



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:01 PM UTC

PDB ID : 1ANX / pdb_00001anx
Title : THE CRYSTAL STRUCTURE OF A NEW HIGH-CALCIUM FORM OF ANNEXIN V
Authors : Sopkova, J.; Renouard, M.; Lewit-Bentley, A.
Deposited on : 1993-10-26
Resolution : 1.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

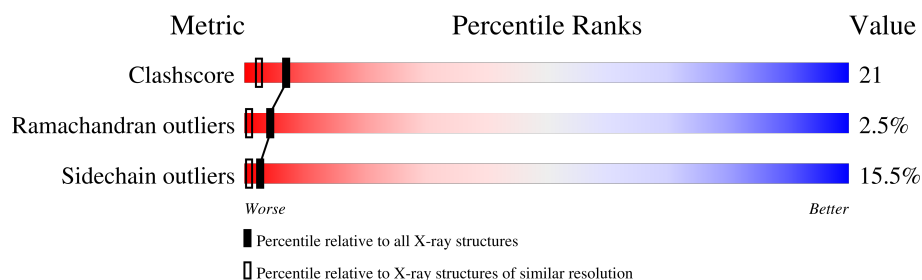
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	319	39% 35% 21% • •
1	B	319	40% 39% 14% 6% •
1	C	319	39% 36% 18% 7% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7990 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 ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	5	0
			2519	1587	428	496	8			
1	B	316	Total	C	N	O	S	0	4	0
			2513	1584	425	496	8			
1	C	316	Total	C	N	O	S	0	4	0
			2513	1584	425	496	8			

- 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		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

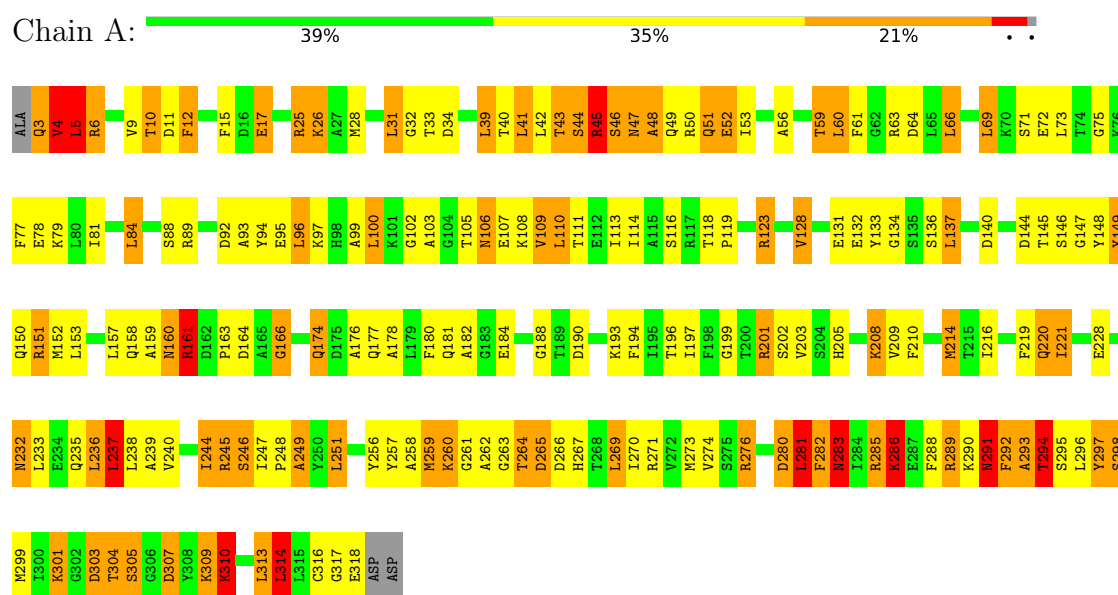
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	133	Total	O	0	0
			133	133		
4	C	134	Total	O	0	0
			134	134		

3 Residue-property plots

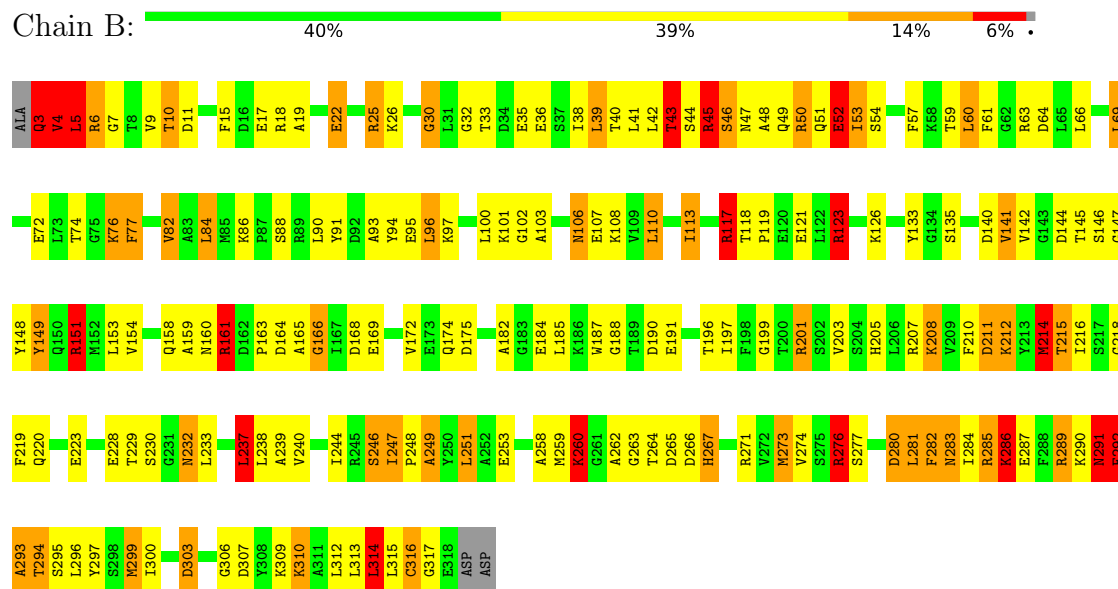
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

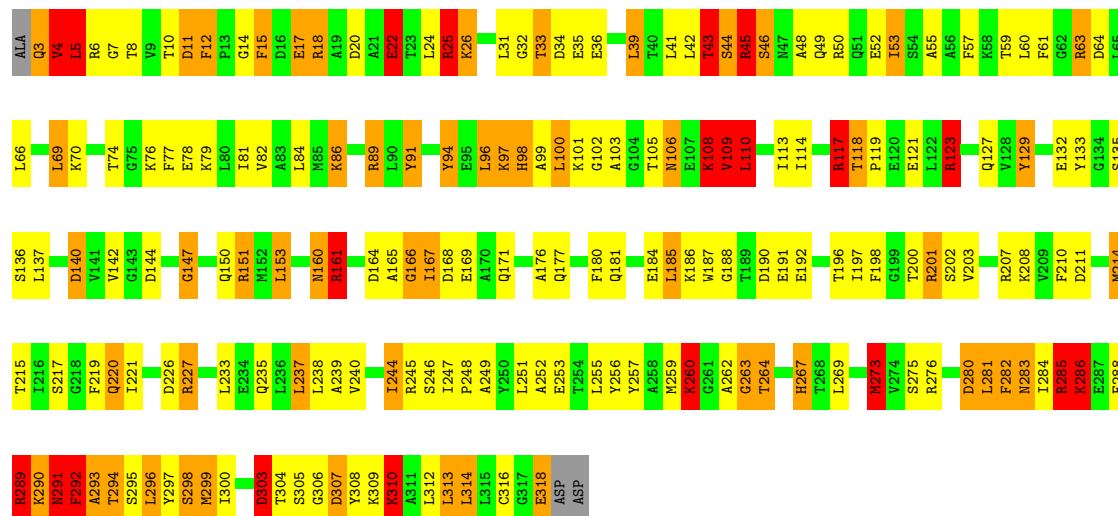


• Molecule 1: ANNEXIN V



● Molecule 1: ANNEXIN V

Chain C: 39% 36% 18% 7%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.20Å 91.30Å 36.20Å 82.40° 82.40° 118.20°	Depositor
Resolution (Å)	12.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7990	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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, SO4

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	1.19	6/2579 (0.2%)	2.51	204/3468 (5.9%)
1	B	1.20	6/2568 (0.2%)	2.44	189/3454 (5.5%)
1	C	1.20	5/2568 (0.2%)	2.53	204/3454 (5.9%)
All	All	1.20	17/7715 (0.2%)	2.49	597/10376 (5.8%)

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	5
1	B	0	9
1	C	0	11
All	All	0	25

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	SER	C-N	-11.11	1.19	1.33
1	C	263	GLY	C-N	-8.77	1.22	1.33
1	C	166	GLY	C-N	-5.92	1.26	1.33
1	B	153	LEU	N-CA	5.67	1.53	1.46
1	A	176	ALA	N-CA	5.54	1.52	1.46
1	A	44	SER	C-N	-5.54	1.25	1.33
1	A	40	THR	C-N	-5.53	1.26	1.33
1	B	19	ALA	C-N	5.43	1.41	1.33
1	C	7	GLY	C-N	-5.42	1.26	1.33
1	A	180	PHE	N-CA	5.29	1.52	1.46
1	B	7	GLY	C-N	-5.29	1.25	1.33
1	A	88	SER	C-N	-5.28	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	THR	CA-CB	5.25	1.61	1.53
1	B	166	GLY	N-CA	5.24	1.52	1.45
1	B	247	ILE	N-CA	5.18	1.52	1.46
1	C	176	ALA	N-CA	5.15	1.52	1.46
1	C	239	ALA	N-CA	5.02	1.52	1.46

All (597) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ASN	CA-CB-CG	13.51	126.11	112.60
1	C	292	PHE	CA-CB-CG	-12.99	100.81	113.80
1	B	45	ARG	NE-CZ-NH2	12.86	130.77	119.20
1	B	25	ARG	NE-CZ-NH2	11.78	129.80	119.20
1	C	81	ILE	CA-C-O	-11.31	108.86	120.85
1	B	88	SER	CA-C-N	11.22	135.75	120.38
1	B	88	SER	C-N-CA	11.22	135.75	120.38
1	B	9	VAL	CA-C-O	10.67	131.79	120.48
1	C	53	ILE	CA-C-O	10.53	132.33	121.17
1	A	201	ARG	NE-CZ-NH2	10.42	128.57	119.20
1	C	44	SER	CA-C-O	10.38	132.51	119.95
1	A	128	VAL	CA-C-O	-10.21	110.33	120.95
1	C	307	ASP	N-CA-C	-10.16	100.29	111.36
1	C	61	PHE	CA-C-O	-10.14	107.90	119.05
1	A	32	GLY	CA-C-O	9.91	131.69	122.57
1	B	296	LEU	N-CA-C	-9.91	100.44	111.14
1	C	64	ASP	CA-C-O	-9.55	109.74	120.43
1	A	271	ARG	CA-C-O	-9.43	110.81	120.90
1	B	4	VAL	O-C-N	9.30	134.20	122.57
1	C	41	LEU	O-C-N	9.27	132.10	122.09
1	C	57	PHE	O-C-N	9.25	133.04	122.22
1	B	203	VAL	CA-C-O	-9.24	111.05	120.85
1	C	74	THR	CA-C-N	9.14	134.78	120.07
1	C	74	THR	C-N-CA	9.14	134.78	120.07
1	A	17	GLU	CA-C-O	-9.05	109.57	119.97
1	C	238	LEU	O-C-N	8.98	132.39	122.15
1	B	300	ILE	O-C-N	8.98	130.71	121.91
1	C	288	PHE	CA-CB-CG	8.90	122.70	113.80
1	A	151[A]	ARG	CD-NE-CZ	-8.89	111.96	124.40
1	A	151[B]	ARG	CD-NE-CZ	-8.89	111.96	124.40
1	A	123	ARG	CD-NE-CZ	8.86	136.80	124.40
1	C	188	GLY	N-CA-C	-8.82	99.15	111.76
1	A	265	ASP	O-C-N	8.74	133.78	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	LYS	N-CA-C	-8.74	101.71	114.39
1	C	4	VAL	O-C-N	8.71	133.46	122.57
1	B	282	PHE	N-CA-C	-8.70	101.38	111.03
1	A	92	ASP	CA-CB-CG	8.62	121.22	112.60
1	C	292	PHE	CA-C-O	-8.51	108.34	120.51
1	C	244	ILE	O-C-N	8.50	130.12	121.87
1	A	164	ASP	CA-CB-CG	-8.50	104.10	112.60
1	B	307	ASP	N-CA-C	-8.48	101.98	111.14
1	C	220	GLN	CA-C-O	-8.48	111.72	121.47
1	C	221	ILE	O-C-N	-8.47	113.31	121.87
1	B	45	ARG	CA-C-O	-8.47	111.55	120.70
1	A	238	LEU	CA-C-O	-8.38	110.34	119.97
1	A	48	ALA	O-C-N	8.27	130.88	122.12
1	A	94	TYR	CA-C-O	8.25	129.19	120.70
1	A	64	ASP	CA-CB-CG	-8.23	104.37	112.60
1	B	271	ARG	CD-NE-CZ	8.22	135.90	124.40
1	B	216	ILE	N-CA-C	8.21	118.25	110.53
1	A	161	ARG	NH1-CZ-NH2	8.20	129.97	119.30
1	A	49	GLN	CA-C-O	-8.20	111.72	120.42
1	B	45	ARG	NE-CZ-NH1	-8.19	113.31	121.50
1	A	235	GLN	CA-C-O	8.14	129.18	120.55
1	A	4	VAL	O-C-N	8.12	132.73	122.57
1	C	198	PHE	CA-C-N	8.09	128.96	119.98
1	C	198	PHE	C-N-CA	8.09	128.96	119.98
1	B	119	PRO	O-C-N	8.08	130.90	122.18
1	C	310	LYS	CA-C-O	8.05	128.96	120.42
1	C	81	ILE	O-C-N	8.00	130.07	121.83
1	C	45	ARG	CD-NE-CZ	-7.97	113.24	124.40
1	B	166	GLY	CA-C-O	7.96	134.42	120.57
1	A	188	GLY	O-C-N	-7.94	116.08	122.90
1	A	180	PHE	CA-C-O	7.93	129.15	120.82
1	B	25	ARG	CD-NE-CZ	-7.89	113.36	124.40
1	C	168	ASP	CA-C-O	-7.89	112.72	120.92
1	B	296	LEU	CB-CA-C	7.89	123.36	110.90
1	A	292	PHE	CA-CB-CG	-7.88	105.92	113.80
1	A	205	HIS	CA-C-O	-7.80	112.67	120.70
1	A	180	PHE	O-C-N	-7.77	114.06	122.07
1	B	187	TRP	CA-C-O	-7.75	112.61	120.98
1	B	201	ARG	CD-NE-CZ	7.74	135.24	124.40
1	B	82	VAL	CA-CB-CG2	7.72	123.53	110.40
1	B	190	ASP	CA-C-O	-7.70	113.42	122.13
1	A	4	VAL	N-CA-C	7.68	125.33	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	SER	O-C-N	7.68	131.60	122.85
1	B	110	LEU	CA-C-O	7.63	129.47	121.07
1	C	91	TYR	O-C-N	-7.63	113.91	122.08
1	B	53	ILE	CA-C-O	7.58	128.83	120.95
1	B	232	ASN	OD1-CG-ND2	7.57	130.17	122.60
1	C	48	ALA	O-C-N	7.55	129.85	122.07
1	C	123	ARG	N-CA-C	-7.51	102.70	111.03
1	C	150	GLN	OE1-CD-NE2	7.50	130.10	122.60
1	C	102	GLY	N-CA-C	-7.49	104.93	114.37
1	C	49	GLN	CA-C-O	-7.47	112.64	120.55
1	A	161	ARG	NE-CZ-NH1	-7.45	114.05	121.50
1	C	296	LEU	N-CA-C	-7.45	103.18	111.82
1	B	188	GLY	N-CA-C	-7.45	101.07	112.84
1	B	296	LEU	CA-C-O	-7.44	113.04	120.70
1	C	164	ASP	CA-CB-CG	-7.44	105.16	112.60
1	B	32	GLY	CA-C-O	7.42	130.30	122.59
1	B	61	PHE	CA-C-O	-7.41	110.50	119.32
1	B	238	LEU	CA-C-O	-7.40	112.58	120.42
1	C	252	ALA	CA-C-O	7.40	128.59	120.82
1	B	175	ASP	CA-C-O	-7.39	112.59	120.42
1	A	132	GLU	CA-C-O	-7.37	112.61	120.42
1	B	149	TYR	CA-C-O	7.37	128.55	120.82
1	A	3	GLN	O-C-N	7.36	134.78	123.00
1	C	11	ASP	CA-CB-CG	-7.35	105.25	112.60
1	A	266	ASP	O-C-N	7.30	131.72	122.23
1	A	26	LYS	CA-C-O	-7.28	113.06	121.07
1	A	64	ASP	CA-C-O	-7.27	112.29	120.43
1	A	296	LEU	N-CA-C	-7.26	102.76	111.69
1	B	215	THR	N-CA-C	-7.21	103.50	111.36
1	C	45	ARG	CA-C-O	-7.20	112.58	120.36
1	A	140	ASP	CA-C-O	-7.20	112.79	120.42
1	B	145	THR	CA-CB-OG1	-7.20	98.80	109.60
1	B	164	ASP	CB-CA-C	7.19	121.28	109.70
1	C	140	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	238	LEU	O-C-N	7.18	130.34	122.15
1	C	300	ILE	O-C-N	7.15	128.80	121.87
1	C	245	ARG	O-C-N	7.14	129.80	122.09
1	A	177	GLN	OE1-CD-NE2	7.14	129.74	122.60
1	C	238	LEU	CA-C-O	-7.13	112.86	120.42
1	B	296	LEU	O-C-N	7.13	129.79	122.09
1	A	181	GLN	O-C-N	-7.09	113.92	122.22
1	A	5	LEU	O-C-N	-7.09	113.16	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	CA-C-O	-7.08	113.85	121.56
1	A	12	PHE	CA-C-O	7.07	127.88	120.25
1	B	164	ASP	CA-CB-CG	-7.07	105.53	112.60
1	A	265	ASP	CA-C-O	-7.06	113.58	120.92
1	B	166	GLY	CA-C-N	7.06	130.02	120.63
1	B	166	GLY	C-N-CA	7.06	130.02	120.63
1	B	249	ALA	O-C-N	7.04	129.58	122.12
1	A	220	GLN	CA-C-O	-7.03	113.39	121.47
1	A	132	GLU	N-CA-C	7.00	118.99	111.36
1	C	4	VAL	N-CA-C	7.00	123.90	109.34
1	B	271	ARG	CA-C-O	-7.00	113.41	120.90
1	A	160	ASN	N-CA-CB	-7.00	101.08	111.43
1	C	273	MET	CA-CB-CG	-7.00	100.11	114.10
1	A	166	GLY	CA-C-O	6.99	132.73	120.57
1	A	174	GLN	CA-CB-CG	6.99	128.08	114.10
1	A	232	ASN	OD1-CG-ND2	6.99	129.59	122.60
1	A	31	LEU	O-C-N	6.97	131.43	123.06
1	C	153	LEU	CA-C-O	-6.97	113.03	120.42
1	C	177	GLN	OE1-CD-NE2	6.97	129.57	122.60
1	B	57	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	216	ILE	N-CA-C	6.96	117.07	110.53
1	C	202	SER	CA-C-O	6.93	129.91	121.87
1	B	218	GLY	CA-C-N	6.93	132.98	122.93
1	B	218	GLY	C-N-CA	6.93	132.98	122.93
1	C	150	GLN	CG-CD-NE2	-6.93	106.01	116.40
1	B	110	LEU	N-CA-CB	-6.91	99.32	109.82
1	C	4	VAL	CA-C-N	6.90	134.72	121.54
1	C	4	VAL	C-N-CA	6.90	134.72	121.54
1	C	98	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	52	GLU	CG-CD-OE1	-6.89	102.55	118.40
1	C	262	ALA	N-CA-C	-6.89	101.10	110.68
1	A	282	PHE	CA-CB-CG	-6.89	106.91	113.80
1	A	238	LEU	O-C-N	6.86	130.71	122.27
1	A	51	GLN	CA-C-O	-6.85	113.16	120.42
1	A	267	HIS	CA-CB-CG	-6.85	106.95	113.80
1	C	26	LYS	CB-CG-CD	6.84	127.03	111.30
1	B	106	ASN	CA-C-O	-6.82	113.47	120.84
1	B	4	VAL	CA-C-N	6.81	134.55	121.54
1	B	4	VAL	C-N-CA	6.81	134.55	121.54
1	B	74	THR	CA-C-N	6.81	131.04	120.07
1	B	74	THR	C-N-CA	6.81	131.04	120.07
1	A	52	GLU	CG-CD-OE2	6.81	134.06	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ALA	CA-C-N	-6.80	108.08	121.41
1	C	165	ALA	C-N-CA	-6.80	108.08	121.41
1	C	201	ARG	O-C-N	6.80	130.64	122.96
1	C	135	SER	O-C-N	6.79	130.55	122.94
1	A	164	ASP	CB-CA-C	6.79	120.98	109.72
1	B	17	GLU	CA-C-O	-6.77	111.30	119.49
1	B	190	ASP	O-C-N	6.77	130.20	122.55
1	A	148	TYR	O-C-N	6.76	131.49	122.43
1	B	49	GLN	OE1-CD-NE2	6.76	129.36	122.60
1	C	239	ALA	CA-C-O	6.75	127.70	120.55
1	C	99	ALA	N-CA-C	-6.75	104.06	112.90
1	C	203	VAL	CA-C-O	-6.74	113.57	121.05
1	C	50	ARG	CA-C-N	6.73	129.85	120.29
1	C	50	ARG	C-N-CA	6.73	129.85	120.29
1	B	52	GLU	CA-CB-CG	6.73	127.56	114.10
1	C	295	SER	O-C-N	6.71	130.54	122.96
1	B	216	ILE	N-CA-CB	-6.69	102.01	110.57
1	A	4	VAL	CB-CA-C	-6.68	100.34	111.29
1	A	3	GLN	CA-C-N	6.67	133.98	121.97
1	A	3	GLN	C-N-CA	6.67	133.98	121.97
1	B	146	SER	CA-C-O	-6.67	114.12	121.33
1	C	52	GLU	CG-CD-OE1	-6.67	103.06	118.40
1	A	51	GLN	CG-CD-NE2	6.67	126.40	116.40
1	A	246	SER	CA-C-N	-6.67	115.00	120.33
1	A	246	SER	C-N-CA	-6.67	115.00	120.33
1	A	199	GLY	CA-C-O	-6.66	112.98	120.30
1	A	249	ALA	O-C-N	6.65	129.17	122.12
1	A	297	TYR	CA-CB-CG	6.65	125.87	113.90
1	B	142	VAL	CA-C-O	6.65	128.19	121.27
1	A	56	ALA	CA-C-N	6.64	129.18	120.28
1	A	56	ALA	C-N-CA	6.64	129.18	120.28
1	B	94	TYR	CA-C-O	6.64	127.54	120.70
1	C	12	PHE	CB-CA-C	6.64	118.23	108.87
1	B	3	GLN	O-C-N	6.61	133.58	123.00
1	C	48	ALA	CA-C-O	-6.59	113.89	120.82
1	B	57	PHE	O-C-N	6.59	129.93	122.22
1	C	4	VAL	CB-CA-C	-6.59	100.48	111.29
1	C	142	VAL	N-CA-CB	-6.58	103.20	110.51
1	B	214	MET	CA-C-O	-6.58	113.44	120.42
1	B	214	MET	CG-SD-CE	6.58	115.38	100.90
1	B	184	GLU	CA-C-O	-6.56	113.93	120.82
1	B	307	ASP	CB-CA-C	6.54	121.23	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLY	N-CA-C	-6.53	102.52	112.84
1	A	197	ILE	O-C-N	6.53	128.69	121.90
1	C	89	ARG	CA-C-O	-6.52	111.60	119.49
1	C	41	LEU	CA-C-O	-6.49	114.02	120.70
1	C	307	ASP	O-C-N	6.48	129.54	122.15
1	B	315	LEU	CA-C-N	6.48	129.20	120.65
1	B	315	LEU	C-N-CA	6.48	129.20	120.65
1	C	167	ILE	N-CA-C	6.47	117.67	108.93
1	C	77	PHE	N-CA-C	-6.47	104.31	111.36
1	A	259	MET	CA-C-N	-6.47	109.19	121.54
1	A	259	MET	C-N-CA	-6.47	109.19	121.54
1	C	102	GLY	CA-C-N	6.46	133.88	121.54
1	C	102	GLY	C-N-CA	6.46	133.88	121.54
1	A	158	GLN	CG-CD-NE2	6.46	126.08	116.40
1	A	197	ILE	CA-C-O	-6.45	113.89	121.05
1	B	307	ASP	O-C-N	6.45	129.05	122.09
1	B	4	VAL	N-CA-C	6.44	122.73	109.34
1	B	50	ARG	NH1-CZ-NH2	6.44	127.67	119.30
1	A	249	ALA	CA-C-O	-6.43	113.73	120.55
1	B	161	ARG	CB-CA-C	6.42	121.35	109.54
1	C	69	LEU	CB-CA-C	6.41	121.07	110.81
1	C	289	ARG	CG-CD-NE	6.41	126.10	112.00
1	B	77	PHE	O-C-N	6.41	128.91	122.12
1	A	161	ARG	CA-C-N	6.40	130.39	120.60
1	A	161	ARG	C-N-CA	6.40	130.39	120.60
1	C	69	LEU	N-CA-CB	-6.40	100.41	109.94
1	B	273	MET	CA-CB-CG	-6.38	101.33	114.10
1	B	292	PHE	CA-C-O	-6.38	111.39	120.51
1	B	230	SER	CA-C-N	6.38	130.39	120.00
1	B	230	SER	C-N-CA	6.38	130.39	120.00
1	C	22	GLU	N-CA-CB	6.36	119.58	110.16
1	C	57	PHE	CA-C-N	-6.36	109.87	120.68
1	C	57	PHE	C-N-CA	-6.36	109.87	120.68
1	C	44	SER	CA-C-N	6.34	131.93	122.99
1	C	44	SER	C-N-CA	6.34	131.93	122.99
1	C	226	ASP	CA-CB-CG	-6.33	106.27	112.60
1	A	174	GLN	N-CA-CB	-6.32	100.81	110.16
1	B	196	THR	CA-C-N	-6.32	112.48	120.56
1	B	196	THR	C-N-CA	-6.32	112.48	120.56
1	C	291	ASN	N-CA-C	-6.30	97.38	110.80
1	A	73	LEU	O-C-N	6.30	130.15	123.03
1	A	210	PHE	CA-CB-CG	6.29	120.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	A	64	ASP	CB-CA-C	6.28	120.70	110.22
1	B	276	ARG	NH1-CZ-NH2	-6.28	111.14	119.30
1	A	201	ARG	CD-NE-CZ	6.27	133.18	124.40
1	C	282	PHE	N-CA-C	-6.27	104.07	111.03
1	C	31	LEU	O-C-N	6.27	130.93	122.59
1	A	12	PHE	CB-CA-C	6.26	119.25	109.42
1	C	113	ILE	CA-C-O	-6.25	113.52	120.96
1	B	69	LEU	CB-CA-C	6.24	120.68	110.88
1	A	59	THR	CA-CB-CG2	6.24	121.10	110.50
1	C	15	PHE	CA-CB-CG	6.22	120.02	113.80
1	C	285	ARG	O-C-N	6.22	128.49	122.03
1	B	117	ARG	CA-C-O	-6.21	113.77	120.92
1	C	117	ARG	CA-C-O	-6.21	113.77	120.92
1	B	142	VAL	CA-C-N	6.21	126.88	119.98
1	B	142	VAL	C-N-CA	6.21	126.88	119.98
1	C	22	GLU	CA-C-N	-6.21	112.37	120.44
1	C	22	GLU	C-N-CA	-6.21	112.37	120.44
1	A	310	LYS	CA-C-O	6.21	127.00	120.42
1	B	22	GLU	O-C-N	6.21	129.22	122.15
1	C	185	LEU	N-CA-CB	-6.20	100.37	110.42
1	A	47	ASN	O-C-N	6.19	128.68	122.12
1	B	165	ALA	CA-C-N	-6.18	109.30	121.41
1	B	165	ALA	C-N-CA	-6.18	109.30	121.41
1	B	295	SER	CA-C-O	6.16	129.10	121.89
1	C	45	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	B	294	THR	N-CA-CB	6.15	120.89	110.49
1	B	199	GLY	CA-C-O	-6.15	113.51	120.09
1	C	161	ARG	NH1-CZ-NH2	6.14	127.28	119.30
1	C	304	THR	N-CA-C	6.14	119.17	110.14
1	C	260	LYS	N-CA-CB	6.14	120.86	110.49
1	C	291	ASN	CB-CA-C	6.13	122.63	110.42
1	A	209	VAL	O-C-N	6.13	127.81	121.87
1	C	275	SER	O-C-N	-6.13	115.21	122.20
1	A	109	VAL	CA-C-O	-6.12	114.25	121.05
1	A	66	LEU	CA-C-O	-6.11	114.41	120.82
1	A	317	GLY	CA-C-N	6.08	132.65	121.70
1	A	317	GLY	C-N-CA	6.08	132.65	121.70
1	B	287	GLU	N-CA-CB	6.07	120.47	110.39
1	A	285	ARG	O-C-N	6.06	128.33	122.03
1	C	94	TYR	CA-C-O	6.06	126.84	120.42
1	C	50	ARG	NE-CZ-NH1	-6.05	115.45	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ILE	CA-C-O	6.04	122.74	118.69
1	A	239	ALA	CA-C-O	6.04	126.95	120.55
1	A	61	PHE	CA-C-O	-6.03	112.41	119.05
1	C	160	ASN	N-CA-C	6.02	120.35	111.87
1	A	164	ASP	CA-C-O	-6.00	114.59	121.19
1	B	113	ILE	CA-C-O	-6.00	113.82	120.96
1	A	184	GLU	O-C-N	-6.00	115.86	122.09
1	A	220	GLN	CG-CD-NE2	5.99	125.39	116.40
1	B	69	LEU	N-CA-CB	-5.99	101.32	110.01
1	C	20	ASP	O-C-N	5.99	128.98	122.15
1	A	73	LEU	CA-C-N	-5.98	112.52	122.21
1	A	73	LEU	C-N-CA	-5.98	112.52	122.21
1	B	126	LYS	O-C-N	5.98	128.97	122.15
1	C	25	ARG	NE-CZ-NH2	5.98	124.59	119.20
1	B	276	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	B	280	ASP	OD1-CG-OD2	-5.98	108.55	122.90
1	C	102	GLY	CA-C-O	5.98	125.31	119.27
1	A	286	LYS	CB-CG-CD	5.98	125.05	111.30
1	B	246	SER	CA-C-N	-5.98	115.55	120.33
1	B	246	SER	C-N-CA	-5.98	115.55	120.33
1	B	229	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	271	ARG	O-C-N	5.97	128.30	122.09
1	C	210	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	214	MET	CG-SD-CE	-5.96	87.80	100.90
1	B	210	PHE	CA-C-O	-5.96	114.24	120.55
1	C	109	VAL	CA-C-O	-5.95	113.83	120.25
1	B	123	ARG	CD-NE-CZ	5.94	132.72	124.40
1	C	267	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	17	GLU	O-C-N	5.92	129.55	122.27
1	A	245	ARG	O-C-N	5.91	128.47	122.09
1	B	160	ASN	OD1-CG-ND2	5.90	128.50	122.60
1	A	93	ALA	CA-C-N	5.90	128.47	120.44
1	A	93	ALA	C-N-CA	5.90	128.47	120.44
1	A	46	SER	N-CA-C	-5.90	103.16	110.41
1	C	282	PHE	O-C-N	5.90	128.40	122.03
1	C	132	GLU	CA-C-O	-5.88	112.85	119.79
1	A	102	GLY	N-CA-C	-5.88	107.64	115.40
1	B	191	GLU	N-CA-CB	5.87	118.75	110.12
1	A	149	TYR	CA-C-N	5.87	128.07	120.44
1	A	149	TYR	C-N-CA	5.87	128.07	120.44
1	C	200	THR	N-CA-CB	-5.87	102.78	110.88
1	C	17	GLU	CA-C-O	-5.87	113.47	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	VAL	CA-C-O	5.86	126.84	120.57
1	A	280	ASP	N-CA-CB	-5.86	102.53	111.66
1	A	289	ARG	O-C-N	5.85	128.09	122.07
1	B	174	GLN	CA-CB-CG	5.84	125.78	114.10
1	A	283	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	B	146	SER	O-C-N	5.83	129.90	123.25
1	C	306	GLY	N-CA-C	5.83	127.00	113.18
1	B	316	CYS	N-CA-C	5.82	117.31	110.97
1	A	196	THR	CA-C-N	-5.82	113.11	120.56
1	A	196	THR	C-N-CA	-5.82	113.11	120.56
1	A	291	ASN	CA-C-N	5.81	132.65	121.54
1	A	291	ASN	C-N-CA	5.81	132.65	121.54
1	A	4	VAL	CA-C-N	5.80	132.62	121.54
1	A	4	VAL	C-N-CA	5.80	132.62	121.54
1	B	182	ALA	CA-C-O	5.80	126.50	119.31
1	C	32	GLY	CA-C-N	5.80	131.98	121.89
1	C	32	GLY	C-N-CA	5.80	131.98	121.89
1	C	165	ALA	CA-C-O	-5.79	114.52	119.97
1	A	245	ARG	CA-C-O	-5.78	114.74	120.70
1	A	285	ARG	NE-CZ-NH2	5.78	124.41	119.20
1	A	202	SER	CA-C-O	5.78	128.57	121.87
1	C	119	PRO	O-C-N	5.78	128.70	122.17
1	B	218	GLY	O-C-N	-5.78	115.00	122.34
1	B	76	LYS	O-C-N	5.78	128.73	122.15
1	B	74	THR	CA-C-O	5.76	127.97	121.51
1	A	10	THR	N-CA-CB	-5.76	101.53	111.55
1	C	298	SER	O-C-N	5.76	128.22	122.12
1	A	296	LEU	CB-CA-C	5.75	121.23	110.70
1	B	48	ALA	O-C-N	5.75	128.22	122.12
1	A	47	ASN	CA-C-O	-5.75	114.46	120.55
1	A	77	PHE	O-C-N	5.74	128.21	122.12
1	A	17	GLU	CG-CD-OE2	-5.73	105.21	118.40
1	B	229	THR	CA-CB-CG2	5.73	120.24	110.50
1	B	188	GLY	O-C-N	-5.73	117.97	122.90
1	B	77	PHE	N-CA-C	-5.72	105.05	111.28
1	B	161	ARG	CA-CB-CG	5.72	125.53	114.10
1	A	221	ILE	O-C-N	-5.71	116.33	121.87
1	C	166	GLY	CA-C-N	5.70	129.10	120.77
1	C	166	GLY	C-N-CA	5.70	129.10	120.77
1	C	187	TRP	CA-C-O	-5.70	114.83	120.98
1	A	274	VAL	CA-C-O	-5.70	114.18	120.96
1	B	205	HIS	O-C-N	-5.69	115.94	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	GLU	CA-C-N	-5.69	112.85	123.03
1	A	228	GLU	C-N-CA	-5.69	112.85	123.03
1	A	296	LEU	O-C-N	5.69	129.62	122.23
1	C	167	ILE	N-CA-CB	-5.69	103.95	110.49
1	A	34	ASP	N-CA-C	-5.68	101.09	109.62
1	B	291	ASN	N-CA-C	-5.67	100.92	109.60
1	A	259	MET	CA-CB-CG	-5.67	102.77	114.10
1	C	260	LYS	CG-CD-CE	5.67	124.33	111.30
1	C	318	GLU	CA-CB-CG	5.67	125.43	114.10
1	B	154	VAL	CB-CA-C	5.67	119.22	111.97
1	C	147	GLY	O-C-N	5.66	128.35	122.86
1	A	314	LEU	CB-CA-C	5.66	121.54	110.67
1	B	4	VAL	CB-CA-C	-5.66	102.00	111.29
1	C	167	ILE	O-C-N	5.66	128.72	122.66
1	A	26	LYS	O-C-N	5.65	128.13	122.08
1	B	237	LEU	CB-CA-C	5.64	120.16	110.79
1	C	286	LYS	CA-C-O	-5.64	114.57	120.55
1	A	137	LEU	O-C-N	5.64	127.96	122.09
1	B	30	GLY	CA-C-N	5.64	132.31	121.54
1	B	30	GLY	C-N-CA	5.64	132.31	121.54
1	B	207	ARG	N-CA-C	-5.63	105.22	111.36
1	C	307	ASP	CB-CA-C	5.63	120.43	110.85
1	A	307	ASP	N-CA-C	-5.63	105.22	111.36
1	B	283	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	C	50	ARG	NH1-CZ-NH2	5.62	126.61	119.30
1	C	280	ASP	OD1-CG-OD2	-5.62	109.41	122.90
1	A	262	ALA	N-CA-C	-5.62	98.83	110.80
1	B	286	LYS	CA-C-O	-5.62	114.92	120.82
1	C	160	ASN	N-CA-CB	-5.61	102.63	111.39
1	A	61	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	148	TYR	CA-C-O	-5.61	112.48	119.38
1	A	245	ARG	CG-CD-NE	5.61	124.34	112.00
1	A	106	ASN	OD1-CG-ND2	-5.61	117.00	122.60
1	A	196	THR	N-CA-CB	5.60	118.14	110.01
1	A	220	GLN	N-CA-C	-5.60	102.19	110.48
1	C	63	ARG	CA-CB-CG	-5.60	102.90	114.10
1	C	108	LYS	CA-C-O	-5.60	114.61	120.55
1	A	84	LEU	CA-C-O	-5.60	113.53	119.97
1	C	292	PHE	N-CA-C	5.59	122.71	110.80
1	C	17	GLU	CG-CD-OE2	-5.59	105.55	118.40
1	C	280	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	31	LEU	N-CA-C	-5.58	102.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	HIS	CA-CB-CG	-5.58	108.22	113.80
1	A	47	ASN	CB-CG-ND2	5.58	124.77	116.40
1	B	228	GLU	CA-C-O	-5.57	113.01	119.14
1	A	281	LEU	CA-C-O	5.56	126.39	120.10
1	A	265	ASP	N-CA-C	-5.55	98.22	107.99
1	B	46	SER	CA-C-N	5.55	127.99	120.38
1	B	46	SER	C-N-CA	5.55	127.99	120.38
1	A	53	ILE	CA-C-O	5.55	126.72	120.95
1	A	313	LEU	O-C-N	5.54	128.70	122.22
1	C	12	PHE	N-CA-C	-5.54	103.09	110.07
1	A	106	ASN	CA-C-O	-5.54	115.16	120.92
1	C	77	PHE	CA-CB-CG	5.54	119.34	113.80
1	A	194	PHE	CB-CG-CD1	-5.53	111.30	120.70
1	A	301	LYS	O-C-N	5.53	127.76	122.07
1	C	53	ILE	O-C-N	-5.53	116.49	121.91
1	C	207	ARG	N-CA-C	-5.53	105.33	111.36
1	B	314	LEU	N-CA-C	-5.52	105.42	111.82
1	C	136	SER	CA-CB-OG	5.51	122.13	111.10
1	B	22	GLU	CA-C-N	-5.51	113.28	120.44
1	B	22	GLU	C-N-CA	-5.51	113.28	120.44
1	A	305	SER	CA-C-N	5.51	132.20	121.41
1	A	305	SER	C-N-CA	5.51	132.20	121.41
1	C	166	GLY	O-C-N	5.50	129.85	122.70
1	C	77	PHE	O-C-N	5.49	128.41	122.15
1	C	191	GLU	N-CA-CB	5.49	118.67	110.22
1	C	129	TYR	CA-C-O	5.49	126.56	120.63
1	A	304	THR	N-CA-C	5.47	118.62	110.14
1	C	35	GLU	CA-C-O	5.47	126.54	120.63
1	B	19	ALA	O-C-N	5.47	128.38	122.15
1	A	251	LEU	CB-CA-C	5.45	120.11	110.85
1	A	134	GLY	O-C-N	5.44	129.78	122.70
1	A	283	ASN	CA-C-O	-5.44	114.76	120.63
1	B	54	SER	CA-CB-OG	-5.44	100.23	111.10
1	B	228	GLU	O-C-N	5.44	129.78	122.49
1	C	289	ARG	CA-CB-CG	5.44	124.97	114.10
1	A	51	GLN	O-C-N	5.44	128.35	122.15
1	B	163	PRO	CB-CA-C	5.43	118.74	110.21
1	C	34	ASP	CA-C-O	-5.43	116.12	122.37
1	A	131	GLU	O-C-N	-5.43	116.44	122.09
1	B	184	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	95	GLU	CB-CA-C	5.42	119.39	110.88
1	B	72	GLU	CB-CG-CD	5.41	121.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	GLY	O-C-N	5.39	128.64	122.33
1	A	276	ARG	N-CA-C	5.39	119.96	113.17
1	B	168	ASP	CA-C-O	-5.38	114.56	120.70
1	C	45	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	A	34	ASP	CA-C-O	-5.38	115.69	122.63
1	A	295	SER	N-CA-C	-5.38	103.28	110.55
1	B	17	GLU	CG-CD-OE2	-5.38	106.02	118.40
1	C	123	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	A	178	ALA	O-C-N	-5.37	116.43	122.12
1	A	6[A]	ARG	N-CA-C	5.37	117.42	108.99
1	A	6[B]	ARG	N-CA-C	5.37	117.42	108.99
1	B	25	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	93	ALA	CA-C-N	5.36	127.72	120.44
1	B	93	ALA	C-N-CA	5.36	127.72	120.44
1	C	184	GLU	CA-C-O	-5.35	115.17	120.90
1	B	317	GLY	CA-C-N	5.35	131.33	121.70
1	B	317	GLY	C-N-CA	5.35	131.33	121.70
1	C	18	ARG	CD-NE-CZ	5.35	131.89	124.40
1	B	107	GLU	CG-CD-OE2	-5.34	106.11	118.40
1	B	50	ARG	CA-C-O	5.34	126.14	120.10
1	C	49	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	B	316	CYS	CA-C-N	5.33	129.17	121.44
1	B	316	CYS	C-N-CA	5.33	129.17	121.44
1	C	135	SER	CA-C-O	-5.32	115.44	121.72
1	B	174	GLN	N-CA-CB	-5.32	102.30	110.12
1	B	164	ASP	CA-C-O	-5.32	115.30	121.15
1	A	45	ARG	CA-C-O	-5.31	114.96	120.70
1	A	25	ARG	CA-C-O	5.31	126.39	120.82
1	C	17	GLU	CG-CD-OE1	5.31	130.60	118.40
1	B	196	THR	O-C-N	5.30	127.53	122.07
1	C	10	THR	CA-CB-OG1	-5.30	101.64	109.60
1	B	197	ILE	O-C-N	5.29	127.40	121.90
1	C	283	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	132	GLU	N-CA-C	5.29	118.89	112.23
1	B	223	GLU	CA-CB-CG	5.28	124.67	114.10
1	C	70	LYS	O-C-N	5.28	128.40	122.22
1	C	161	ARG	N-CA-CB	-5.28	102.27	110.04
1	C	285	ARG	CA-C-O	-5.28	115.45	121.00
1	B	211	ASP	O-C-N	5.28	127.80	122.09
1	B	158	GLN	N-CA-CB	5.28	119.15	110.39
1	A	203	VAL	CA-C-O	-5.28	115.19	121.05
1	A	214	MET	CB-CG-SD	-5.28	96.88	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	GLY	N-CA-C	-5.27	105.79	114.76
1	C	63	ARG	CA-C-O	-5.26	115.13	120.71
1	A	291	ASN	CB-CA-C	5.26	120.89	110.42
1	C	255	LEU	O-C-N	5.26	127.50	122.03
1	A	60	LEU	CA-C-N	5.25	130.60	122.26
1	A	60	LEU	C-N-CA	5.25	130.60	122.26
1	A	264	THR	CA-CB-OG1	-5.25	101.73	109.60
1	B	205	HIS	CA-CB-CG	5.25	119.05	113.80
1	C	289	ARG	CA-C-N	5.24	128.07	120.79
1	C	289	ARG	C-N-CA	5.24	128.07	120.79
1	C	55	ALA	CA-C-O	-5.24	114.87	120.42
1	C	46	SER	CA-C-N	5.24	127.30	120.28
1	C	46	SER	C-N-CA	5.24	127.30	120.28
1	C	184	GLU	CB-CG-CD	5.23	121.49	112.60
1	A	292	PHE	N-CA-C	5.23	121.93	110.80
1	C	208	LYS	CA-C-N	5.22	127.61	120.46
1	C	208	LYS	C-N-CA	5.22	127.61	120.46
1	A	298	SER	O-C-N	5.20	127.63	122.12
1	C	217	SER	N-CA-C	5.19	119.89	113.50
1	B	43	THR	N-CA-CB	-5.19	102.32	110.46
1	A	17	GLU	CG-CD-OE1	5.18	130.32	118.40
1	B	285	ARG	O-C-N	5.18	127.41	122.07
1	B	197	ILE	CA-C-O	-5.18	115.30	121.05
1	C	296	LEU	CB-CA-C	5.18	120.61	110.67
1	B	40	THR	N-CA-C	5.17	117.66	111.71
1	B	174	GLN	CB-CA-C	5.17	119.38	110.79
1	A	160	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	B	314	LEU	O-C-N	5.17	128.63	122.27
1	C	113	ILE	O-C-N	5.17	128.62	121.90
1	C	181	GLN	CA-CB-CG	-5.17	103.76	114.10
1	A	237	LEU	CB-CA-C	5.17	119.36	110.79
1	B	10	THR	N-CA-CB	-5.17	101.97	111.37
1	B	306	GLY	N-CA-C	5.16	125.41	113.18
1	A	244	ILE	O-C-N	5.16	126.88	121.87
1	B	52	GLU	CG-CD-OE1	-5.16	106.53	118.40
1	A	84	LEU	O-C-N	5.16	128.61	122.27
1	A	282	PHE	N-CA-C	-5.16	99.82	110.80
1	C	66	LEU	CB-CA-C	5.15	119.04	110.90
1	C	186	LYS	N-CA-C	5.15	118.21	109.76
1	A	160	ASN	N-CA-C	5.15	118.66	111.30
1	B	30	GLY	CA-C-O	5.15	129.53	120.57
1	A	205	HIS	CA-CB-CG	5.15	118.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	C	303	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	148	TYR	CA-C-N	-5.13	113.77	120.44
1	A	148	TYR	C-N-CA	-5.13	113.77	120.44
1	C	185	LEU	CB-CA-C	5.13	119.86	110.11
1	B	239	ALA	CA-C-O	5.13	125.99	120.55
1	B	164	ASP	N-CA-C	-5.12	103.02	110.24
1	B	50	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	B	141	VAL	CB-CA-C	5.12	118.72	112.02
1	C	190	ASP	CA-C-O	-5.11	116.35	122.13
1	A	107	GLU	CG-CD-OE1	5.11	130.15	118.40
1	B	64	ASP	CA-C-O	-5.11	114.71	120.43
1	A	258	ALA	N-CA-CB	5.10	118.15	110.30
1	A	270	ILE	O-C-N	5.10	127.39	121.94
1	B	228	GLU	N-CA-C	5.09	119.77	113.50
1	C	180	PHE	O-C-N	-5.09	116.83	122.07
1	C	161	ARG	CB-CA-C	5.09	118.72	109.62
1	A	158	GLN	N-CA-C	-5.08	106.34	112.54
1	A	216	ILE	N-CA-CB	-5.08	104.06	110.57
1	B	57	PHE	CA-C-N	-5.08	112.04	120.68
1	B	57	PHE	C-N-CA	-5.08	112.04	120.68
1	C	33	THR	CA-C-O	-5.08	113.36	120.21
1	C	196	THR	CA-C-N	-5.08	114.06	120.56
1	C	196	THR	C-N-CA	-5.08	114.06	120.56
1	A	12	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	44	SER	CA-C-O	5.07	126.09	119.95
1	C	164	ASP	CB-CA-C	5.07	118.13	109.72
1	C	280	ASP	N-CA-CB	-5.07	103.75	111.66
1	B	144	ASP	CA-CB-CG	-5.06	107.54	112.60
1	C	3	GLN	O-C-N	5.06	131.10	123.00
1	C	25	ARG	CD-NE-CZ	-5.06	117.31	124.40
1	C	106	ASN	CA-C-O	-5.06	114.93	120.70
1	A	95	GLU	N-CA-C	-5.05	105.66	111.07
1	C	142	VAL	CB-CA-C	5.05	118.35	111.88
1	A	296	LEU	CA-C-O	-5.05	114.63	120.24
1	C	5	LEU	N-CA-CB	5.05	119.02	110.49
1	C	135	SER	CA-C-N	-5.05	113.44	122.07
1	C	135	SER	C-N-CA	-5.05	113.44	122.07
1	B	216	ILE	CB-CG1-CD1	-5.05	103.20	113.80
1	C	101	LYS	N-CA-C	5.04	116.34	109.18
1	B	260	LYS	N-CA-CB	5.04	117.64	110.98
1	C	110	LEU	CA-C-O	5.04	126.11	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	LEU	CA-C-N	-5.04	115.14	122.65
1	B	185	LEU	C-N-CA	-5.04	115.14	122.65
1	B	312	LEU	CB-CA-C	5.04	118.79	110.88
1	B	210	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	146	SER	CA-C-O	-5.02	115.91	121.33
1	C	43	THR	N-CA-CB	-5.02	102.22	110.40
1	A	45	ARG	O-C-N	5.02	129.75	123.23
1	A	161	ARG	CA-CB-CG	5.02	124.13	114.10
1	C	118	THR	CA-C-N	5.01	124.18	118.97
1	C	118	THR	C-N-CA	5.01	124.18	118.97
1	A	88	SER	CA-C-N	5.01	127.69	120.38
1	A	88	SER	C-N-CA	5.01	127.69	120.38
1	A	99	ALA	N-CA-C	-5.01	106.68	112.89
1	B	215	THR	CA-C-O	-5.01	115.11	120.42
1	C	57	PHE	CA-CB-CG	5.01	118.81	113.80
1	B	32	GLY	CA-C-N	5.00	130.97	122.37
1	B	32	GLY	C-N-CA	5.00	130.97	122.37
1	C	197	ILE	O-C-N	5.00	127.10	121.90

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	6[A]	ARG	Sidechain
1	A	6[B]	ARG	Sidechain
1	A	63	ARG	Sidechain
1	B	117	ARG	Sidechain
1	B	151[A]	ARG	Sidechain
1	B	151[B]	ARG	Sidechain
1	B	161	ARG	Sidechain
1	B	25	ARG	Sidechain
1	B	276	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	50	ARG	Sidechain
1	B	63	ARG	Sidechain
1	C	117	ARG	Sidechain
1	C	123	ARG	Sidechain
1	C	151[A]	ARG	Sidechain
1	C	151[B]	ARG	Sidechain
1	C	161	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	227	ARG	Sidechain
1	C	25	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	289	ARG	Sidechain
1	C	45	ARG	Sidechain
1	C	63	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2519	0	2540	104	0
1	B	2513	0	2530	107	0
1	C	2513	0	2531	111	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	151	0	0	7	0
4	B	133	0	0	7	0
4	C	134	0	0	9	0
All	All	7990	0	7601	322	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 21.

All (322) 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:A:3:GLN:HG2	1:A:247:ILE:HD13	1.28	1.07
1:B:3:GLN:HG2	1:B:247:ILE:HD13	1.33	1.07
1:B:123:ARG:NH2	1:B:159:ALA:O	1.94	0.99
1:B:3:GLN:N	4:B:378:HOH:O	1.99	0.96
1:A:41:LEU:HD13	1:A:45:ARG:HH11	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLN:NE2	1:B:121:GLU:OE1	1.99	0.94
1:A:3:GLN:N	4:A:452:HOH:O	2.00	0.94
1:A:41:LEU:HD13	1:A:45:ARG:NH1	1.83	0.94
1:A:3:GLN:NE2	1:A:116:SER:O	2.02	0.91
1:A:286:LYS:HZ1	1:A:289:ARG:HH11	1.21	0.86
1:C:3:GLN:NE2	1:C:121:GLU:OE1	2.09	0.85
1:C:273:MET:HE2	1:C:281:LEU:HD11	1.58	0.85
1:A:3:GLN:HG3	1:A:118:THR:HG23	1.59	0.84
1:B:3:GLN:HG3	1:B:118:THR:HG23	1.61	0.82
1:B:286:LYS:NZ	1:B:289:ARG:HE	1.76	0.82
1:C:3:GLN:OE1	1:C:247:ILE:HG21	1.79	0.81
1:A:286:LYS:HZ1	1:A:289:ARG:NH1	1.78	0.81
1:B:6:ARG:H	1:B:283:ASN:HD21	1.25	0.81
1:C:6:ARG:H	1:C:283:ASN:HD21	1.23	0.81
1:B:286:LYS:NZ	1:B:289:ARG:NE	2.29	0.80
1:C:214:MET:HE2	1:C:219:PHE:C	2.06	0.79
1:B:41:LEU:HG	1:B:45:ARG:NH1	1.97	0.79
1:A:152:MET:HG2	1:A:236:LEU:HD13	1.65	0.79
1:B:100:LEU:HD11	1:B:110:LEU:HD11	1.64	0.78
1:B:6:ARG:HG3	1:B:6:ARG:HH11	1.45	0.78
1:B:286:LYS:HZ3	1:B:289:ARG:NE	1.81	0.77
1:B:286:LYS:HZ1	1:B:289:ARG:HE	1.30	0.77
1:B:289:ARG:HD3	4:B:381:HOH:O	1.83	0.77
1:A:100:LEU:HD13	1:A:110:LEU:HD11	1.68	0.75
1:B:273:MET:HE2	1:B:281:LEU:HD11	1.67	0.75
1:A:96:LEU:HD13	1:A:113:ILE:HD12	1.66	0.75
1:A:265:ASP:O	1:A:269:LEU:HB2	1.85	0.75
1:A:297:TYR:CE1	1:A:313:LEU:HD13	2.21	0.75
1:A:273:MET:HE2	1:A:281:LEU:HD11	1.70	0.74
1:C:3:GLN:HG2	1:C:118:THR:HG23	1.68	0.74
1:A:285:ARG:HH11	1:A:289:ARG:HH22	1.33	0.74
1:C:293:ALA:O	1:C:294:THR:HB	1.88	0.73
1:A:305:SER:O	1:A:309:LYS:HB2	1.89	0.72
1:C:310:LYS:HE2	1:C:310:LYS:HA	1.70	0.72
1:B:3:GLN:OE1	1:B:247:ILE:HG21	1.89	0.72
1:C:259:MET:HG2	1:C:264:THR:HG23	1.71	0.71
1:A:41:LEU:HD12	1:A:41:LEU:C	2.15	0.71
1:A:291:ASN:O	1:A:293:ALA:N	2.20	0.71
1:C:22:GLU:O	1:C:26:LYS:HG2	1.90	0.71
1:C:3:GLN:O	1:C:280:ASP:OD2	2.08	0.71
1:B:39:LEU:O	1:B:43:THR:HB	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:O	1:A:314:LEU:HB2	1.92	0.70
1:A:285:ARG:HD2	1:A:289:ARG:NH2	2.07	0.69
1:A:233:LEU:HG	1:A:237:LEU:HD22	1.73	0.69
1:A:304:THR:OG1	1:A:309:LYS:HG2	1.92	0.69
1:C:297:TYR:CD2	1:C:318:GLU:HB2	2.28	0.69
1:A:259:MET:HG2	1:A:264:THR:HG23	1.73	0.69
1:B:310:LYS:O	1:B:314:LEU:HD22	1.93	0.68
1:C:108:LYS:HG3	4:C:380:HOH:O	1.91	0.68
1:B:273:MET:CE	1:B:281:LEU:HD11	2.21	0.68
1:A:97:LYS:HD3	1:A:133:TYR:CG	2.29	0.68
1:C:39:LEU:O	1:C:43:THR:HB	1.94	0.67
1:B:6:ARG:H	1:B:283:ASN:ND2	1.93	0.67
1:B:66:LEU:HD11	1:B:82:VAL:HG12	1.77	0.66
1:B:214:MET:CE	1:B:219:PHE:C	2.68	0.66
1:C:297:TYR:HD2	1:C:318:GLU:HB2	1.60	0.66
1:C:22:GLU:HB3	1:C:26:LYS:HE2	1.77	0.66
1:C:211:ASP:O	1:C:215:THR:HG23	1.94	0.66
1:A:43:THR:HG21	1:A:314:LEU:HG	1.78	0.66
1:A:261:GLY:O	1:A:263:GLY:N	2.30	0.65
1:A:293:ALA:O	1:A:294:THR:HB	1.95	0.65
1:B:297:TYR:CE1	1:B:313:LEU:HD13	2.32	0.65
1:B:220:GLN:NE2	4:B:396:HOH:O	2.29	0.65
1:B:22:GLU:O	1:B:26:LYS:HG2	1.97	0.65
1:C:286:LYS:HZ3	1:C:289:ARG:HD3	1.62	0.65
1:A:39:LEU:O	1:A:43:THR:HB	1.97	0.64
1:A:41:LEU:C	1:A:41:LEU:CD1	2.71	0.63
1:A:240:VAL:O	1:A:244:ILE:HG12	1.98	0.63
1:C:246:SER:HB3	1:C:249:ALA:HB3	1.80	0.63
1:B:147:GLY:O	1:B:151[A]:ARG:HD3	1.99	0.63
1:B:291:ASN:O	1:B:293:ALA:N	2.26	0.63
1:A:220:GLN:NE2	4:A:411:HOH:O	2.31	0.62
1:C:233:LEU:HG	1:C:237:LEU:HD22	1.81	0.62
1:A:297:TYR:CD1	1:A:313:LEU:HD22	2.34	0.62
1:A:3:GLN:CD	1:A:276:ARG:HH22	2.07	0.62
1:C:12:PHE:HB2	1:C:44:SER:O	2.00	0.62
1:A:286:LYS:NZ	1:A:289:ARG:NH1	2.47	0.62
1:C:3:GLN:CG	1:C:118:THR:HG23	2.30	0.62
1:B:3:GLN:O	1:B:280:ASP:OD2	2.17	0.62
1:B:246:SER:HB3	1:B:249:ALA:HB3	1.82	0.61
1:C:4:VAL:HA	1:C:280:ASP:HB3	1.82	0.61
1:B:3:GLN:HG2	1:B:247:ILE:CD1	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASN:O	1:C:293:ALA:N	2.29	0.61
1:A:294:THR:HG21	1:A:299:MET:CE	2.31	0.61
1:B:22:GLU:HB3	1:B:26:LYS:HE3	1.83	0.61
1:C:285:ARG:HH12	1:C:289:ARG:HH12	1.49	0.60
1:B:233:LEU:HG	1:B:237:LEU:HD22	1.83	0.60
1:A:299:MET:O	1:A:303:ASP:HB2	2.02	0.60
1:C:281:LEU:O	1:C:285:ARG:HG3	2.01	0.60
1:B:258:ALA:HB1	1:B:265:ASP:HB3	1.84	0.59
1:B:172:VAL:HG12	1:B:212:LYS:HD2	1.84	0.59
1:A:286:LYS:HZ2	1:A:286:LYS:HA	1.68	0.59
1:B:6:ARG:N	1:B:283:ASN:HD21	1.98	0.59
1:A:294:THR:HG21	1:A:299:MET:HE3	1.86	0.58
1:B:280:ASP:O	1:B:284:ILE:HG13	2.04	0.58
1:C:5:LEU:HB3	1:C:283:ASN:OD1	2.03	0.58
1:B:91:TYR:OH	4:B:339:HOH:O	2.16	0.57
1:B:240:VAL:O	1:B:244:ILE:HG12	2.05	0.57
1:C:293:ALA:O	1:C:294:THR:CB	2.53	0.57
1:B:6:ARG:O	1:B:282:PHE:HB3	2.04	0.56
1:C:285:ARG:HH11	1:C:289:ARG:HH22	1.52	0.56
1:A:246:SER:HB3	1:A:249:ALA:HB3	1.87	0.56
1:B:4:VAL:HA	1:B:280:ASP:HB3	1.88	0.56
1:C:22:GLU:HB3	1:C:26:LYS:CE	2.36	0.56
1:C:256:TYR:HD2	1:C:257:TYR:CE1	2.24	0.55
1:C:91:TYR:OH	4:C:361:HOH:O	2.15	0.54
1:B:309:LYS:HZ3	1:B:310:LYS:HZ2	1.54	0.54
1:A:5:LEU:HB3	1:A:283:ASN:OD1	2.08	0.54
1:B:41:LEU:O	1:B:45:ARG:HG2	2.07	0.54
1:C:263:GLY:O	4:C:413:HOH:O	2.19	0.54
1:C:308:TYR:CE1	1:C:312:LEU:HD11	2.43	0.54
1:B:100:LEU:HD11	1:B:110:LEU:CD1	2.36	0.54
1:C:105:THR:OG1	1:C:144:ASP:HB3	2.06	0.54
1:A:11:ASP:OD1	1:A:46:SER:OG	2.15	0.53
1:B:47:ASN:O	1:B:51:GLN:HG2	2.07	0.53
1:C:6:ARG:N	1:C:283:ASN:HD21	2.01	0.53
1:C:273:MET:HE2	1:C:281:LEU:CD1	2.36	0.53
1:B:96:LEU:O	1:B:100:LEU:HD13	2.09	0.53
1:C:285:ARG:HH11	1:C:289:ARG:NH2	2.07	0.53
1:B:151[B]:ARG:NH2	4:B:426:HOH:O	2.40	0.53
1:C:8:THR:HG23	1:C:281:LEU:HB3	1.91	0.53
1:C:285:ARG:NH1	1:C:289:ARG:HH12	2.07	0.53
1:C:214:MET:HE2	1:C:219:PHE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:HD2	1:B:286:LYS:N	2.24	0.52
1:B:3:GLN:OE1	1:B:276:ARG:NH2	2.42	0.52
1:B:15:PHE:CE2	1:B:52:GLU:HG3	2.44	0.52
1:C:18:ARG:NH2	4:C:326:HOH:O	2.43	0.52
1:A:28:MET:SD	1:A:72:GLU:HG3	2.49	0.52
1:A:282:PHE:O	1:A:285:ARG:HB2	2.09	0.52
1:B:66:LEU:CD1	1:B:82:VAL:HG12	2.40	0.52
1:C:253:GLU:HG3	1:C:257:TYR:HE1	1.74	0.52
1:A:152:MET:CG	1:A:236:LEU:HD13	2.38	0.52
1:A:305:SER:C	1:A:309:LYS:HB2	2.35	0.52
1:B:3:GLN:NE2	1:B:117:ARG:HA	2.25	0.51
1:B:259:MET:HG2	1:B:264:THR:HG23	1.92	0.51
1:C:253:GLU:HG3	1:C:257:TYR:CE1	2.45	0.51
1:A:3:GLN:HB2	4:A:415:HOH:O	2.10	0.51
1:A:214:MET:HA	1:A:219:PHE:O	2.10	0.51
1:B:15:PHE:HE2	1:B:52:GLU:HG3	1.74	0.51
1:B:211:ASP:O	1:B:215:THR:HG23	2.11	0.51
1:C:292:PHE:O	1:C:293:ALA:O	2.29	0.51
1:A:149:TYR:CD1	1:A:232:ASN:HB3	2.45	0.51
1:B:214:MET:HE2	1:B:219:PHE:C	2.35	0.51
1:A:256:TYR:HD2	1:A:257:TYR:CD1	2.27	0.51
1:A:307:ASP:N	4:A:421:HOH:O	2.44	0.51
1:C:259:MET:HE3	1:C:299:MET:HG2	1.92	0.51
1:A:12:PHE:HB2	1:A:44:SER:O	2.12	0.50
1:C:6:ARG:H	1:C:283:ASN:ND2	1.99	0.50
1:C:273:MET:HE1	1:C:316:CYS:HB2	1.93	0.50
1:A:118:THR:HB	1:A:119:PRO:CD	2.41	0.50
1:A:97:LYS:HD3	1:A:133:TYR:CD1	2.46	0.49
1:A:147:GLY:O	1:A:151[B]:ARG:HG3	2.12	0.49
1:A:214:MET:HE2	1:A:220:GLN:OE1	2.12	0.49
1:A:273:MET:HE1	1:A:316:CYS:HB2	1.94	0.49
1:B:310:LYS:HE3	1:B:313:LEU:HD12	1.94	0.49
1:B:11:ASP:OD1	1:B:46:SER:OG	2.15	0.49
1:A:208:LYS:NZ	4:A:442:HOH:O	2.46	0.49
1:C:285:ARG:NH1	1:C:289:ARG:HH22	2.10	0.49
1:A:301:LYS:HA	1:A:309:LYS:HD3	1.95	0.49
1:B:18:ARG:O	1:B:22:GLU:HG3	2.12	0.49
1:B:273:MET:HE3	1:B:281:LEU:HD21	1.95	0.49
1:A:3:GLN:O	1:A:280:ASP:OD2	2.31	0.49
1:C:100:LEU:HD13	1:C:110:LEU:HD11	1.94	0.49
1:C:294:THR:HG21	1:C:299:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:OE1	1:A:276:ARG:NH1	2.41	0.49
1:B:214:MET:HE3	1:B:219:PHE:C	2.38	0.49
1:B:297:TYR:CD1	1:B:313:LEU:HD22	2.48	0.49
1:B:309:LYS:NZ	1:B:310:LYS:HZ2	2.10	0.49
1:C:309:LYS:O	1:C:313:LEU:HD22	2.13	0.49
1:B:263:GLY:O	4:B:452:HOH:O	2.20	0.48
1:C:282:PHE:O	1:C:285:ARG:HB2	2.13	0.48
1:B:82:VAL:O	1:B:86[A]:LYS:HG2	2.13	0.48
1:C:260:LYS:HE2	1:C:260:LYS:O	2.13	0.48
1:C:307:ASP:N	4:C:444:HOH:O	2.36	0.48
1:A:285:ARG:HH11	1:A:289:ARG:NH2	2.06	0.48
1:B:253:GLU:HA	1:B:292:PHE:CE2	2.48	0.48
1:A:25:ARG:NH1	4:A:378:HOH:O	2.46	0.48
1:B:259:MET:CE	1:B:299:MET:HG2	2.43	0.48
1:A:261:GLY:C	1:A:263:GLY:N	2.69	0.48
1:C:4:VAL:HG23	1:C:5:LEU:N	2.28	0.48
1:A:297:TYR:HE1	1:A:313:LEU:HD13	1.74	0.48
1:C:3:GLN:NE2	1:C:117:ARG:HA	2.28	0.48
1:B:161:ARG:HG3	1:B:201:ARG:O	2.14	0.48
1:A:43:THR:HG21	1:A:314:LEU:CG	2.42	0.48
1:C:106:ASN:ND2	1:C:109:VAL:HG12	2.29	0.48
1:C:108:LYS:HE3	4:C:380:HOH:O	2.13	0.48
1:B:264:THR:OG1	1:B:303:ASP:OD2	2.31	0.47
1:B:292:PHE:O	1:B:293:ALA:O	2.32	0.47
1:C:3:GLN:OE1	1:C:276:ARG:NH2	2.48	0.47
1:A:105:THR:OG1	1:A:144:ASP:HB3	2.15	0.47
1:B:309:LYS:NZ	1:B:310:LYS:NZ	2.62	0.47
1:C:3:GLN:CD	1:C:276:ARG:HH22	2.23	0.47
1:B:6:ARG:HG3	1:B:6:ARG:NH1	2.20	0.47
1:B:214:MET:HE3	1:B:220:GLN:N	2.29	0.47
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.80	0.47
1:B:101:LYS:HB3	1:B:102:GLY:H	1.40	0.47
1:C:43:THR:HG21	1:C:314:LEU:HB3	1.96	0.47
1:C:167:ILE:HG22	1:C:169[B]:GLU:OE1	2.14	0.47
1:A:106:ASN:ND2	1:A:109:VAL:HG23	2.30	0.47
1:B:96:LEU:HD13	1:B:113:ILE:HD12	1.97	0.47
1:C:240:VAL:O	1:C:244:ILE:HG12	2.15	0.47
1:C:276:ARG:HH21	1:C:280:ASP:CG	2.23	0.46
1:C:297:TYR:CE1	1:C:313:LEU:HG	2.49	0.46
1:C:3:GLN:HA	1:C:247:ILE:HD13	1.98	0.46
1:C:214:MET:CE	1:C:219:PHE:C	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HB	1:A:119:PRO:HD2	1.97	0.46
1:B:299:MET:HE3	1:B:299:MET:HB2	1.72	0.46
1:C:108:LYS:HZ1	1:C:235:GLN:HB3	1.80	0.46
1:B:299:MET:O	1:B:303:ASP:HB2	2.15	0.46
1:B:39:LEU:HB3	1:B:77:PHE:CZ	2.51	0.46
1:B:149:TYR:CD1	1:B:232:ASN:HB3	2.50	0.46
1:C:256:TYR:CD2	1:C:292:PHE:CE1	3.04	0.46
1:B:273:MET:O	1:B:277:SER:HB3	2.16	0.46
1:A:285:ARG:NH1	1:A:318:GLU:HB3	2.31	0.45
1:B:18:ARG:NH2	4:B:371:HOH:O	2.12	0.45
1:B:260:LYS:HA	1:B:260:LYS:HD2	1.47	0.45
1:B:276:ARG:HH21	1:B:280:ASP:CG	2.23	0.45
1:B:297:TYR:HE1	1:B:313:LEU:HD13	1.79	0.45
1:A:41:LEU:O	1:A:45:ARG:HG2	2.15	0.45
1:B:84:LEU:HD13	1:B:274:VAL:HG22	1.97	0.45
1:C:247:ILE:N	1:C:248:PRO:CD	2.80	0.45
1:C:214:MET:HE3	1:C:220:GLN:NE2	2.31	0.45
1:B:4:VAL:HB	1:B:5:LEU:H	1.44	0.45
1:B:310:LYS:HD3	1:B:310:LYS:HA	1.63	0.45
1:A:4:VAL:HB	1:A:5:LEU:H	1.39	0.45
1:A:48:ALA:O	1:A:52:GLU:HG3	2.16	0.45
1:C:192:GLU:HG3	4:C:404:HOH:O	2.16	0.45
1:C:97:LYS:HD3	1:C:133:TYR:CG	2.51	0.45
1:C:15:PHE:CZ	1:C:17:GLU:HB3	2.52	0.44
1:C:24:LEU:HD12	1:C:53:ILE:HG21	1.99	0.44
1:A:174:GLN:HG3	4:A:439:HOH:O	2.17	0.44
1:C:161:ARG:HG3	1:C:201:ARG:O	2.16	0.44
1:A:79:LYS:N	1:A:79:LYS:HD2	2.33	0.44
1:B:35:GLU:HA	1:B:38:ILE:HD12	2.00	0.44
1:B:247:ILE:N	1:B:248:PRO:CD	2.80	0.44
1:A:247:ILE:N	1:A:248:PRO:CD	2.80	0.44
1:A:259:MET:HE3	1:A:299:MET:HG2	1.99	0.44
1:C:253:GLU:O	1:C:257:TYR:HD1	2.00	0.44
1:A:69:LEU:HG	1:A:81:ILE:HG21	2.00	0.44
1:B:3:GLN:HB3	1:B:276:ARG:HH22	1.82	0.44
1:B:39:LEU:HB3	1:B:77:PHE:HZ	1.82	0.44
1:C:285:ARG:HG2	1:C:296:LEU:HD23	1.98	0.44
1:A:123:ARG:NH2	1:A:159:ALA:O	2.50	0.44
1:C:280:ASP:HA	1:C:283:ASN:HD22	1.82	0.44
1:A:190:ASP:OD2	1:A:193[A]:LYS:HE2	2.17	0.44
1:A:46:SER:O	1:A:50:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:THR:CG2	1:C:314:LEU:HB3	2.48	0.44
1:C:280:ASP:O	1:C:284:ILE:HG13	2.18	0.44
1:B:97:LYS:HD3	1:B:133:TYR:CD1	2.53	0.43
1:C:5:LEU:HD22	1:C:5:LEU:HA	1.77	0.43
1:C:257:TYR:CD1	1:C:257:TYR:N	2.86	0.43
1:C:123:ARG:HD2	4:C:351:HOH:O	2.17	0.43
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.79	0.43
1:A:245:ARG:HG2	1:A:245:ARG:HH11	1.83	0.43
1:B:5:LEU:HB3	1:B:283:ASN:OD1	2.18	0.43
1:B:3:GLN:HE21	1:B:121:GLU:CD	2.16	0.43
1:C:147:GLY:O	1:C:151[A]:ARG:HD2	2.18	0.43
1:A:15:PHE:CZ	1:A:17:GLU:HB3	2.53	0.43
1:A:214:MET:CE	1:A:220:GLN:OE1	2.67	0.43
1:A:285:ARG:HH12	1:A:318:GLU:HB3	1.84	0.43
1:C:43:THR:HG21	1:C:314:LEU:HG	2.00	0.43
1:A:3:GLN:HB3	1:A:276:ARG:HH22	1.84	0.43
1:C:108:LYS:NZ	1:C:235:GLN:HB3	2.34	0.43
1:B:5:LEU:HD22	1:B:5:LEU:HA	1.91	0.43
1:B:208:LYS:NZ	1:B:208:LYS:HB3	2.34	0.43
1:C:94:TYR:O	1:C:98:HIS:HD2	2.02	0.43
1:C:4:VAL:CG2	1:C:5:LEU:N	2.78	0.42
1:C:43:THR:HG21	1:C:314:LEU:CG	2.49	0.42
1:C:151[B]:ARG:NH2	4:C:425:HOH:O	2.49	0.42
1:A:41:LEU:HD22	1:A:45:ARG:HH12	1.85	0.42
1:B:15:PHE:HZ	1:B:53:ILE:HG13	1.84	0.42
1:A:260:LYS:HA	1:A:260:LYS:HD2	1.57	0.42
1:B:148:TYR:CE1	1:B:151[B]:ARG:NH1	2.88	0.42
1:C:267:HIS:HD2	1:C:267:HIS:O	2.03	0.42
1:B:106:ASN:OD1	1:B:108:LYS:HB3	2.19	0.42
1:C:273:MET:HE3	1:C:281:LEU:HD21	2.01	0.42
1:C:96:LEU:HD12	1:C:110:LEU:HD12	2.02	0.42
1:A:114:ILE:HD12	1:A:153:LEU:HD22	2.01	0.42
1:A:145:THR:O	1:A:150:GLN:NE2	2.53	0.42
1:B:100:LEU:HD23	1:B:140:ASP:HB3	2.02	0.42
1:B:251:LEU:HB3	1:B:284:ILE:HD13	2.02	0.41
1:C:11:ASP:OD1	1:C:46:SER:OG	2.38	0.41
1:C:78:GLU:O	1:C:79:LYS:C	2.63	0.41
1:A:47:ASN:O	1:A:51:GLN:HG2	2.19	0.41
1:A:75:GLY:O	1:A:79:LYS:HD3	2.19	0.41
1:B:3:GLN:NE2	1:B:121:GLU:CD	2.74	0.41
1:C:290:LYS:C	1:C:291:ASN:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151[B]:ARG:HH11	1:A:151[B]:ARG:HD2	1.58	0.41
1:A:221:ILE:HD12	1:A:221:ILE:HA	1.91	0.41
1:B:247:ILE:HB	1:B:248:PRO:HD3	2.01	0.41
1:C:82:VAL:O	1:C:86[B]:LYS:HG2	2.21	0.41
1:C:114:ILE:HD12	1:C:153:LEU:HD22	2.03	0.41
1:A:259:MET:CE	1:A:299:MET:HG2	2.50	0.41
1:A:286:LYS:NZ	1:A:289:ARG:HD2	2.36	0.41
1:C:129:TYR:OH	1:C:140:ASP:OD2	2.31	0.41
1:C:299:MET:HE3	1:C:299:MET:HB2	1.67	0.41
1:C:310:LYS:O	1:C:314:LEU:HD22	2.21	0.41
1:A:161:ARG:HG3	1:A:201:ARG:O	2.20	0.41
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.90	0.41
1:C:285:ARG:HH11	1:C:285:ARG:HD2	1.64	0.41
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.92	0.41
1:A:182:ALA:HB1	1:A:190:ASP:HB3	2.03	0.41
1:C:285:ARG:O	1:C:289:ARG:HD2	2.20	0.41
1:B:76:LYS:HE2	1:B:266:ASP:OD2	2.21	0.40
1:C:3:GLN:NE2	1:C:276:ARG:HH12	2.20	0.40
1:C:286:LYS:HA	1:C:289:ARG:HG2	2.03	0.40
1:C:299:MET:O	1:C:303:ASP:HB2	2.21	0.40
1:A:256:TYR:HB2	1:A:288:PHE:CE1	2.57	0.40
1:C:4:VAL:HB	1:C:5:LEU:H	1.37	0.40
1:B:41:LEU:HG	1:B:45:ARG:HH12	1.84	0.40
1:B:95:GLU:CD	1:B:267:HIS:HE2	2.27	0.40
1:B:285:ARG:HD3	1:B:316:CYS:SG	2.62	0.40
1:C:26:LYS:N	1:C:26:LYS:HD3	2.37	0.40
1:C:310:LYS:NZ	1:C:314:LEU:HD22	2.37	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	319/319 (100%)	293 (92%)	18 (6%)	8 (2%)	4	1
1	B	318/319 (100%)	296 (93%)	13 (4%)	9 (3%)	4	0
1	C	318/319 (100%)	294 (92%)	17 (5%)	7 (2%)	5	1
All	All	955/957 (100%)	883 (92%)	48 (5%)	24 (2%)	4	1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	103	ALA
1	A	292	PHE
1	A	294	THR
1	B	5	LEU
1	B	292	PHE
1	B	293	ALA
1	B	294	THR
1	C	5	LEU
1	C	103	ALA
1	C	292	PHE
1	C	294	THR
1	A	291	ASN
1	A	293	ALA
1	B	103	ALA
1	B	262	ALA
1	C	293	ALA
1	A	4	VAL
1	B	30	GLY
1	A	166	GLY
1	C	4	VAL
1	B	166	GLY
1	B	4	VAL
1	C	166	GLY

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	274/271 (101%)	232 (85%)	42 (15%)	3	1
1	B	273/271 (101%)	236 (86%)	37 (14%)	3	1
1	C	273/271 (101%)	224 (82%)	49 (18%)	2	0
All	All	820/813 (101%)	692 (84%)	128 (16%)	2	1

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	THR
1	A	26	LYS
1	A	31	LEU
1	A	33	THR
1	A	39	LEU
1	A	41	LEU
1	A	42	LEU
1	A	43	THR
1	A	59	THR
1	A	60	LEU
1	A	69	LEU
1	A	71	SER
1	A	78	GLU
1	A	84	LEU
1	A	89	ARG
1	A	96	LEU
1	A	100	LEU
1	A	108	LYS
1	A	110	LEU
1	A	128	VAL
1	A	136	SER
1	A	137	LEU
1	A	160	ASN
1	A	163	PRO
1	A	208	LYS
1	A	236	LEU
1	A	237	LEU
1	A	251	LEU
1	A	260	LYS
1	A	269	LEU
1	A	281	LEU
1	A	283	ASN
1	A	286	LYS

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Mol	Chain	Res	Type
1	A	290	LYS
1	A	291	ASN
1	A	294	THR
1	A	298	SER
1	A	303	ASP
1	A	309	LYS
1	A	310	LYS
1	A	314	LEU
1	B	3	GLN
1	B	5	LEU
1	B	6	ARG
1	B	10	THR
1	B	33	THR
1	B	36	GLU
1	B	39	LEU
1	B	42	LEU
1	B	43	THR
1	B	52	GLU
1	B	59	THR
1	B	60	LEU
1	B	69	LEU
1	B	84	LEU
1	B	90	LEU
1	B	96	LEU
1	B	123	ARG
1	B	141	VAL
1	B	151[A]	ARG
1	B	151[B]	ARG
1	B	169[A]	GLU
1	B	169[B]	GLU
1	B	208	LYS
1	B	212	LYS
1	B	214	MET
1	B	237	LEU
1	B	251	LEU
1	B	260	LYS
1	B	281	LEU
1	B	286	LYS
1	B	289	ARG
1	B	290	LYS
1	B	291	ASN
1	B	299	MET

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Mol	Chain	Res	Type
1	B	303	ASP
1	B	310	LYS
1	B	314	LEU
1	C	5	LEU
1	C	22	GLU
1	C	25	ARG
1	C	33	THR
1	C	36	GLU
1	C	39	LEU
1	C	42	LEU
1	C	43	THR
1	C	45	ARG
1	C	59	THR
1	C	60	LEU
1	C	69	LEU
1	C	76	LYS
1	C	84	LEU
1	C	86[A]	LYS
1	C	86[B]	LYS
1	C	89	ARG
1	C	96	LEU
1	C	97	LYS
1	C	100	LEU
1	C	108	LYS
1	C	109	VAL
1	C	110	LEU
1	C	117	ARG
1	C	123	ARG
1	C	127	GLN
1	C	137	LEU
1	C	160	ASN
1	C	185	LEU
1	C	214	MET
1	C	227	ARG
1	C	237	LEU
1	C	251	LEU
1	C	260	LYS
1	C	264	THR
1	C	269	LEU
1	C	273	MET
1	C	281	LEU
1	C	286	LYS

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Mol	Chain	Res	Type
1	C	289	ARG
1	C	290	LYS
1	C	291	ASN
1	C	298	SER
1	C	299	MET
1	C	303	ASP
1	C	305	SER
1	C	310	LYS
1	C	313	LEU
1	C	314	LEU

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

Mol	Chain	Res	Type
1	A	98	HIS
1	A	127	GLN
1	A	177	GLN
1	A	181	GLN
1	A	283	ASN
1	B	150	GLN
1	B	160	ASN
1	B	171	GLN
1	B	174	GLN
1	B	177	GLN
1	B	181	GLN
1	B	220	GLN
1	B	235	GLN
1	B	283	ASN
1	C	150	GLN
1	C	158	GLN
1	C	160	ASN
1	C	232	ASN
1	C	283	ASN

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](#)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	322	2	4,4,4	1.49	1 (25%)	6,6,6	0.51	0
3	SO4	C	322	2	4,4,4	1.60	1 (25%)	6,6,6	0.95	0
3	SO4	A	322	2	4,4,4	1.48	1 (25%)	6,6,6	0.94	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	322	SO4	O1-S	2.77	1.61	1.44
3	B	322	SO4	O1-S	2.60	1.60	1.44
3	A	322	SO4	O1-S	2.42	1.59	1.44

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	88:SER	C	89:ARG	N	1.19

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.