS:H	1:E:265:LYS:HD2	1.65	0.61
1:C:258:LYS:HA	1:C:258:LYS:NZ	2.15	0.61
1:E:113:CYS:HA	1:E:154:MET:HE2	1.83	0.61
1:B:203:GLN:HE21	1:B:203:GLN:HA	1.66	0.60
1:A:89:PHE:O	1:A:93:GLN:HG2	2.02	0.60
1:C:258:LYS:HA	1:C:258:LYS:CE	2.32	0.59
1:F:258:LYS:HA	1:F:258:LYS:NZ	2.16	0.59
1:F:258:LYS:HA	1:F:258:LYS:HZ2	1.67	0.59
1:D:113:CYS:HA	1:D:154:MET:HE2	1.83	0.59
1:E:293:SER:HB3	1:E:296:GLU:HG3	1.84	0.59
1:A:265:LYS:HD2	1:A:265:LYS:N	2.18	0.58
1:A:165:VAL:HA	1:A:203:GLN:HE21	1.69	0.58
1:F:258:LYS:HA	1:F:258:LYS:CE	2.33	0.58
1:A:166:ASN:H	1:A:203:GLN:NE2	2.02	0.57
1:B:258:LYS:HA	1:B:258:LYS:NZ	2.19	0.57
1:E:258:LYS:HA	1:E:258:LYS:CE	2.33	0.57
1:E:258:LYS:HA	1:E:258:LYS:HZ2	1.70	0.57
1:F:34:LYS:HD2	1:F:34:LYS:N	2.20	0.57
1:C:113:CYS:HA	1:C:154:MET:HE2	1.85	0.56
1:B:293:SER:HB3	1:B:296:GLU:HG3	1.88	0.55
1:F:203:GLN:HE21	1:F:203:GLN:HA	1.72	0.55
1:E:283:LYS:HG2	1:E:294:LEU:HD23	1.88	0.55
1:C:34:LYS:H	1:C:34:LYS:HD2	1.71	0.54
1:B:6:THR:OG1	1:B:279:LEU:HD23	2.08	0.54
1:C:6:THR:OG1	1:C:279:LEU:HD23	2.08	0.54
1:C:293:SER:HB3	1:C:296:GLU:HG3	1.90	0.54
1:E:203:GLN:HA	1:E:203:GLN:HE21	1.73	0.54
1:D:258:LYS:NZ	1:D:258:LYS:HA	2.22	0.54
1:C:165:VAL:HA	1:C:203:GLN:NE2	2.23	0.53
1:E:34:LYS:HD2	1:E:34:LYS:H	1.74	0.53
1:E:258:LYS:HA	1:E:258:LYS:NZ	2.23	0.53
1:C:203:GLN:HE21	1:C:203:GLN:HA	1.73	0.53
1:C:115:GLN:HG3	1:C:119:GLN:HB2	1.89	0.53
1:A:258:LYS:HA	1:A:258:LYS:CE	2.39	0.53
1:D:258:LYS:HA	1:D:258:LYS:CE	2.39	0.52
1:C:150:LEU:HD22	1:C:231:ILE:HD12	1.92	0.52
1:B:39:ILE:O	1:B:43:ARG:HD3	2.09	0.52
1:D:166:ASN:H	1:D:203:GLN:NE2	2.07	0.52
1:D:6:THR:OG1	1:D:279:LEU:HD23	2.10	0.51
1:B:113:CYS:HA	1:B:154:MET:HE2	1.92	0.51
1:F:29:ILE:HD12	1:F:29:ILE:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:GLY:HA3	1:D:275:SER:O	2.11	0.50
1:B:283:LYS:HG2	1:B:294:LEU:HD23	1.92	0.50
1:A:258:LYS:HA	1:A:258:LYS:NZ	2.26	0.49
1:B:258:LYS:HA	1:B:258:LYS:CE	2.42	0.49
1:C:34:LYS:HD2	1:C:34:LYS:N	2.27	0.49
1:F:33:GLU:HB2	1:F:34:LYS:NZ	2.27	0.49
1:C:165:VAL:HA	1:C:203:GLN:HE21	1.77	0.49
1:C:258:LYS:HA	1:C:258:LYS:HZ2	1.76	0.49
1:C:33:GLU:HB2	1:C:34:LYS:NZ	2.28	0.49
1:D:293:SER:HB3	1:D:296:GLU:HG3	1.93	0.49
1:A:115:GLN:HG3	1:A:119:GLN:HB2	1.94	0.49
1:C:283:LYS:HG2	1:C:294:LEU:HD23	1.95	0.48
1:A:111:ILE:O	1:A:115:GLN:NE2	2.45	0.48
1:A:113:CYS:HA	1:A:154:MET:HE2	1.95	0.48
1:D:34:LYS:HD2	1:D:34:LYS:H	1.78	0.48
1:D:166:ASN:H	1:D:203:GLN:HE22	1.61	0.48
1:F:6:THR:OG1	1:F:279:LEU:HD23	2.13	0.48
1:A:165:VAL:HA	1:A:203:GLN:NE2	2.28	0.48
1:D:29:ILE:H	1:D:29:ILE:HD12	1.79	0.48
1:F:182:GLU:OE1	1:F:217:LYS:NZ	2.47	0.48
1:E:150:LEU:HD22	1:E:231:ILE:HD12	1.95	0.48
1:B:165:VAL:HA	1:B:203:GLN:NE2	2.29	0.47
1:D:150:LEU:HD22	1:D:231:ILE:HD12	1.96	0.47
1:A:6:THR:OG1	1:A:279:LEU:HD23	2.14	0.47
1:C:281:ASN:O	1:C:284:GLU:HG2	2.15	0.47
1:A:29:ILE:HD12	1:A:29:ILE:H	1.80	0.47
1:C:3:VAL:HA	1:C:281:ASN:OD1	2.14	0.47
1:D:34:LYS:HD2	1:D:34:LYS:N	2.29	0.47
1:D:3:VAL:HG23	1:D:278:ASP:HB3	1.97	0.47
1:F:166:ASN:H	1:F:203:GLN:NE2	2.13	0.47
1:A:189:GLU:HG2	1:A:227:PHE:HE1	1.79	0.47
1:D:120:ILE:HD13	1:D:120:ILE:HA	1.75	0.47
1:D:258:LYS:HA	1:D:258:LYS:HZ2	1.78	0.47
1:F:85:LYS:HZ2	1:F:88:GLU:HG3	1.79	0.46
1:B:189:GLU:HG2	1:B:227:PHE:HE1	1.81	0.46
1:D:3:VAL:HA	1:D:281:ASN:OD1	2.16	0.46
1:C:29:ILE:H	1:C:29:ILE:HD12	1.81	0.46
1:A:206:GLN:O	1:A:210:GLU:HG2	2.17	0.45
1:E:29:ILE:HD12	1:E:29:ILE:H	1.82	0.45
1:F:189:GLU:HG2	1:F:227:PHE:HE1	1.81	0.45
1:A:33:GLU:HB2	1:A:34:LYS:HZ2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HH12	1:C:163:GLU:CD	2.24	0.45
1:B:269:ARG:HH11	1:B:269:ARG:HD3	1.62	0.45
1:F:3:VAL:HA	1:F:281:ASN:OD1	2.16	0.45
1:A:281:ASN:O	1:A:284:GLU:HG2	2.16	0.45
1:F:238:ILE:O	1:F:242:VAL:HG23	2.17	0.45
1:E:34:LYS:HD2	1:E:34:LYS:N	2.32	0.45
1:F:165:VAL:HA	1:F:203:GLN:NE2	2.32	0.45
1:A:33:GLU:HB2	1:A:34:LYS:NZ	2.32	0.45
1:A:166:ASN:H	1:A:203:GLN:HE22	1.63	0.44
1:F:76:GLU:O	1:F:80:LEU:HB2	2.17	0.44
1:D:115:GLN:HG3	1:D:119:GLN:CB	2.47	0.44
1:D:189:GLU:HG2	1:D:227:PHE:HE1	1.82	0.44
1:D:115:GLN:HG3	1:D:119:GLN:HB2	1.99	0.44
1:A:313:ILE:HD13	1:A:313:ILE:HG21	1.72	0.44
1:B:120:ILE:HD13	1:B:120:ILE:HA	1.81	0.44
1:B:307:LYS:NZ	1:B:308:ASP:OD1	2.51	0.44
1:C:120:ILE:HD13	1:C:120:ILE:HA	1.90	0.44
1:E:110:ASP:OD2	1:E:252:ARG:NH1	2.50	0.44
1:A:150:LEU:HD22	1:A:231:ILE:HD12	2.00	0.44
1:B:150:LEU:HD22	1:B:231:ILE:HD12	2.00	0.44
1:F:240:LYS:NZ	1:F:251:GLU:OE1	2.49	0.44
1:B:45:ASN:O	1:B:49:GLN:HG2	2.17	0.43
1:F:120:ILE:HD13	1:F:120:ILE:HA	1.80	0.43
1:F:166:ASN:H	1:F:203:GLN:HE22	1.66	0.43
1:A:258:LYS:HA	1:A:258:LYS:HZ1	1.83	0.43
1:A:195:VAL:O	1:A:199:ARG:HG2	2.18	0.43
1:C:33:GLU:HB2	1:C:34:LYS:HZ2	1.83	0.43
1:D:47:GLN:O	1:D:51:ILE:HG13	2.19	0.43
1:B:23:ARG:HG3	1:B:59:PHE:CZ	2.54	0.43
1:A:110:ASP:OD2	1:A:252:ARG:NH1	2.52	0.43
1:B:29:ILE:HD12	1:B:29:ILE:H	1.84	0.43
1:C:240:LYS:NZ	1:C:251:GLU:OE2	2.51	0.43
1:F:307:LYS:NZ	1:F:308:ASP:OD1	2.52	0.43
1:E:115:GLN:HG3	1:E:119:GLN:HB2	2.00	0.42
1:F:23:ARG:HG3	1:F:59:PHE:CZ	2.54	0.42
1:F:33:GLU:HB2	1:F:34:LYS:HZ3	1.84	0.42
1:F:115:GLN:HG3	1:F:119:GLN:HB2	2.00	0.42
1:F:281:ASN:O	1:F:284:GLU:HG2	2.19	0.42
1:A:163:GLU:HA	1:A:164:PRO:HD3	1.79	0.42
1:D:203:GLN:HE21	1:D:203:GLN:HA	1.84	0.42
1:D:238:ILE:O	1:D:242:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LYS:NZ	1:C:308:ASP:OD1	2.53	0.42
1:F:110:ASP:OD1	1:F:252:ARG:NH1	2.52	0.42
1:B:34:LYS:HD2	1:B:34:LYS:N	2.35	0.42
1:E:199:ARG:HH11	1:E:199:ARG:HD2	1.69	0.42
1:F:150:LEU:O	1:F:154:MET:HG2	2.20	0.42
1:A:23:ARG:HG3	1:A:59:PHE:CE2	2.54	0.42
1:A:34:LYS:HD2	1:A:34:LYS:N	2.35	0.42
1:C:101:LEU:HD11	1:F:81:ALA:HB2	2.00	0.42
1:E:6:THR:OG1	1:E:279:LEU:HD23	2.19	0.42
1:F:165:VAL:HA	1:F:203:GLN:HE21	1.85	0.42
1:C:110:ASP:OD1	1:C:252:ARG:NH1	2.49	0.42
1:C:269:ARG:HH11	1:C:269:ARG:HD3	1.67	0.42
1:A:180:ALA:O	1:A:187:THR:HA	2.20	0.42
1:D:131:TYR:C	1:D:133:GLU:H	2.28	0.42
1:F:20:GLU:OE1	1:F:24:LYS:NZ	2.53	0.41
1:E:281:ASN:O	1:E:284:GLU:HG2	2.20	0.41
1:A:247:ALA:O	1:A:251:GLU:HB2	2.20	0.41
1:B:34:LYS:HD2	1:B:34:LYS:H	1.85	0.41
1:A:5:GLY:HA3	1:A:275:SER:O	2.21	0.41
1:C:14:ASN:ND2	1:C:17:GLU:HB2	2.35	0.41
1:D:115:GLN:HB3	1:D:120:ILE:HG12	2.02	0.41
1:F:139:ILE:HD13	1:F:139:ILE:HA	1.94	0.41
1:B:115:GLN:HB3	1:B:120:ILE:HG12	2.03	0.41
1:C:189:GLU:HG2	1:C:227:PHE:HE1	1.85	0.41
1:C:265:LYS:HD2	1:C:265:LYS:N	2.34	0.41
1:C:274:ARG:NH1	1:C:278:ASP:OD2	2.54	0.41
1:E:189:GLU:HG2	1:E:227:PHE:HE1	1.85	0.41
1:B:180:ALA:O	1:B:187:THR:HA	2.21	0.41
1:C:81:ALA:HB2	1:F:101:LEU:HD11	2.03	0.41
1:F:3:VAL:HG23	1:F:278:ASP:HB3	2.03	0.41
1:B:177:ILE:HD13	1:B:177:ILE:HG21	1.80	0.41
1:B:220:LEU:O	1:B:224:GLU:HB2	2.21	0.41
1:D:43:ARG:O	1:D:48:ARG:NH2	2.54	0.41
1:E:204:LEU:HD23	1:E:204:LEU:HA	1.91	0.41
1:A:34:LYS:HD2	1:A:34:LYS:H	1.84	0.41
1:B:76:GLU:O	1:B:80:LEU:HB2	2.21	0.41
1:C:165:VAL:HG13	1:C:206:GLN:HG2	2.03	0.40
1:A:81:ALA:HB2	1:E:101:LEU:HD11	2.02	0.40
1:A:269:ARG:HH11	1:A:269:ARG:HD3	1.65	0.40
1:A:307:LYS:O	1:A:311:LEU:HG	2.21	0.40
1:C:203:GLN:NE2	1:C:203:GLN:HA	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:LYS:HZ2	1:E:305:ASP:CG	2.28	0.40
1:F:21:THR:HG21	1:F:39:ILE:HD11	2.04	0.40
1:D:85:LYS:HA	1:D:86:PRO:HD3	1.89	0.40
1:D:110:ASP:OD1	1:D:252:ARG:NH1	2.54	0.40
1:E:21:THR:HG21	1:E:39:ILE:HD11	2.03	0.40
1:E:163:GLU:OE1	1:E:199:ARG:HA	2.21	0.40
1:E:265:LYS:HD2	1:E:265:LYS:N	2.35	0.40
1:F:163:GLU:HB3	1:F:200:SER:HB3	2.04	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	313/315 (99%)	302 (96%)	9 (3%)	2 (1%)	21	51
1	B	313/315 (99%)	304 (97%)	7 (2%)	2 (1%)	21	51
1	C	313/315 (99%)	302 (96%)	9 (3%)	2 (1%)	21	51
1	D	313/315 (99%)	305 (97%)	7 (2%)	1 (0%)	36	66
1	E	313/315 (99%)	301 (96%)	11 (4%)	1 (0%)	36	66
1	F	313/315 (99%)	302 (96%)	9 (3%)	2 (1%)	21	51
All	All	1878/1890 (99%)	1816 (97%)	52 (3%)	10 (0%)	24	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLY
1	B	186	GLY
1	B	132	LYS
1	C	186	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	132	LYS
1	F	132	LYS
1	C	132	LYS
1	E	132	LYS
1	F	186	GLY
1	A	132	LYS

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	260/260 (100%)	238 (92%)	22 (8%)	10	31
1	B	260/260 (100%)	232 (89%)	28 (11%)	6	21
1	C	260/260 (100%)	235 (90%)	25 (10%)	8	26
1	D	260/260 (100%)	232 (89%)	28 (11%)	6	21
1	E	260/260 (100%)	235 (90%)	25 (10%)	8	26
1	F	260/260 (100%)	234 (90%)	26 (10%)	7	24
All	All	1560/1560 (100%)	1406 (90%)	154 (10%)	7	24

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	24	LYS
1	A	31	THR
1	A	34	LYS
1	A	35	SER
1	A	63	LEU
1	A	80	LEU
1	A	82	LEU
1	A	85	LYS
1	A	106	ASN
1	A	115	GLN
1	A	129	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	132	LYS
1	A	137	LYS
1	A	144	SER
1	A	220	LEU
1	A	232	LYS
1	A	240	LYS
1	A	258	LYS
1	A	260	LEU
1	A	301	ASP
1	A	307	LYS
1	B	3	VAL
1	B	15	SER
1	B	24	LYS
1	B	31	THR
1	B	34	LYS
1	B	35	SER
1	B	39	ILE
1	B	63	LEU
1	B	80	LEU
1	B	82	LEU
1	B	85	LYS
1	B	101	LEU
1	B	115	GLN
1	B	120	ILE
1	B	129	LEU
1	B	132	LYS
1	B	137	LYS
1	B	144	SER
1	B	199	ARG
1	B	203	GLN
1	B	216	ASN
1	B	220	LEU
1	B	232	LYS
1	B	240	LYS
1	B	258	LYS
1	B	260	LEU
1	B	301	ASP
1	B	307	LYS
1	C	3	VAL
1	C	24	LYS
1	C	29	ILE
1	C	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	34	LYS
1	C	63	LEU
1	C	80	LEU
1	C	82	LEU
1	C	85	LYS
1	C	101	LEU
1	C	115	GLN
1	C	120	ILE
1	C	124	LYS
1	C	132	LYS
1	C	137	LYS
1	C	144	SER
1	C	220	LEU
1	C	232	LYS
1	C	240	LYS
1	C	258	LYS
1	C	260	LEU
1	C	265	LYS
1	C	301	ASP
1	C	307	LYS
1	C	310	LEU
1	D	3	VAL
1	D	15	SER
1	D	24	LYS
1	D	29	ILE
1	D	31	THR
1	D	34	LYS
1	D	63	LEU
1	D	69	SER
1	D	80	LEU
1	D	82	LEU
1	D	85	LYS
1	D	106	ASN
1	D	115	GLN
1	D	120	ILE
1	D	132	LYS
1	D	137	LYS
1	D	144	SER
1	D	199	ARG
1	D	216	ASN
1	D	220	LEU
1	D	232	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	240	LYS
1	D	258	LYS
1	D	260	LEU
1	D	265	LYS
1	D	301	ASP
1	D	307	LYS
1	D	310	LEU
1	E	3	VAL
1	E	24	LYS
1	E	34	LYS
1	E	63	LEU
1	E	80	LEU
1	E	82	LEU
1	E	85	LYS
1	E	115	GLN
1	E	120	ILE
1	E	132	LYS
1	E	137	LYS
1	E	144	SER
1	E	150	LEU
1	E	193	ASN
1	E	199	ARG
1	E	203	GLN
1	E	220	LEU
1	E	232	LYS
1	E	240	LYS
1	E	258	LYS
1	E	260	LEU
1	E	274	ARG
1	E	301	ASP
1	E	307	LYS
1	E	310	LEU
1	F	3	VAL
1	F	15	SER
1	F	24	LYS
1	F	29	ILE
1	F	31	THR
1	F	34	LYS
1	F	63	LEU
1	F	80	LEU
1	F	82	LEU
1	F	85	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	101	LEU
1	F	106	ASN
1	F	115	GLN
1	F	124	LYS
1	F	132	LYS
1	F	137	LYS
1	F	144	SER
1	F	199	ARG
1	F	203	GLN
1	F	220	LEU
1	F	232	LYS
1	F	240	LYS
1	F	258	LYS
1	F	260	LEU
1	F	301	ASP
1	F	307	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	45	ASN
1	A	62	HIS
1	A	119	GLN
1	A	203	GLN
1	A	216	ASN
1	A	244	ASN
1	B	14	ASN
1	B	45	ASN
1	B	62	HIS
1	B	95	HIS
1	B	106	ASN
1	B	119	GLN
1	B	203	GLN
1	B	244	ASN
1	C	14	ASN
1	C	45	ASN
1	C	93	GLN
1	C	121	HIS
1	C	193	ASN
1	C	203	GLN
1	C	216	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	244	ASN
1	C	316	HIS
1	D	62	HIS
1	D	119	GLN
1	D	203	GLN
1	D	216	ASN
1	E	14	ASN
1	E	45	ASN
1	E	62	HIS
1	E	93	GLN
1	E	106	ASN
1	E	203	GLN
1	E	216	ASN
1	E	225	ASN
1	E	244	ASN
1	E	316	HIS
1	F	93	GLN
1	F	106	ASN
1	F	119	GLN
1	F	203	GLN
1	F	216	ASN
1	F	244	ASN

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

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.