



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 08:16 AM BST

PDB ID : 1AEI
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

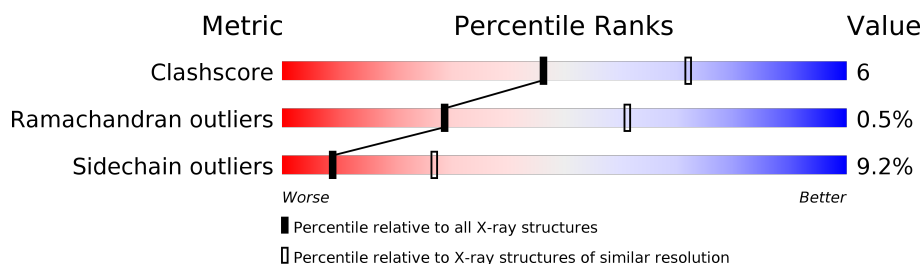
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 on 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 (three-letter code: CA) (formula: Ca).

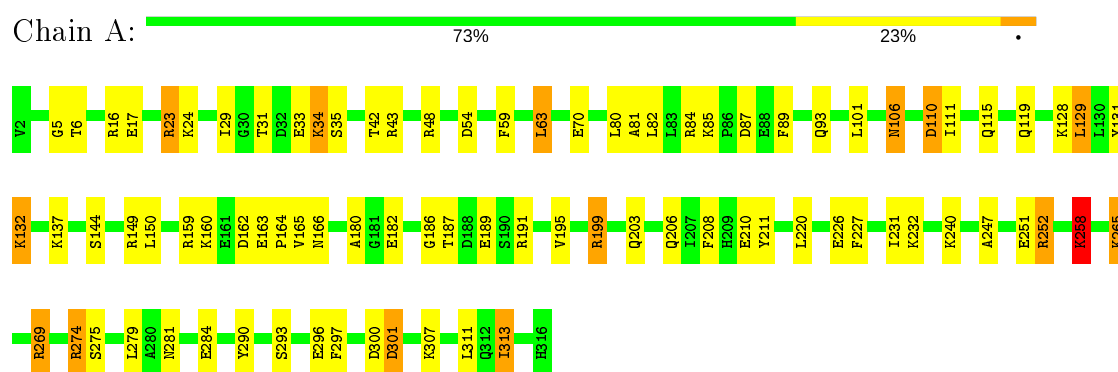
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	4	Total	Ca	0	0
			4	4		
2	E	4	Total	Ca	0	0
			4	4		
2	B	4	Total	Ca	0	0
			4	4		
2	C	4	Total	Ca	0	0
			4	4		
2	A	4	Total	Ca	0	0
			4	4		
2	F	4	Total	Ca	0	0
			4	4		

3 Residue-property plots

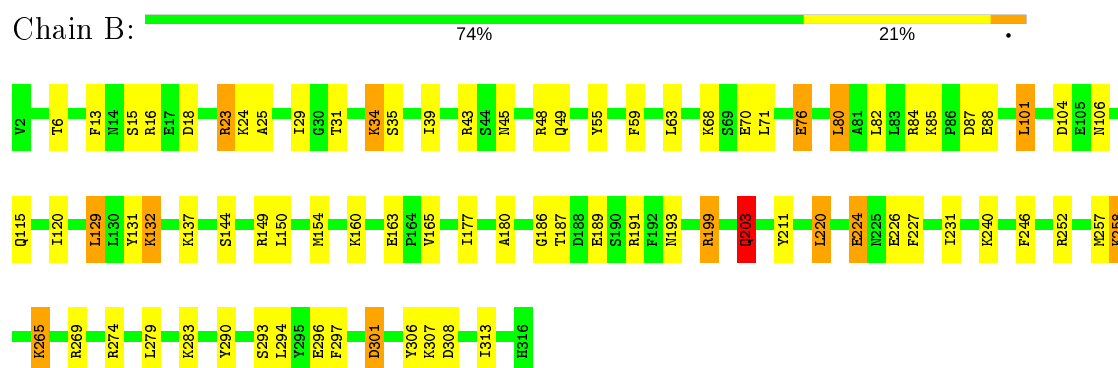
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

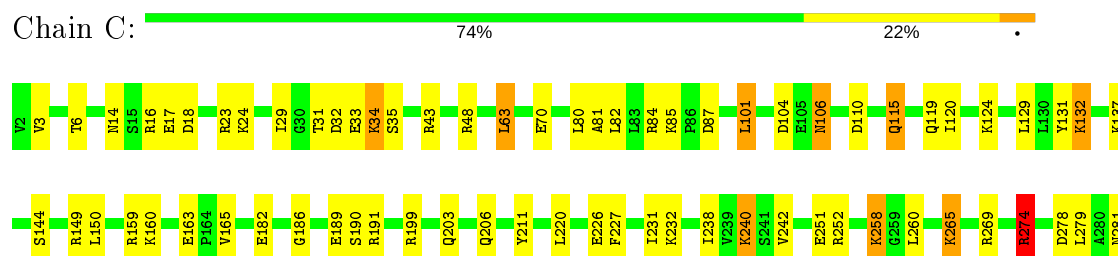
• Molecule 1: ANNEXIN XII



• Molecule 1: ANNEXIN XII



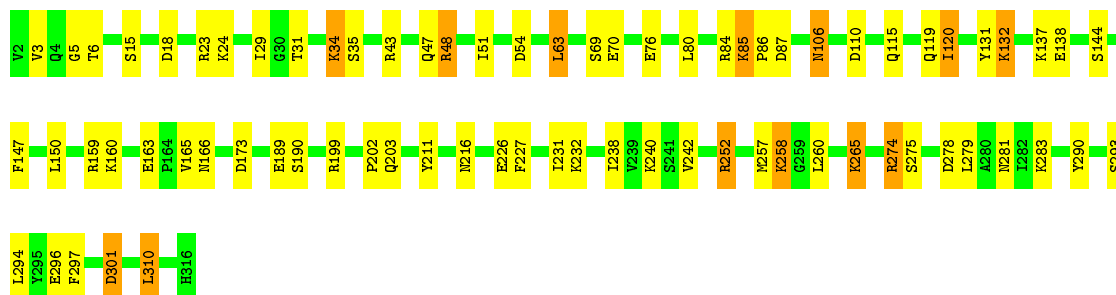
• Molecule 1: ANNEXIN XII





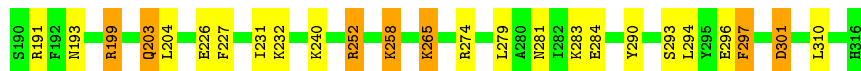
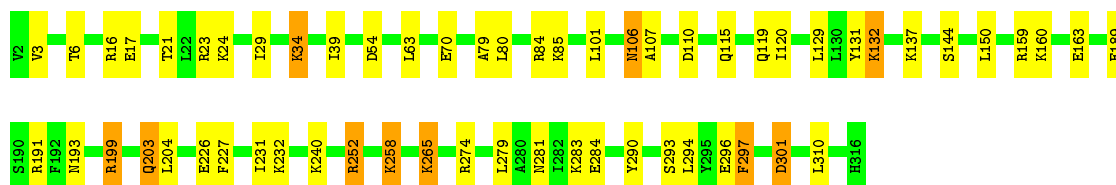
• Molecule 1: ANNEXIN XII

Chain D: 76% 20%



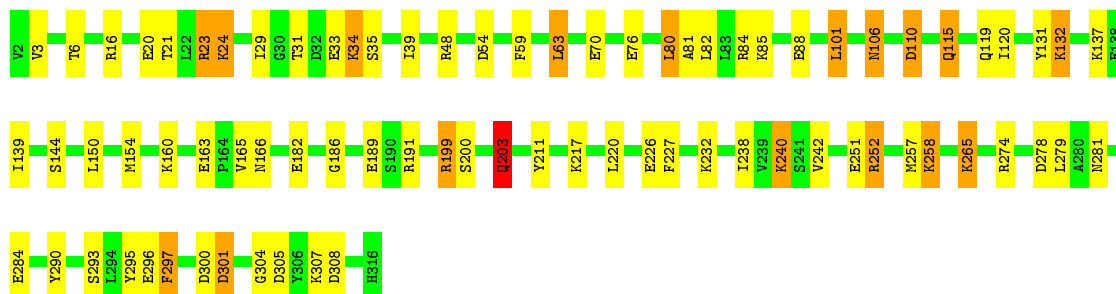
• Molecule 1: ANNEXIN XII

Chain E: 81% 16%



• Molecule 1: ANNEXIN XII

Chain F: 75% 19% 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	71.20 Å 179.20 Å 100.70 Å 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

5.1 Standard geometry

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	1.06	0/2498	1.62	37/3361 (1.1%)
1	B	1.05	3/2498 (0.1%)	1.60	33/3361 (1.0%)
1	C	1.10	1/2498 (0.0%)	1.66	31/3361 (0.9%)
1	D	1.04	0/2498	1.58	26/3361 (0.8%)
1	E	1.05	0/2498	1.61	20/3361 (0.6%)
1	F	1.07	1/2498 (0.0%)	1.61	27/3361 (0.8%)
All	All	1.06	5/14988 (0.0%)	1.61	174/20166 (0.9%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	GLU	CD-OE1	-5.87	1.19	1.25
1	B	15	SER	CA-CB	-5.85	1.44	1.52
1	C	35	SER	CA-CB	-5.85	1.44	1.52
1	F	88	GLU	CA-CB	-5.62	1.41	1.53
1	B	88	GLU	CA-CB	-5.29	1.42	1.53

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ASP	CB-CG-OD1	11.91	129.02	118.30
1	A	84	ARG	NE-CZ-NH2	-11.89	114.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	ASP	CB-CG-OD1	11.67	128.81	118.30
1	D	301	ASP	CB-CG-OD1	10.66	127.90	118.30
1	B	84	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	D	84	ARG	NE-CZ-NH2	-10.27	115.16	120.30
1	C	274	ARG	NE-CZ-NH2	10.13	125.37	120.30
1	B	301	ASP	CB-CG-OD1	9.82	127.14	118.30
1	C	191	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	43	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	E	159	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	159	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	D	70	GLU	OE1-CD-OE2	-8.97	112.54	123.30
1	F	301	ASP	CB-CG-OD1	8.96	126.36	118.30
1	B	70	GLU	OE1-CD-OE2	-8.96	112.55	123.30
1	F	226	GLU	OE1-CD-OE2	-8.90	112.61	123.30
1	C	131	TYR	CB-CG-CD1	-8.90	115.66	121.00
1	B	48	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	F	48	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	E	70	GLU	OE1-CD-OE2	-8.71	112.84	123.30
1	E	226	GLU	OE1-CD-OE2	-8.64	112.93	123.30
1	E	301	ASP	CB-CG-OD1	8.46	125.92	118.30
1	C	43	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	E	131	TYR	CB-CG-CD1	-8.39	115.97	121.00
1	C	226	GLU	OE1-CD-OE2	-8.35	113.28	123.30
1	F	70	GLU	OE1-CD-OE2	-8.29	113.35	123.30
1	A	70	GLU	OE1-CD-OE2	-8.15	113.52	123.30
1	B	226	GLU	OE1-CD-OE2	-8.06	113.63	123.30
1	C	300	ASP	CB-CG-OD1	8.03	125.53	118.30
1	F	84	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	E	84	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	131	TYR	CB-CG-CD1	-7.90	116.26	121.00
1	C	290	TYR	CB-CG-CD1	-7.82	116.31	121.00
1	A	226	GLU	OE1-CD-OE2	-7.75	114.00	123.30
1	F	54	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	290	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	C	70	GLU	OE1-CD-OE2	-7.50	114.30	123.30
1	E	159	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	C	16	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	D	301	ASP	OD1-CG-OD2	-7.33	109.37	123.30
1	D	131	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	B	154	MET	CG-SD-CE	7.27	111.84	100.20
1	D	84	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	84	ARG	NE-CZ-NH2	-7.16	116.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	191	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	E	252	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	A	43	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	84	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	F	304	GLY	O-C-N	7.08	134.03	122.70
1	F	191	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	199	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	C	211	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	B	76	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	C	18	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	199	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	A	162	ASP	CB-CG-OD2	6.86	124.47	118.30
1	D	226	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	C	301	ASP	OD1-CG-OD2	-6.82	110.34	123.30
1	A	313	ILE	CB-CG1-CD1	-6.76	94.97	113.90
1	B	131	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	A	301	ASP	OD1-CG-OD2	-6.71	110.55	123.30
1	E	129	LEU	CB-CG-CD1	-6.53	99.90	111.00
1	D	18	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	211	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	F	290	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	B	18	ASP	CB-CG-OD1	6.46	124.11	118.30
1	E	16	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	A	159	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	48	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	252	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	C	306	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	16	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	B	301	ASP	OD1-CG-OD2	-6.29	111.35	123.30
1	D	290	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	F	106	ASN	CB-CG-ND2	6.23	131.65	116.70
1	C	106	ASN	CB-CG-ND2	6.22	131.62	116.70
1	F	301	ASP	OD1-CG-OD2	-6.16	111.60	123.30
1	A	182	GLU	OE1-CD-OE2	-6.11	115.97	123.30
1	C	131	TYR	CB-CG-CD2	6.10	124.66	121.00
1	B	104	ASP	CB-CG-OD1	6.09	123.78	118.30
1	F	203	GLN	OE1-CD-NE2	-6.09	107.90	121.90
1	D	252	ARG	CG-CD-NE	6.06	124.53	111.80
1	E	290	TYR	CB-CG-CD1	-6.06	117.36	121.00
1	F	199	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	F	211	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	B	306	TYR	CB-CG-CD2	-5.99	117.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	131	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	A	54	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	290	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	B	87	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	211	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	48	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	F	295	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	D	159	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	191	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	E	252	ARG	CG-CD-NE	5.83	124.03	111.80
1	A	17	GLU	CA-CB-CG	5.82	126.20	113.40
1	B	131	TYR	CB-CG-CD2	5.80	124.48	121.00
1	D	257	MET	CA-CB-CG	-5.80	103.44	113.30
1	B	191	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	E	301	ASP	OD1-CG-OD2	-5.75	112.36	123.30
1	B	313	ILE	CB-CG1-CD1	-5.73	97.86	113.90
1	F	300	ASP	CB-CG-OD1	5.73	123.45	118.30
1	D	138	GLU	OE1-CD-OE2	-5.70	116.47	123.30
1	B	101	LEU	CA-CB-CG	5.69	128.40	115.30
1	D	106	ASN	CB-CG-ND2	5.66	130.28	116.70
1	A	274	ARG	CD-NE-CZ	-5.62	115.72	123.60
1	A	101	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	274	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	84	ARG	CB-CG-CD	-5.58	97.08	111.60
1	A	208	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	D	310	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	F	297	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	D	76	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	B	68	LYS	CB-CG-CD	-5.52	97.24	111.60
1	B	211	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	F	305	ASP	CB-CG-OD1	5.52	123.27	118.30
1	E	54	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	54	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	257	MET	CA-CB-CG	-5.50	103.94	113.30
1	B	25	ALA	CB-CA-C	-5.49	101.86	110.10
1	D	147	PHE	CB-CG-CD2	-5.49	116.96	120.80
1	A	269	ARG	CD-NE-CZ	-5.46	115.95	123.60
1	F	63	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	C	129	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	F	16	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	129	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	C	159	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	106	ASN	CB-CG-OD1	-5.40	110.79	121.60
1	C	289	MET	CA-CB-CG	5.39	122.47	113.30
1	A	300	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	32	ASP	CB-CG-OD1	5.37	123.13	118.30
1	E	17	GLU	CA-CB-CG	5.36	125.19	113.40
1	C	149	ARG	CA-CB-CG	-5.36	101.61	113.40
1	F	110	ASP	CB-CA-C	-5.35	99.70	110.40
1	C	63	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	B	224	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	E	107	ALA	CB-CA-C	-5.32	102.12	110.10
1	B	149	ARG	CA-CB-CG	-5.30	101.74	113.40
1	C	190	SER	CA-CB-OG	5.27	125.43	111.20
1	A	110	ASP	CB-CA-C	-5.27	99.86	110.40
1	D	48	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	106	ASN	CB-CG-ND2	5.26	129.32	116.70
1	F	257	MET	O-C-N	-5.26	114.29	122.70
1	F	252	ARG	CG-CD-NE	5.25	122.83	111.80
1	A	87	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	104	ASP	N-CA-C	-5.23	96.87	111.00
1	E	79	ALA	O-C-N	-5.23	114.34	122.70
1	A	191	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	252	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	173	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	203	GLN	OE1-CD-NE2	-5.19	109.97	121.90
1	D	190	SER	CA-CB-OG	5.17	125.17	111.20
1	F	203	GLN	CG-CD-NE2	5.17	129.10	116.70
1	B	71	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	106	ASN	CB-CG-ND2	5.16	129.08	116.70
1	C	296	GLU	CA-CB-CG	5.15	124.74	113.40
1	D	63	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	A	149	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	42	THR	CA-CB-CG2	-5.13	105.22	112.40
1	A	63	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	B	246	PHE	CB-CG-CD2	-5.11	117.23	120.80
1	C	274	ARG	CG-CD-NE	5.10	122.51	111.80
1	A	297	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	A	128	LYS	CA-CB-CG	5.08	124.58	113.40
1	C	87	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	131	TYR	CB-CG-CD2	5.05	124.03	121.00
1	B	129	LEU	CB-CG-CD1	-5.04	102.42	111.00
1	D	87	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	13	PHE	CB-CG-CD2	-5.03	117.28	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	E	84	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	202	PRO	CA-N-CD	-5.02	104.48	111.50
1	C	182	GLU	OE1-CD-OE2	-5.01	117.29	123.30

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	34	0
1	B	2462	576	2450	28	0
1	C	2462	576	2450	36	0
1	D	2462	576	2450	30	0
1	E	2462	576	2450	25	0
1	F	2462	576	2450	38	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	187	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 6.

All (187) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:258:LYS:HA	1:C:258:LYS:HZ2	1.62	0.62
1:F:34:LYS:HD2	1:F:34:LYS:H	1.63	0.62
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:B:203:GLN:HA	1:B:203:GLN:HE21	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:NZ	1:F:258:LYS:HA	2.16	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:NZ	1:B:258:LYS:HA	2.19	0.57
1:B:258:LYS:HZ2	1:B:258:LYS:HA	1.67	0.57
1:E:258:LYS:HA	1:E:258:LYS:CE	2.33	0.57
1:F:34:LYS:HD2	1:F:34:LYS:N	2.20	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:GLN:HA	1:E:203:GLN:HE21	1.73	0.54
1:D:258:LYS:HA	1:D:258:LYS:NZ	2.22	0.54
1:C:165:VAL:HA	1:C:203:GLN:NE2	2.23	0.53
1:E:258:LYS:HA	1:E:258:LYS:NZ	2.23	0.53
1:E:34:LYS:HD2	1:E:34:LYS:H	1.74	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:C:258:LYS:HZ1	1:C:297:PHE:HE1	1.57	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:F:29:ILE:H	1:F:29:ILE:HD12	1.75	0.51
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:CE	1:B:258:LYS:HA	2.42	0.49
1:C:34:LYS:N	1:C:34:LYS:HD2	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: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:D:34:LYS:H	1:D:34:LYS:HD2	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:F:258:LYS:HZ2	1:F:258:LYS:HA	1.77	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:F:258:LYS:HZ1	1:F:297:PHE:HE2	1.62	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:C:3:VAL:HA	1:C:281:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:H	1:A:29:ILE:HD12	1.80	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: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:HD12	1:C:29:ILE:H	1.81	0.46
1:F:33:GLU:HB2	1:F:34:LYS:HZ3	1.81	0.45
1:A:206:GLN:O	1:A:210:GLU:HG2	2.17	0.45
1:E:29:ILE:H	1:E:29:ILE:HD12	1.82	0.45
1:F:189:GLU:HG2	1:F:227:PHE:HE1	1.81	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:N	1:E:34:LYS:HD2	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:E:258:LYS:HA	1:E:258:LYS:HZ2	1.81	0.44
1:E:258:LYS:HZ1	1:E:297:PHE:HE2	1.64	0.44
1:A:313:ILE:HD13	1:A:313:ILE:HG21	1.72	0.44
1:B:120:ILE:HA	1:B:120:ILE:HD13	1.81	0.44
1:B:307:LYS:NZ	1:B:308:ASP:OD1	2.51	0.44
1:C:120:ILE:HA	1:C:120:ILE:HD13	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:HA	1:F:120:ILE:HD13	1.80	0.43
1:F:166:ASN:H	1:F:203:GLN:HE22	1.66	0.43
1:A:195:VAL:O	1:A:199:ARG:HG2	2.18	0.43
1:D:47:GLN:O	1:D:51:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:29:ILE:HD12	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:115:GLN:HG3	1:F:119:GLN:HB2	2.00	0.42
1:F:23:ARG:HG3	1:F:59:PHE:CZ	2.54	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
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:N	1:B:34:LYS:HD2	2.35	0.42
1:E:199:ARG:HD2	1:E:199:ARG:HH11	1.69	0.42
1:F:150:LEU:O	1:F:154:MET:HG2	2.20	0.42
1:A:34:LYS:HD2	1:A:34:LYS:N	2.35	0.42
1:A:23:ARG:HG3	1:A:59:PHE:CE2	2.54	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:101:LEU:HD11	1:F:81:ALA:HB2	2.00	0.42
1:C:110:ASP:OD1	1:C:252:ARG:NH1	2.49	0.42
1:C:269:ARG:HD3	1:C:269:ARG:HH11	1.67	0.42
1:A:180:ALA:O	1:A:187:THR:HA	2.20	0.42
1:A:33:GLU:HB2	1:A:34:LYS:HZ2	1.85	0.42
1:B:258:LYS:HZ1	1:B:297:PHE:HE2	1.68	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:HA	1:F:139:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:43:ARG:O	1:D:48:ARG:NH2	2.54	0.41
1:B:220:LEU:O	1:B:224:GLU:HB2	2.21	0.41
1:E:204:LEU:HA	1:E:204:LEU:HD23	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:B:16:ARG:HH12	1:C:163:GLU:CD	2.24	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:HA	1:C:203:GLN:NE2	2.36	0.40
1:F:21:THR:HG21	1:F:39:ILE:HD11	2.04	0.40
1:D:110:ASP:OD1	1:D:252:ARG:NH1	2.54	0.40
1:D:85:LYS:HA	1:D:86:PRO:HD3	1.89	0.40
1:E:163:GLU:OE1	1:E:199:ARG:HA	2.21	0.40
1:E:21:THR:HG21	1:E:39:ILE:HD11	2.03	0.40
1:C:289:MET:HB3	1:C:289:MET:HE2	1.94	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	313/315 (99%)	302 (96%)	9 (3%)	2 (1%)	25 56
1	B	313/315 (99%)	304 (97%)	7 (2%)	2 (1%)	25 56
1	C	313/315 (99%)	302 (96%)	9 (3%)	2 (1%)	25 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	313/315 (99%)	305 (97%)	7 (2%)	1 (0%)	41	72
1	E	313/315 (99%)	301 (96%)	11 (4%)	1 (0%)	41	72
1	F	313/315 (99%)	302 (96%)	9 (3%)	2 (1%)	25	56
All	All	1878/1890 (99%)	1816 (97%)	52 (3%)	10 (0%)	29	61

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
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%)	236 (91%)	24 (9%)	9	27
1	C	260/260 (100%)	235 (90%)	25 (10%)	8	24
1	D	260/260 (100%)	234 (90%)	26 (10%)	7	22
1	E	260/260 (100%)	238 (92%)	22 (8%)	10	31
1	F	260/260 (100%)	236 (91%)	24 (9%)	9	27
All	All	1560/1560 (100%)	1417 (91%)	143 (9%)	9	27

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
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	129	LEU
1	A	132	LYS
1	A	137	LYS
1	A	144	SER
1	A	199	ARG
1	A	220	LEU
1	A	232	LYS
1	A	240	LYS
1	A	258	LYS
1	A	265	LYS
1	A	274	ARG
1	A	301	ASP
1	B	23	ARG
1	B	24	LYS
1	B	31	THR
1	B	34	LYS
1	B	35	SER
1	B	63	LEU
1	B	80	LEU
1	B	82	LEU
1	B	85	LYS
1	B	101	LEU
1	B	106	ASN
1	B	129	LEU
1	B	132	LYS
1	B	137	LYS
1	B	144	SER
1	B	193	ASN
1	B	199	ARG
1	B	203	GLN
1	B	220	LEU
1	B	240	LYS
1	B	258	LYS

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Mol	Chain	Res	Type
1	B	265	LYS
1	B	274	ARG
1	B	301	ASP
1	C	23	ARG
1	C	24	LYS
1	C	31	THR
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	106	ASN
1	C	115	GLN
1	C	124	LYS
1	C	132	LYS
1	C	137	LYS
1	C	144	SER
1	C	199	ARG
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	274	ARG
1	C	297	PHE
1	C	301	ASP
1	D	15	SER
1	D	23	ARG
1	D	24	LYS
1	D	31	THR
1	D	34	LYS
1	D	35	SER
1	D	63	LEU
1	D	69	SER
1	D	80	LEU
1	D	85	LYS
1	D	106	ASN
1	D	120	ILE
1	D	132	LYS
1	D	137	LYS

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Mol	Chain	Res	Type
1	D	144	SER
1	D	199	ARG
1	D	216	ASN
1	D	232	LYS
1	D	240	LYS
1	D	258	LYS
1	D	260	LEU
1	D	265	LYS
1	D	274	ARG
1	D	297	PHE
1	D	301	ASP
1	D	310	LEU
1	E	23	ARG
1	E	24	LYS
1	E	34	LYS
1	E	63	LEU
1	E	80	LEU
1	E	85	LYS
1	E	106	ASN
1	E	120	ILE
1	E	132	LYS
1	E	137	LYS
1	E	144	SER
1	E	193	ASN
1	E	199	ARG
1	E	203	GLN
1	E	232	LYS
1	E	240	LYS
1	E	258	LYS
1	E	265	LYS
1	E	274	ARG
1	E	297	PHE
1	E	301	ASP
1	E	310	LEU
1	F	23	ARG
1	F	24	LYS
1	F	31	THR
1	F	34	LYS
1	F	35	SER
1	F	63	LEU
1	F	80	LEU
1	F	82	LEU

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Mol	Chain	Res	Type
1	F	85	LYS
1	F	101	LEU
1	F	106	ASN
1	F	115	GLN
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	265	LYS
1	F	274	ARG
1	F	301	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	203	GLN
1	B	62	HIS
1	B	119	GLN
1	B	203	GLN
1	C	203	GLN
1	D	119	GLN
1	D	203	GLN
1	E	62	HIS
1	E	203	GLN
1	F	119	GLN
1	F	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.