



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:58 AM UTC

PDB ID : 7R1R / pdb_00007r1r
Title : RIBONUCLEOTIDE REDUCTASE E441Q MUTANT R1 PROTEIN FROM
ESCHERICHIA COLI
Authors : Eriksson, M.; Eklund, H.
Deposited on : 1997-09-17
Resolution : 3.10 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

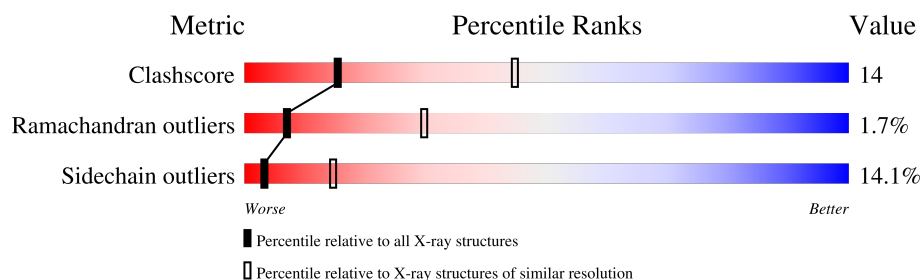
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	761	
1	B	761	
1	C	761	
2	D	20	
2	E	20	
2	F	20	
2	P	20	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18166 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 RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			
1	B	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			
1	C	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLN	GLU	engineered mutation	UNP P00452
B	441	GLN	GLU	engineered mutation	UNP P00452
C	441	GLN	GLU	engineered mutation	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOTIDE REDUCTASE R2 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	E	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	F	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	P	4	Total	C	N	O	0	0	0
			31	22	4	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		

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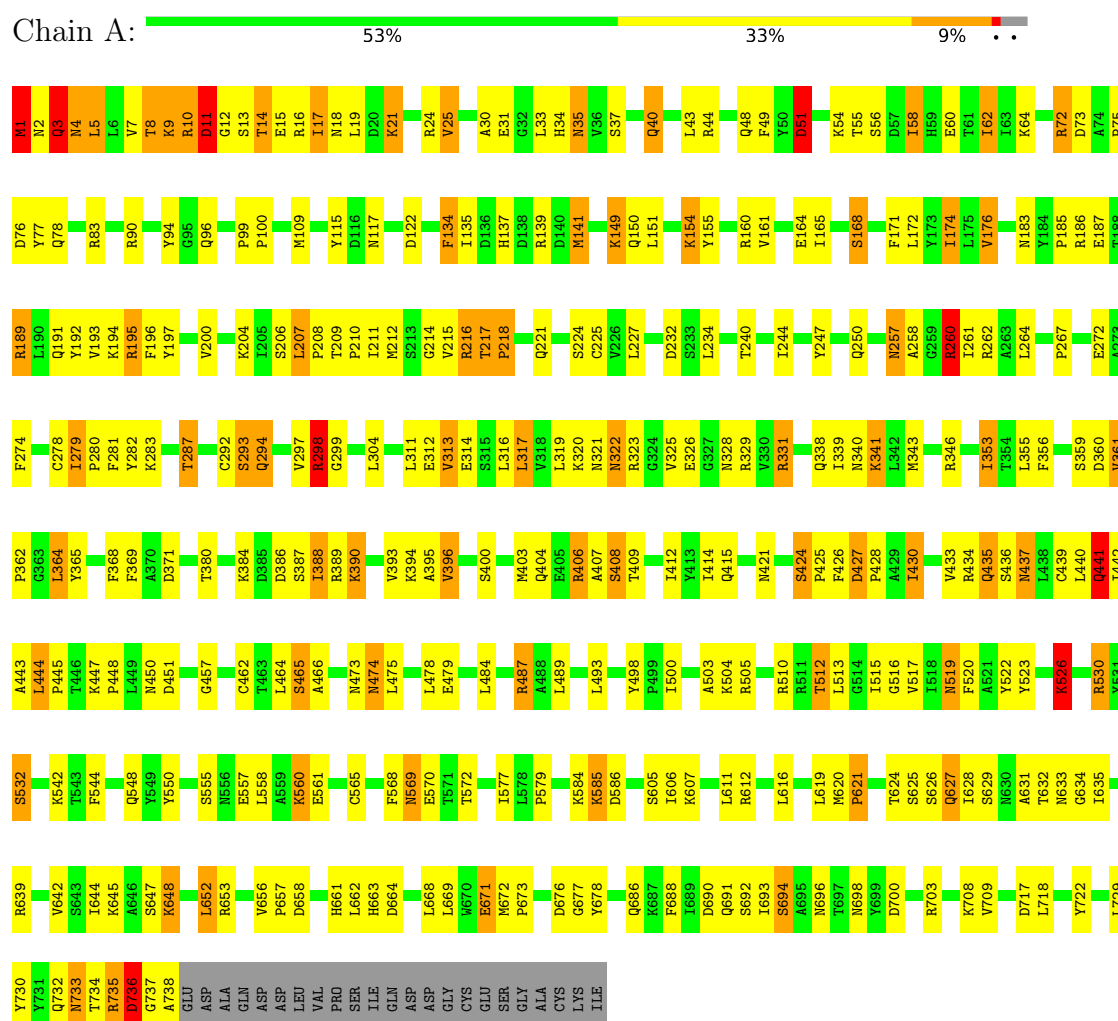
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	C	32	Total	O	0	0
			32	32		

3 Residue-property plots

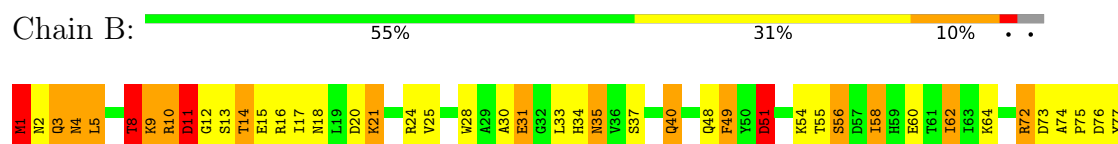
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

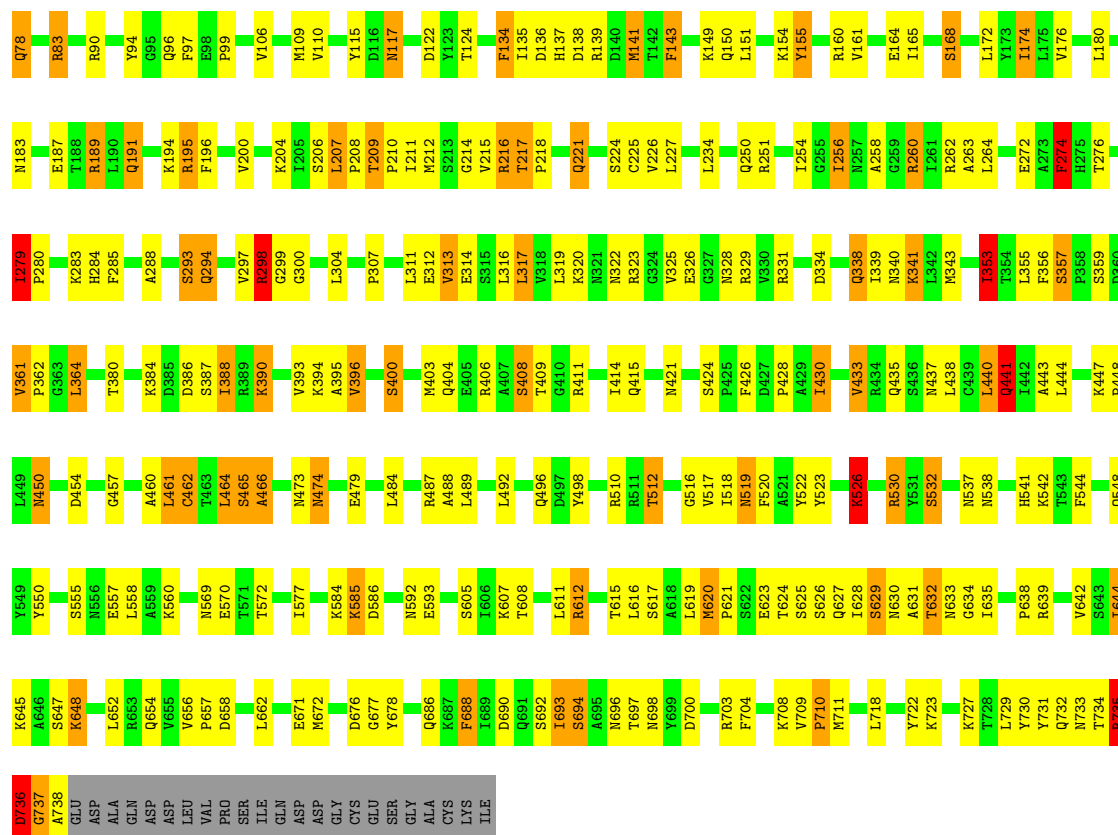
Note EDS was not executed.

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



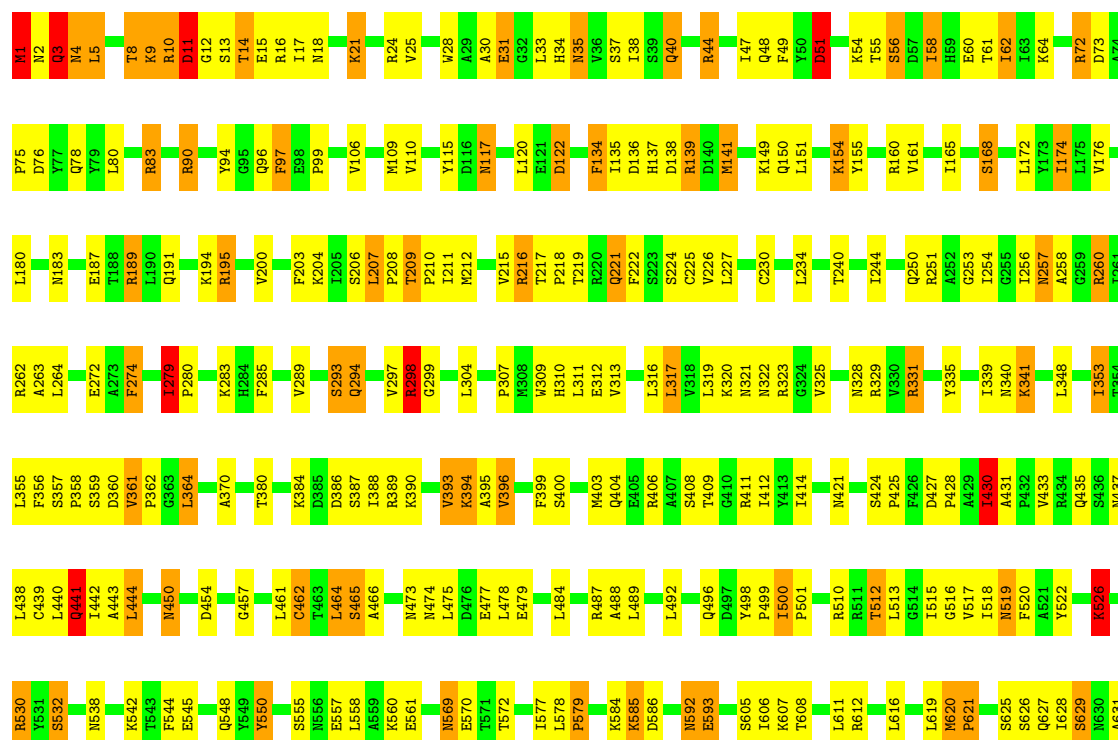
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

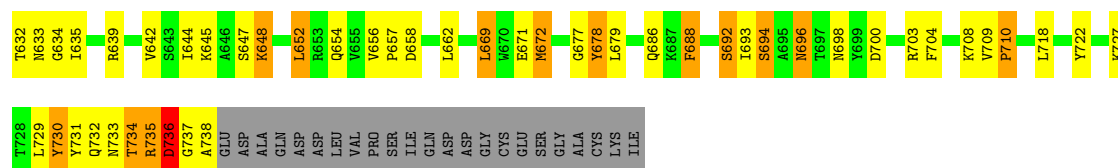




● Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain C: 54% 32% 10% ..

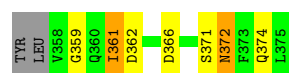




• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



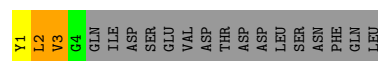
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.56Å 224.56Å 335.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	91.2 (20.00-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.200 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18166	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/6003	1.78	135/8130 (1.7%)
1	B	0.60	0/6003	1.80	137/8130 (1.7%)
1	C	0.65	0/6003	1.83	140/8130 (1.7%)
2	D	0.48	0/140	1.49	1/188 (0.5%)
2	E	0.46	0/140	1.45	1/188 (0.5%)
2	F	0.51	0/140	1.55	1/188 (0.5%)
2	P	1.14	0/31	2.86	4/41 (9.8%)
All	All	0.62	0/18460	1.80	419/24995 (1.7%)

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
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (419) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	736	ASP	CA-CB-CG	12.84	125.44	112.60
1	C	195	ARG	CD-NE-CZ	12.77	142.27	124.40
1	B	736	ASP	CA-CB-CG	11.22	123.82	112.60
1	B	703	ARG	NE-CZ-NH2	-10.74	109.54	119.20
1	B	195	ARG	CD-NE-CZ	10.54	139.15	124.40
1	A	736	ASP	CA-CB-CG	10.48	123.08	112.60
1	A	464	LEU	N-CA-C	10.12	125.83	110.14
1	A	24	ARG	CD-NE-CZ	10.07	138.50	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	421	ASN	CA-CB-CG	-9.80	102.80	112.60
1	B	338	GLN	OE1-CD-NE2	9.74	132.34	122.60
1	A	195	ARG	CD-NE-CZ	9.70	137.98	124.40
1	B	464	LEU	N-CA-C	9.20	124.38	109.85
1	A	703	ARG	NE-CZ-NH2	-9.14	110.97	119.20
1	C	464	LEU	N-CA-C	9.10	124.25	110.14
1	B	421	ASN	CA-CB-CG	-9.04	103.56	112.60
1	B	642	VAL	CA-C-O	-8.95	110.99	120.39
1	C	83	ARG	NE-CZ-NH2	-8.93	111.17	119.20
1	C	450	ASN	CA-CB-CG	-8.71	103.89	112.60
1	B	450	ASN	CA-CB-CG	-8.66	103.94	112.60
1	A	441	GLN	OE1-CD-NE2	-8.63	113.97	122.60
1	C	515	ILE	CA-C-O	-8.53	111.44	120.57
1	C	293	SER	CA-C-N	8.46	137.70	121.54
1	C	293	SER	C-N-CA	8.46	137.70	121.54
1	B	532	SER	N-CA-C	8.45	123.40	113.18
1	A	293	SER	CA-C-O	8.40	130.68	120.60
1	A	4	ASN	N-CA-C	8.35	123.99	111.04
1	B	24	ARG	CD-NE-CZ	8.35	136.09	124.40
1	C	72	ARG	NE-CZ-NH2	8.34	126.71	119.20
2	P	3	VAL	N-CA-C	8.25	126.49	109.34
1	B	441	GLN	OE1-CD-NE2	-8.22	114.38	122.60
1	A	293	SER	CA-C-N	8.19	137.19	121.54
1	A	293	SER	C-N-CA	8.19	137.19	121.54
1	C	732	GLN	CA-C-O	-8.17	111.33	120.32
1	B	293	SER	CA-C-N	8.17	137.14	121.54
1	B	293	SER	C-N-CA	8.17	137.14	121.54
1	A	450	ASN	CA-CB-CG	-8.13	104.47	112.60
1	A	72	ARG	NE-CZ-NH2	8.08	126.47	119.20
1	C	24	ARG	CD-NE-CZ	8.03	135.64	124.40
1	B	703	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	B	51	ASP	CA-C-O	-7.91	109.20	120.51
1	A	732	GLN	CA-C-O	-7.89	111.86	120.30
1	C	703	ARG	NE-CZ-NH1	7.87	129.37	121.50
1	A	154	LYS	N-CA-CB	-7.83	102.40	111.79
1	B	293	SER	CA-C-O	7.81	129.97	120.60
1	C	4	ASN	N-CA-C	7.75	123.05	111.04
1	C	257	ASN	CA-C-O	-7.62	112.20	120.36
1	B	732	GLN	CA-C-O	-7.61	112.16	120.30
1	C	532	SER	N-CA-C	7.61	122.39	113.18
1	C	393	VAL	N-CA-CB	7.56	123.85	111.45
1	A	441	GLN	CG-CD-OE1	7.54	135.88	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	SER	CA-C-O	7.54	129.55	120.28
1	B	4	ASN	N-CA-C	7.43	122.56	111.04
1	A	532	SER	N-CA-C	7.40	122.13	113.18
1	A	224	SER	N-CA-CB	7.37	123.16	110.34
1	A	444	LEU	CA-C-O	7.35	127.26	120.50
1	C	370	ALA	N-CA-C	7.24	122.38	112.90
1	C	620	MET	CB-CA-C	-7.22	97.89	109.37
1	A	642	VAL	CA-C-O	-7.18	112.92	120.39
1	A	160	ARG	CD-NE-CZ	7.14	134.39	124.40
1	B	160	ARG	CD-NE-CZ	7.13	134.39	124.40
1	A	530	ARG	NE-CZ-NH1	7.13	128.63	121.50
1	C	703	ARG	NE-CZ-NH2	-7.08	112.83	119.20
1	C	669	LEU	CA-C-O	-7.07	113.33	120.90
1	C	331	ARG	N-CA-C	7.07	121.14	112.23
1	A	51	ASP	CA-C-O	-7.03	110.46	120.51
1	B	353	ILE	CA-C-O	-7.03	113.08	120.39
1	C	621	PRO	CA-C-O	-7.01	112.89	122.15
1	A	690	ASP	CA-CB-CG	-7.00	105.60	112.60
1	C	209	THR	CA-C-O	6.99	125.58	118.73
1	A	224	SER	N-CA-C	-6.96	103.67	112.93
1	C	183	ASN	CA-CB-CG	-6.93	105.67	112.60
1	C	557	GLU	CA-CB-CG	6.88	127.86	114.10
1	C	439	CYS	CA-C-N	6.87	132.18	122.08
1	C	439	CYS	C-N-CA	6.87	132.18	122.08
1	C	396	VAL	CB-CA-C	-6.85	102.89	112.14
1	A	207	LEU	CA-C-N	6.83	126.85	119.89
1	A	207	LEU	C-N-CA	6.83	126.85	119.89
1	A	671	GLU	N-CA-C	-6.82	104.77	113.23
1	A	11	ASP	CA-C-O	6.82	130.26	120.51
1	B	462	CYS	CA-C-N	-6.81	113.39	122.85
1	B	462	CYS	C-N-CA	-6.81	113.39	122.85
1	B	72	ARG	NE-CZ-NH2	6.80	125.33	119.20
1	A	421	ASN	CA-CB-CG	-6.79	105.81	112.60
1	C	671	GLU	N-CA-C	-6.78	105.16	113.50
1	B	298	ARG	N-CA-C	6.76	119.87	108.23
1	A	389	ARG	CD-NE-CZ	6.73	133.82	124.40
1	C	154	LYS	N-CA-CB	-6.70	99.69	111.42
1	B	544	PHE	CA-CB-CG	-6.70	107.10	113.80
1	C	11	ASP	CA-C-O	6.69	130.08	120.51
1	A	362	PRO	N-CA-CB	6.68	109.20	103.19
1	A	515	ILE	CA-C-O	-6.62	113.16	120.84
1	B	438	LEU	CA-C-O	-6.62	113.82	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	LEU	N-CA-C	6.61	117.86	108.54
1	C	253	GLY	CA-C-O	-6.59	115.38	121.18
1	B	211	ILE	CA-C-O	-6.59	113.74	121.05
1	B	319	LEU	CA-C-O	-6.59	111.52	119.49
1	C	545	GLU	CA-C-O	-6.58	113.57	120.55
1	A	298	ARG	N-CA-C	6.58	119.55	108.23
1	C	500	ILE	CB-CA-C	-6.58	103.22	110.52
1	A	2	ASN	CA-CB-CG	6.57	119.17	112.60
1	B	1	MET	CA-C-N	6.55	134.05	121.54
1	B	1	MET	C-N-CA	6.55	134.05	121.54
1	C	425	PRO	N-CA-CB	6.51	109.53	103.41
1	C	544	PHE	CA-CB-CG	-6.48	107.32	113.80
1	A	530	ARG	NE-CZ-NH2	-6.47	113.37	119.20
1	B	11	ASP	CA-C-O	6.46	129.75	120.51
1	C	51	ASP	CA-C-O	-6.43	111.31	120.51
1	A	183	ASN	CA-CB-CG	-6.41	106.19	112.60
1	B	77	TYR	CA-C-O	-6.40	113.71	120.63
1	A	1	MET	CA-C-N	6.40	133.76	121.54
1	A	1	MET	C-N-CA	6.40	133.76	121.54
1	C	498	TYR	CA-C-O	6.39	125.47	119.59
1	A	703	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	B	396	VAL	CB-CA-C	-6.38	103.71	111.88
1	B	612	ARG	NH1-CZ-NH2	6.38	127.60	119.30
1	A	154	LYS	N-CA-C	6.38	117.94	110.41
1	B	356	PHE	CA-C-O	-6.38	112.70	120.54
1	C	441	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	C	362	PRO	N-CA-CB	6.36	108.92	103.19
1	B	72	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	B	362	PRO	N-CA-CB	6.35	108.91	103.19
1	C	230	CYS	CA-C-O	-6.35	113.37	120.54
1	A	396	VAL	CB-CA-C	-6.34	103.59	112.14
1	B	671	GLU	N-CA-C	-6.33	105.38	113.23
1	A	517	VAL	CA-C-N	6.33	130.80	122.51
1	A	517	VAL	C-N-CA	6.33	130.80	122.51
1	A	544	PHE	CA-CB-CG	-6.33	107.47	113.80
1	B	474	ASN	OD1-CG-ND2	6.33	128.93	122.60
1	A	353	ILE	CA-C-O	-6.32	113.82	120.39
1	A	299	GLY	CA-C-O	-6.31	117.88	122.23
1	B	466	ALA	CA-C-O	6.30	128.05	120.99
1	C	61	THR	CA-C-O	-6.29	114.22	120.82
1	A	584	LYS	CA-C-O	6.26	127.84	120.58
1	A	648	LYS	N-CA-C	-6.25	105.48	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	PHE	CA-CB-CG	6.21	120.02	113.80
1	C	608	THR	N-CA-C	6.20	117.92	111.03
1	C	688	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	388	ILE	N-CA-C	6.20	117.71	108.54
1	A	627	GLN	CA-C-O	-6.19	113.99	120.55
1	A	35	ASN	CA-CB-CG	-6.18	106.42	112.60
1	B	307	PRO	N-CA-CB	6.18	109.08	103.33
1	C	1	MET	CA-C-N	6.18	133.34	121.54
1	C	1	MET	C-N-CA	6.18	133.34	121.54
1	A	462	CYS	CA-C-N	-6.17	114.27	122.85
1	A	462	CYS	C-N-CA	-6.17	114.27	122.85
1	B	440	LEU	N-CA-C	6.16	120.10	112.47
1	B	426	PHE	CA-CB-CG	-6.15	107.65	113.80
1	A	356	PHE	CA-CB-CG	6.13	119.94	113.80
1	C	441	GLN	CG-CD-OE1	6.13	133.06	120.80
1	B	441	GLN	CG-CD-OE1	6.13	133.06	120.80
1	C	299	GLY	CA-C-O	-6.10	118.02	122.23
1	C	648	LYS	N-CA-C	-6.09	105.67	113.23
1	B	530	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	A	694	SER	CA-C-O	-6.07	115.07	122.41
1	A	523	TYR	CA-CB-CG	6.06	124.81	113.90
1	C	428	PRO	N-CA-CB	6.04	109.91	103.39
1	C	654	GLN	OE1-CD-NE2	6.04	128.63	122.60
1	C	526	LYS	N-CA-CB	6.03	119.50	110.22
1	A	257	ASN	CA-C-O	-6.02	114.28	120.54
1	C	62	ILE	CB-CG1-CD1	6.01	126.43	113.80
1	A	217	THR	CA-C-N	6.01	126.12	119.87
1	A	217	THR	C-N-CA	6.01	126.12	119.87
1	B	356	PHE	CA-CB-CG	5.99	119.79	113.80
1	C	517	VAL	CA-C-N	5.97	130.33	122.51
1	C	517	VAL	C-N-CA	5.97	130.33	122.51
1	B	124	THR	CA-C-O	-5.95	114.92	121.89
1	C	183	ASN	OD1-CG-ND2	5.95	128.55	122.60
1	B	183	ASN	CA-CB-CG	-5.93	106.67	112.60
1	B	526	LYS	N-CA-CB	5.93	119.35	110.22
1	C	200	VAL	CA-C-O	-5.93	114.57	120.85
1	B	538	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	B	224	SER	N-CA-C	-5.89	105.75	113.12
1	B	608	THR	N-CA-C	5.89	117.57	111.03
1	B	656	VAL	CA-C-N	5.89	126.19	119.83
1	B	656	VAL	C-N-CA	5.89	126.19	119.83
2	P	3	VAL	N-CA-CB	-5.88	101.52	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	ARG	CD-NE-CZ	5.88	132.63	124.40
1	A	313	VAL	N-CA-C	5.87	116.53	110.36
1	C	356	PHE	CA-CB-CG	5.87	119.67	113.80
1	C	464	LEU	CA-C-O	5.86	128.65	121.56
1	A	218	PRO	N-CA-CB	5.85	108.91	103.41
1	C	251	ARG	CD-NE-CZ	5.84	132.58	124.40
1	B	688	PHE	CA-CB-CG	-5.84	107.96	113.80
1	A	425	PRO	N-CA-CB	5.84	109.11	103.51
1	A	691	GLN	OE1-CD-NE2	5.82	128.42	122.60
1	C	2	ASN	CA-CB-CG	5.82	118.42	112.60
1	C	207	LEU	CA-C-N	5.80	125.81	119.89
1	C	207	LEU	C-N-CA	5.80	125.81	119.89
1	A	447	LYS	CA-C-N	5.79	125.73	119.76
1	A	447	LYS	C-N-CA	5.79	125.73	119.76
1	A	503	ALA	CA-C-O	-5.79	113.81	120.24
1	B	136	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	257	ASN	OD1-CG-ND2	5.78	128.38	122.60
1	C	696	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	C	530	ARG	NE-CZ-NH2	-5.77	114.00	119.20
1	A	733	ASN	N-CA-CB	5.77	120.03	110.52
1	B	544	PHE	CA-C-O	-5.76	112.86	119.60
1	A	457	GLY	N-CA-C	-5.76	103.79	112.89
1	A	3	GLN	CA-C-N	5.75	129.52	120.89
1	A	3	GLN	C-N-CA	5.75	129.52	120.89
1	C	136	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	736	ASP	N-CA-C	5.75	121.59	113.02
2	P	2	LEU	CB-CA-C	-5.75	103.20	111.70
1	A	473	ASN	CA-CB-CG	-5.73	106.87	112.60
1	B	448	PRO	N-CA-CB	5.73	108.41	103.31
1	A	331	ARG	N-CA-C	5.73	119.45	112.23
1	A	322	ASN	N-CA-C	5.72	117.51	111.28
1	B	217	THR	CA-C-N	5.71	126.46	120.12
1	B	217	THR	C-N-CA	5.71	126.46	120.12
1	C	90	ARG	N-CA-CB	5.71	118.35	110.07
1	C	444	LEU	CA-C-O	5.71	125.75	120.50
1	B	557	GLU	CA-CB-CG	5.69	125.48	114.10
1	C	672	MET	CA-C-N	5.68	125.36	119.56
1	C	672	MET	C-N-CA	5.68	125.36	119.56
1	C	358	PRO	N-CA-CB	5.68	109.22	103.25
1	C	474	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	B	208	PRO	N-CA-CB	5.68	108.09	103.32
1	B	433	VAL	CA-C-O	-5.68	114.40	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	SER	N-CA-CB	5.67	119.10	110.42
1	A	214	GLY	N-CA-C	5.67	126.61	113.18
1	B	78	GLN	CB-CA-C	-5.66	101.75	110.81
1	C	72	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	A	371	ASP	N-CA-CB	-5.65	102.09	110.90
1	B	690	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	424	SER	CA-C-N	5.64	125.26	119.56
1	A	424	SER	C-N-CA	5.64	125.26	119.56
1	C	678	TYR	CA-C-O	-5.64	114.89	120.82
1	B	537	ASN	CA-C-O	-5.63	115.08	121.00
1	A	448	PRO	N-CA-CB	5.63	108.32	103.31
1	A	487	ARG	CA-C-O	-5.61	114.60	120.55
2	F	366	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	134	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	732	GLN	OE1-CD-NE2	5.59	128.19	122.60
1	A	624	THR	CA-C-N	5.58	128.08	120.54
1	A	624	THR	C-N-CA	5.58	128.08	120.54
1	A	437	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	C	360	ASP	N-CA-C	5.57	120.07	113.16
1	B	523	TYR	CA-CB-CG	5.57	123.92	113.90
1	C	538	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	C	656	VAL	CA-C-N	5.57	125.84	119.83
1	C	656	VAL	C-N-CA	5.57	125.84	119.83
1	A	208	PRO	N-CA-CB	5.56	107.99	103.32
1	A	211	ILE	CA-C-O	-5.55	114.74	121.18
1	B	183	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	C	457	GLY	N-CA-C	-5.54	104.13	112.89
1	C	679	LEU	O-C-N	-5.54	116.25	122.12
1	B	221	GLN	CB-CG-CD	5.53	122.00	112.60
1	A	164	GLU	CA-CB-CG	5.52	125.14	114.10
1	B	644	ILE	N-CA-C	5.52	116.54	108.53
1	C	498	TYR	CA-C-N	5.52	125.17	119.05
1	C	498	TYR	C-N-CA	5.52	125.17	119.05
1	A	451	ASP	CA-C-O	-5.51	115.33	121.23
1	B	207	LEU	CA-C-N	5.51	125.51	119.89
1	B	207	LEU	C-N-CA	5.51	125.51	119.89
1	B	638	PRO	N-CA-CB	5.51	108.46	103.33
1	A	439	CYS	CA-C-N	5.50	130.17	122.08
1	A	439	CYS	C-N-CA	5.50	130.17	122.08
1	B	326	GLU	N-CA-C	5.50	117.98	111.33
1	A	287	THR	N-CA-CB	5.50	118.80	110.28
1	C	438	LEU	CA-C-O	-5.50	115.02	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	PHE	CA-C-O	5.50	126.03	119.60
1	A	474	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	B	299	GLY	CA-C-O	-5.49	118.65	122.22
1	B	447	LYS	CA-C-N	5.48	125.41	119.76
1	B	447	LYS	C-N-CA	5.48	125.41	119.76
1	C	279	ILE	CA-C-N	5.48	125.57	119.32
1	C	279	ILE	C-N-CA	5.48	125.57	119.32
1	A	717	ASP	CA-CB-CG	-5.47	107.13	112.60
1	C	224	SER	N-CA-CB	5.47	119.52	110.33
1	A	557	GLU	CA-CB-CG	5.47	125.04	114.10
1	C	399	PHE	CA-C-O	-5.47	115.08	120.82
1	C	710	PRO	N-CA-CB	5.47	108.42	103.33
1	B	62	ILE	CB-CG1-CD1	5.47	125.28	113.80
1	C	35	ASN	OD1-CG-ND2	5.46	128.06	122.60
1	C	499	PRO	N-CA-CB	5.46	109.33	103.33
1	C	462	CYS	CA-C-N	-5.46	115.27	122.85
1	C	462	CYS	C-N-CA	-5.46	115.27	122.85
1	B	473	ASN	CA-CB-CG	-5.45	107.15	112.60
1	B	430	ILE	CA-C-O	5.44	123.86	119.29
1	B	357	SER	N-CA-C	-5.42	102.81	109.65
1	A	176	VAL	N-CA-C	-5.42	105.09	110.62
1	B	457	GLY	N-CA-C	-5.42	104.33	112.89
1	A	498	TYR	CA-C-N	5.41	125.06	119.05
1	A	498	TYR	C-N-CA	5.41	125.06	119.05
1	A	361	VAL	CA-C-N	5.41	125.72	119.93
1	A	361	VAL	C-N-CA	5.41	125.72	119.93
1	B	83	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	A	406	ARG	N-CA-C	-5.40	105.30	111.07
1	C	584	LYS	CA-C-O	5.39	126.75	120.49
1	C	253	GLY	CA-C-N	-5.39	116.14	123.10
1	C	253	GLY	C-N-CA	-5.39	116.14	123.10
1	A	663	HIS	N-CA-CB	5.39	117.97	109.94
1	B	612	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	652	LEU	N-CA-CB	5.39	119.20	110.42
1	B	517	VAL	N-CA-CB	-5.39	106.20	112.34
1	A	462	CYS	CA-C-O	-5.39	115.32	120.92
1	C	90	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	B	8	THR	N-CA-CB	5.38	119.01	110.57
1	B	428	PRO	N-CA-CB	5.38	109.20	103.39
1	A	526	LYS	N-CA-CB	5.38	118.50	110.22
1	C	530	ARG	CD-NE-CZ	5.37	131.91	124.40
1	A	43	LEU	CA-C-O	-5.36	115.16	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	461	LEU	N-CA-C	5.33	117.97	109.81
1	A	232	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	221	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	C	335	TYR	CA-CB-CG	-5.32	104.32	113.90
1	C	361	VAL	CA-C-N	5.32	125.62	119.93
1	C	361	VAL	C-N-CA	5.32	125.62	119.93
1	B	530	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	A	2	ASN	CA-C-N	5.31	130.97	122.32
1	A	2	ASN	C-N-CA	5.31	130.97	122.32
1	C	652	LEU	N-CA-CB	5.31	119.07	110.42
1	B	191	GLN	N-CA-C	-5.30	105.19	110.97
1	B	648	LYS	N-CA-C	-5.30	106.66	113.23
1	A	360	ASP	CA-CB-CG	5.30	117.90	112.60
2	E	366	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	334	ASP	CA-C-O	-5.29	115.01	121.36
1	A	664	ASP	CA-C-O	-5.29	112.87	119.38
1	B	693	ILE	CA-C-O	-5.29	114.75	120.67
1	C	298	ARG	N-CA-C	5.28	117.28	107.99
1	A	427	ASP	CA-C-O	5.28	123.52	119.46
1	B	217	THR	N-CA-C	-5.28	103.98	110.31
1	B	388	ILE	N-CA-C	5.28	116.35	108.54
1	C	122	ASP	N-CA-C	5.28	117.94	111.82
1	B	155	TYR	CA-CB-CG	5.27	123.39	113.90
1	B	164	GLU	CA-CB-CG	5.26	124.61	114.10
1	C	569	ASN	CA-C-O	-5.26	113.41	119.61
1	B	90	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	487	ARG	CA-C-O	-5.25	115.30	120.82
1	B	632	THR	CA-C-O	-5.25	115.83	121.56
1	B	251	ARG	CD-NE-CZ	5.25	131.75	124.40
1	B	274	PHE	N-CA-CB	5.25	118.52	110.70
1	A	627	GLN	CB-CG-CD	-5.23	103.70	112.60
1	C	550	TYR	CA-C-O	-5.23	115.00	120.55
1	B	710	PRO	N-CA-CB	5.22	108.19	103.33
1	A	500	ILE	CB-CA-C	-5.22	105.06	110.13
1	B	541	HIS	CA-C-O	-5.22	114.99	120.63
1	C	3	GLN	CA-C-N	5.22	128.72	120.89
1	C	3	GLN	C-N-CA	5.22	128.72	120.89
1	A	346	ARG	CA-C-O	-5.22	114.99	120.63
1	B	361	VAL	CA-C-N	5.22	125.52	119.93
1	B	361	VAL	C-N-CA	5.22	125.52	119.93
1	A	62	ILE	CB-CG1-CD1	5.22	124.76	113.80
1	A	694	SER	CB-CA-C	-5.21	103.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	B	624	THR	N-CA-C	5.21	116.65	110.97
1	C	530	ARG	NE-CZ-NH1	5.21	126.70	121.50
1	A	498	TYR	CA-C-O	5.20	124.38	119.59
1	B	97	PHE	CA-C-O	5.20	125.68	119.60
1	C	642	VAL	CA-C-O	-5.20	114.93	120.39
1	B	735	ARG	NE-CZ-NH2	5.19	123.88	119.20
1	C	430	ILE	CB-CA-C	-5.19	106.50	111.06
1	C	606	ILE	CA-C-O	-5.18	115.17	121.18
1	B	256	ILE	CA-C-O	-5.18	114.99	120.48
1	A	326	GLU	N-CA-C	5.18	117.59	111.33
1	C	473	ASN	CA-CB-CG	-5.18	107.42	112.60
1	B	498	TYR	CA-C-O	5.17	124.35	119.59
1	B	74	ALA	CA-C-N	5.17	124.78	119.56
1	B	74	ALA	C-N-CA	5.17	124.78	119.56
1	B	617	SER	CA-C-O	5.16	126.94	121.11
1	C	211	ILE	CA-C-O	-5.16	115.70	121.17
1	C	592	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	278	CYS	N-CA-C	5.16	116.99	111.36
1	B	143	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	621	PRO	CA-C-O	-5.16	115.34	122.15
1	A	408	SER	CB-CA-C	-5.15	102.76	110.90
1	C	694	SER	CA-C-O	-5.15	116.18	122.41
1	C	431	ALA	CA-C-N	5.14	125.12	120.03
1	C	431	ALA	C-N-CA	5.14	125.12	120.03
1	A	183	ASN	OD1-CG-ND2	5.14	127.74	122.60
1	A	606	ILE	CA-C-O	-5.13	115.23	121.18
1	C	389	ARG	CD-NE-CZ	5.12	131.57	124.40
1	A	4	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	653	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	200	VAL	CA-C-O	-5.11	114.95	120.47
1	B	49	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	435	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	C	80	LEU	CA-C-N	5.10	127.08	120.44
1	C	80	LEU	C-N-CA	5.10	127.08	120.44
1	B	134	PHE	CA-CB-CG	5.10	118.90	113.80
1	B	279	ILE	CA-C-N	5.10	125.14	119.32
1	B	279	ILE	C-N-CA	5.10	125.14	119.32
1	C	399	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	464	LEU	CA-C-O	5.10	127.43	121.46
1	C	139	ARG	O-C-N	-5.10	115.77	122.39
1	C	221	GLN	CB-CG-CD	5.09	121.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	B	313	VAL	N-CA-C	5.09	115.70	110.36
1	C	730	TYR	N-CA-C	5.08	112.94	108.78
1	A	260	ARG	CD-NE-CZ	5.07	131.50	124.40
1	B	20	ASP	CA-CB-CG	-5.07	107.53	112.60
1	B	694	SER	CB-CA-C	-5.07	103.18	111.50
1	B	584	LYS	CA-C-N	5.07	127.39	120.54
1	B	584	LYS	C-N-CA	5.07	127.39	120.54
1	A	4	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	477	GLU	N-CA-CB	5.07	118.92	110.41
1	B	209	THR	CA-C-O	5.06	123.69	118.73
1	A	77	TYR	CA-C-O	-5.06	115.17	120.63
1	C	593	GLU	CA-C-N	5.06	125.50	120.14
1	C	593	GLU	C-N-CA	5.06	125.50	120.14
1	A	100	PRO	N-CA-CB	5.05	108.56	103.25
1	C	44	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	C	307	PRO	N-CA-CB	5.05	108.03	103.33
1	B	2	ASN	CA-CB-CG	5.05	117.65	112.60
1	C	208	PRO	N-CA-CB	5.05	107.56	103.32
1	A	247	TYR	N-CA-C	5.04	117.67	111.82
2	D	361	ILE	N-CA-C	5.04	117.02	109.20
1	B	214	GLY	N-CA-C	5.04	125.12	113.18
1	B	735	ARG	O-C-N	-5.04	115.89	122.59
1	C	154	LYS	N-CA-C	5.04	118.63	112.03
1	A	25	VAL	CB-CA-C	-5.03	105.44	111.88
1	B	196	PHE	CB-CA-C	-5.02	102.99	110.88
1	A	200	VAL	CA-C-O	-5.02	114.83	120.25
1	A	661	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	72	ARG	NE-CZ-NH1	-5.01	116.48	121.50
1	B	408	SER	CB-CA-C	-5.01	102.99	110.90
1	C	38	ILE	CA-C-O	-5.00	115.75	120.95
1	A	267	PRO	N-CA-CB	5.00	107.70	103.35
1	C	734	THR	CA-C-O	-5.00	115.30	120.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	PRO	Mainchain
1	B	620	MET	Mainchain
1	B	697	THR	Mainchain
1	C	579	PRO	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	5875	0	5801	165	0
1	B	5875	0	5801	154	0
1	C	5875	0	5801	164	0
2	D	140	0	123	3	0
2	E	140	0	123	3	0
2	F	140	0	123	3	0
2	P	31	0	34	4	0
3	A	28	0	0	2	0
3	B	30	0	0	3	0
3	C	32	0	0	3	0
All	All	18166	0	17806	485	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 14.

All (485) 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:B:619:LEU:HD12	1:B:693:ILE:HG12	1.46	0.96
1:B:191:GLN:HE21	1:B:195:ARG:HH21	1.11	0.94
1:A:191:GLN:HE21	1:A:195:ARG:HH21	1.12	0.93
1:C:441:GLN:NE2	1:C:620:MET:HB3	1.85	0.92
1:C:441:GLN:HE21	1:C:620:MET:HB3	1.34	0.92
1:C:191:GLN:HE21	1:C:195:ARG:HH21	1.08	0.91
1:B:441:GLN:HE21	1:B:620:MET:HB3	1.31	0.91
1:B:441:GLN:NE2	1:B:620:MET:HB3	1.88	0.89
1:B:37:SER:HB3	1:B:40:GLN:HB2	1.56	0.88
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.56	0.88
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.57	0.86
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.58	0.86
1:C:260:ARG:HG2	1:C:260:ARG:HH11	1.40	0.84
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.59	0.83
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.61	0.82
1:B:294:GLN:HB2	1:B:298:ARG:HB3	1.62	0.82
1:A:294:GLN:HB2	1:A:298:ARG:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.45	0.81
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.63	0.80
1:B:75:PRO:O	1:B:78:GLN:HG3	1.80	0.80
1:A:4:ASN:O	1:A:5:LEU:HB2	1.82	0.79
1:C:75:PRO:O	1:C:78:GLN:HG3	1.83	0.78
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.64	0.78
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.66	0.78
1:B:4:ASN:O	1:B:5:LEU:HB2	1.83	0.78
1:C:294:GLN:HB2	1:C:298:ARG:HB3	1.67	0.77
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.67	0.77
1:C:4:ASN:O	1:C:5:LEU:HB2	1.86	0.75
1:B:215:VAL:O	1:B:216:ARG:HB3	1.85	0.75
1:C:325:VAL:HG13	1:C:328:ASN:HB2	1.69	0.75
1:A:260:ARG:HH11	1:A:260:ARG:HG2	1.50	0.74
1:A:83:ARG:HG2	1:A:141:MET:HG3	1.71	0.73
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.70	0.72
1:A:75:PRO:O	1:A:78:GLN:HG3	1.88	0.72
1:A:150:GLN:OE1	1:A:154:LYS:HE3	1.92	0.70
1:A:325:VAL:HG13	1:A:328:ASN:HB2	1.74	0.70
1:A:686:GLN:HE22	1:A:692:SER:HA	1.56	0.70
1:A:734:THR:O	1:A:735:ARG:HB2	1.91	0.70
1:B:325:VAL:HG13	1:B:328:ASN:HB2	1.73	0.70
1:A:94:TYR:OH	1:A:168:SER:HB3	1.90	0.70
1:A:215:VAL:O	1:A:216:ARG:HB3	1.90	0.70
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.74	0.70
1:C:734:THR:O	1:C:735:ARG:HB2	1.93	0.69
1:B:734:THR:O	1:B:735:ARG:HB2	1.91	0.68
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.76	0.68
1:A:522:TYR:CE2	1:A:526:LYS:HD3	2.29	0.67
1:C:215:VAL:O	1:C:216:ARG:HB3	1.94	0.67
1:A:548:GLN:HA	1:A:548:GLN:HE21	1.59	0.67
1:C:548:GLN:HE21	1:C:548:GLN:HA	1.59	0.67
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.76	0.67
1:A:548:GLN:HA	1:A:548:GLN:NE2	2.11	0.66
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.78	0.65
1:B:519:ASN:ND2	1:B:632:THR:H	1.95	0.65
1:B:548:GLN:HA	1:B:548:GLN:NE2	2.12	0.65
1:B:548:GLN:HA	1:B:548:GLN:HE21	1.62	0.65
1:B:700:ASP:OD2	1:B:736:ASP:HB3	1.97	0.65
1:C:150:GLN:OE1	1:C:154:LYS:HE3	1.95	0.65
1:C:700:ASP:OD2	1:C:736:ASP:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.78	0.64
1:B:94:TYR:OH	1:B:168:SER:HB3	1.98	0.63
1:B:361:VAL:HG21	1:B:364:LEU:HD12	1.79	0.63
1:C:548:GLN:HA	1:C:548:GLN:NE2	2.14	0.63
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.80	0.63
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.81	0.63
1:B:234:LEU:HG	1:B:272:GLU:HG2	1.79	0.63
1:A:532:SER:HA	1:A:677:GLY:HA3	1.81	0.63
1:C:322:ASN:HA	1:C:331:ARG:NH1	2.14	0.63
1:A:620:MET:HB2	1:A:621:PRO:HD2	1.81	0.62
1:C:209:THR:N	1:C:210:PRO:HD2	2.14	0.62
1:A:441:GLN:HE21	1:A:620:MET:HA	1.64	0.62
1:A:441:GLN:NE2	1:A:620:MET:HB3	2.15	0.62
1:C:620:MET:HB2	1:C:621:PRO:HD2	1.82	0.62
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.81	0.62
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.82	0.62
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.81	0.62
1:B:620:MET:HB2	1:B:621:PRO:HD2	1.82	0.62
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.79	0.61
1:C:94:TYR:OH	1:C:168:SER:HB3	2.00	0.61
1:A:234:LEU:HG	1:A:272:GLU:HG2	1.83	0.61
1:C:519:ASN:ND2	1:C:632:THR:H	1.98	0.61
1:C:522:TYR:CE2	1:C:526:LYS:HD3	2.34	0.61
1:C:441:GLN:NE2	1:C:620:MET:CB	2.62	0.61
1:A:569:ASN:H	1:A:569:ASN:HD22	1.48	0.61
1:B:215:VAL:HB	3:B:789:HOH:O	2.00	0.61
1:B:322:ASN:HA	1:B:331:ARG:NH1	2.16	0.61
1:A:176:VAL:HG22	3:A:787:HOH:O	2.01	0.61
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.82	0.60
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.37	0.60
1:C:83:ARG:HG2	1:C:141:MET:HG3	1.83	0.60
1:B:215:VAL:O	1:B:216:ARG:CB	2.50	0.60
1:B:33:LEU:HB3	1:B:76:ASP:HB3	1.83	0.60
1:A:441:GLN:NE2	1:A:620:MET:CB	2.65	0.60
1:A:361:VAL:HG21	1:A:364:LEU:HD12	1.82	0.59
1:B:532:SER:HA	1:B:677:GLY:HA3	1.84	0.59
1:C:532:SER:HA	1:C:677:GLY:HA3	1.84	0.59
1:C:272:GLU:HB3	1:C:274:PHE:HE1	1.66	0.59
1:C:34:HIS:O	1:C:35:ASN:HB2	2.02	0.59
1:C:260:ARG:HG2	1:C:260:ARG:NH1	2.15	0.59
1:B:522:TYR:CE2	1:B:526:LYS:HD3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.83	0.59
1:A:519:ASN:ND2	1:A:632:THR:H	2.00	0.59
1:B:176:VAL:HG22	3:B:789:HOH:O	2.01	0.59
1:B:686:GLN:HE22	1:B:692:SER:HA	1.67	0.59
1:C:191:GLN:NE2	1:C:195:ARG:HH21	1.90	0.59
1:B:698:ASN:ND2	1:B:733:ASN:ND2	2.51	0.58
1:C:361:VAL:HG21	1:C:364:LEU:HD12	1.84	0.58
1:A:700:ASP:OD2	1:A:736:ASP:HB3	2.03	0.58
1:C:122:ASP:O	1:C:189:ARG:NH2	2.36	0.58
1:B:272:GLU:HB3	1:B:274:PHE:HE1	1.68	0.58
1:A:272:GLU:HB3	1:A:274:PHE:HE1	1.68	0.58
1:C:686:GLN:HE22	1:C:692:SER:HA	1.68	0.58
1:A:262:ARG:HB3	1:A:359:SER:HB3	1.86	0.57
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.39	0.57
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.39	0.57
1:A:150:GLN:HE21	1:A:627:GLN:NE2	2.02	0.57
1:A:621:PRO:HD3	1:A:694:SER:OG	2.05	0.57
1:A:34:HIS:O	1:A:35:ASN:HB2	2.05	0.57
1:A:322:ASN:HA	1:A:331:ARG:NH1	2.19	0.57
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.39	0.57
1:A:187:GLU:HB2	3:C:762:HOH:O	2.04	0.57
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.40	0.57
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.87	0.57
1:B:621:PRO:HD3	1:B:694:SER:OG	2.05	0.57
1:A:585:LYS:HD3	1:A:586:ASP:OD1	2.05	0.56
1:C:187:GLU:HB2	3:C:782:HOH:O	2.05	0.56
1:C:215:VAL:O	1:C:216:ARG:CB	2.53	0.56
1:C:262:ARG:HB3	1:C:359:SER:HB3	1.87	0.56
1:A:572:THR:HB	1:A:577:ILE:HB	1.86	0.56
1:B:313:VAL:HG22	1:B:317:LEU:HD22	1.86	0.56
1:C:33:LEU:HB3	1:C:76:ASP:HB3	1.87	0.56
1:A:257:ASN:HB2	1:A:435:GLN:OE1	2.06	0.56
1:B:441:GLN:NE2	1:B:620:MET:CB	2.65	0.56
1:A:569:ASN:H	1:A:569:ASN:ND2	2.04	0.56
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.41	0.56
1:C:172:LEU:O	1:C:176:VAL:HG23	2.06	0.56
1:B:209:THR:N	1:B:210:PRO:HD2	2.20	0.56
1:B:388:ILE:O	1:B:390:LYS:HE3	2.06	0.55
1:A:585:LYS:HD2	1:A:585:LYS:N	2.22	0.55
2:D:372:ASN:H	2:D:372:ASN:ND2	2.03	0.55
1:B:172:LEU:O	1:B:176:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LEU:HD23	1:C:51:ASP:HA	1.87	0.55
1:B:191:GLN:NE2	1:B:195:ARG:HH21	1.93	0.55
1:B:441:GLN:HE21	1:B:620:MET:CB	2.12	0.55
1:C:572:THR:HB	1:C:577:ILE:HB	1.87	0.55
1:A:441:GLN:HE21	1:A:620:MET:CA	2.20	0.55
1:B:262:ARG:HB3	1:B:359:SER:HB3	1.89	0.55
1:A:209:THR:N	1:A:210:PRO:HD2	2.22	0.54
1:B:700:ASP:CG	1:B:736:ASP:HB3	2.32	0.54
1:A:18:ASN:ND2	1:A:21:LYS:HE3	2.23	0.54
1:A:441:GLN:HE21	1:A:620:MET:CB	2.20	0.54
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.42	0.54
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.43	0.54
1:C:21:LYS:O	1:C:25:VAL:HG23	2.08	0.53
1:A:5:LEU:HD23	1:A:51:ASP:HA	1.90	0.53
1:B:312:GLU:O	1:B:316:LEU:HG	2.08	0.53
1:B:572:THR:HB	1:B:577:ILE:HB	1.89	0.53
1:C:10:ARG:O	1:C:11:ASP:C	2.52	0.53
1:C:49:PHE:CZ	1:C:58:ILE:HG23	2.44	0.53
1:C:234:LEU:HG	1:C:272:GLU:HG2	1.90	0.53
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.44	0.53
1:A:215:VAL:O	1:A:216:ARG:CB	2.57	0.53
1:B:122:ASP:O	1:B:189:ARG:NH2	2.42	0.53
2:E:372:ASN:H	2:E:372:ASN:ND2	2.05	0.53
1:A:221:GLN:NE2	1:A:250:GLN:OE1	2.42	0.53
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.90	0.53
1:B:5:LEU:HD23	1:B:51:ASP:HA	1.91	0.53
1:B:9:LYS:HE2	1:B:55:THR:HG21	1.92	0.52
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.91	0.52
1:A:18:ASN:HD22	1:A:21:LYS:HE3	1.74	0.52
1:A:388:ILE:O	1:A:390:LYS:HE3	2.10	0.52
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.09	0.52
1:B:353:ILE:HG13	1:B:395:ALA:HB2	1.91	0.52
1:A:215:VAL:HB	3:A:787:HOH:O	2.10	0.52
1:A:329:ARG:HG3	1:A:331:ARG:NH1	2.25	0.52
1:B:150:GLN:OE1	1:B:154:LYS:HE3	2.09	0.52
1:B:329:ARG:HG3	1:B:331:ARG:NH1	2.24	0.52
1:C:9:LYS:HE2	1:C:55:THR:HG21	1.91	0.52
1:C:56:SER:O	1:C:60:GLU:HG2	2.09	0.52
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.92	0.52
1:C:272:GLU:HB3	1:C:274:PHE:CE1	2.45	0.51
1:C:427:ASP:HB3	1:C:430:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:ASN:ND2	1:C:733:ASN:ND2	2.58	0.51
1:A:172:LEU:O	1:A:176:VAL:HG23	2.11	0.51
1:B:585:LYS:HD3	1:B:586:ASP:OD1	2.10	0.51
1:C:585:LYS:HD3	1:C:586:ASP:OD1	2.10	0.51
1:A:260:ARG:HG2	1:A:260:ARG:NH1	2.23	0.51
1:A:341:LYS:HG2	1:A:722:TYR:OH	2.11	0.51
1:C:47:ILE:HG13	1:C:47:ILE:O	2.10	0.51
1:C:388:ILE:O	1:C:390:LYS:HE3	2.11	0.51
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.41	0.51
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.46	0.51
1:C:700:ASP:CG	1:C:736:ASP:HB3	2.36	0.51
1:A:672:MET:HE1	1:A:678:TYR:HB2	1.93	0.51
1:B:34:HIS:O	1:B:35:ASN:HB2	2.08	0.51
1:B:263:ALA:HB3	1:B:357:SER:HB2	1.92	0.51
1:B:272:GLU:HB3	1:B:274:PHE:CE1	2.46	0.51
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.46	0.50
1:C:672:MET:HE1	1:C:678:TYR:HB2	1.93	0.50
1:C:176:VAL:HG22	3:C:791:HOH:O	2.10	0.50
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.94	0.50
1:B:626:SER:CB	1:B:633:ASN:HD22	2.24	0.50
1:C:260:ARG:HH11	1:C:260:ARG:CG	2.18	0.50
1:B:56:SER:O	1:B:60:GLU:HG2	2.12	0.50
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.94	0.50
1:A:272:GLU:HB3	1:A:274:PHE:CE1	2.47	0.50
1:C:633:ASN:O	1:C:634:GLY:C	2.55	0.50
1:B:585:LYS:HD2	1:B:585:LYS:N	2.26	0.50
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.77	0.50
1:A:585:LYS:HD2	1:A:585:LYS:H	1.76	0.49
1:C:585:LYS:HD2	1:C:585:LYS:N	2.26	0.49
1:A:49:PHE:CZ	1:A:58:ILE:HG23	2.47	0.49
1:A:522:TYR:CD1	1:A:657:PRO:HB2	2.47	0.49
1:B:627:GLN:HG2	1:B:654:GLN:HE22	1.77	0.49
1:C:217:THR:HB	1:C:218:PRO:CD	2.41	0.49
1:A:555:SER:HB3	1:A:611:LEU:HD22	1.95	0.49
1:B:10:ARG:O	1:B:11:ASP:C	2.55	0.49
1:B:522:TYR:CD1	1:B:657:PRO:HB2	2.48	0.49
1:B:672:MET:HE1	1:B:678:TYR:HB2	1.95	0.49
1:A:10:ARG:O	1:A:11:ASP:C	2.56	0.49
1:B:21:LYS:O	1:B:25:VAL:HG23	2.11	0.49
1:C:569:ASN:HD22	1:C:569:ASN:H	1.61	0.49
1:A:698:ASN:ND2	1:A:733:ASN:ND2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:ILE:HA	1:C:634:GLY:HA2	1.95	0.49
1:C:180:LEU:CD1	1:C:488:ALA:HB1	2.43	0.48
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.43	0.48
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.95	0.48
1:B:217:THR:HB	1:B:218:PRO:HD2	1.95	0.48
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.14	0.48
1:C:669:LEU:HD11	1:C:698:ASN:ND2	2.28	0.48
1:A:404:GLN:HG3	2:D:361:ILE:HD11	1.96	0.48
1:A:466:ALA:HA	1:A:516:GLY:O	2.13	0.48
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.38	0.48
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.49	0.48
1:A:279:ILE:HD13	1:A:319:LEU:HD21	1.95	0.48
1:A:415:GLN:HE22	1:A:435:GLN:HA	1.77	0.48
1:A:737:GLY:O	1:A:738:ALA:HB3	2.14	0.48
1:A:626:SER:CB	1:A:633:ASN:HD22	2.26	0.48
1:B:117:ASN:H	1:B:117:ASN:ND2	2.12	0.48
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.49	0.48
1:B:226:VAL:HG12	1:B:461:LEU:CD2	2.44	0.48
1:C:120:LEU:HD13	2:P:1:TYR:CB	2.43	0.48
1:C:150:GLN:HE21	1:C:627:GLN:NE2	2.12	0.48
1:A:353:ILE:HG13	1:A:395:ALA:HB2	1.96	0.48
1:A:519:ASN:ND2	1:A:522:TYR:HB3	2.29	0.48
1:C:1:MET:HA	1:C:3:GLN:HE21	1.77	0.48
1:B:18:ASN:HD22	1:B:21:LYS:HE3	1.79	0.48
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.96	0.48
1:C:329:ARG:HG3	1:C:331:ARG:NH1	2.28	0.48
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.96	0.48
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.96	0.47
1:A:56:SER:O	1:A:60:GLU:HG2	2.14	0.47
1:A:338:GLN:HE21	1:A:415:GLN:NE2	2.12	0.47
1:B:338:GLN:HE21	1:B:415:GLN:NE2	2.13	0.47
1:B:569:ASN:H	1:B:569:ASN:HD22	1.61	0.47
1:C:207:LEU:HD13	1:C:212:MET:HE3	1.97	0.47
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.96	0.47
2:F:372:ASN:ND2	2:F:372:ASN:H	2.10	0.47
1:A:312:GLU:O	1:A:316:LEU:HG	2.14	0.47
1:B:519:ASN:CG	1:B:631:ALA:HB1	2.40	0.47
1:C:120:LEU:HD13	2:P:1:TYR:HB3	1.97	0.47
1:A:700:ASP:CG	1:A:736:ASP:HB3	2.40	0.47
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.49	0.47
1:A:548:GLN:HB2	1:A:688:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ILE:HB	1:B:729:LEU:HB2	1.97	0.47
1:C:737:GLY:O	1:C:738:ALA:HB3	2.14	0.47
1:B:18:ASN:ND2	1:B:21:LYS:HE3	2.30	0.47
1:B:150:GLN:HE21	1:B:627:GLN:NE2	2.12	0.47
1:C:227:LEU:HD11	1:C:437:ASN:HB3	1.96	0.47
1:A:404:GLN:O	1:A:407:ALA:HB3	2.15	0.47
1:B:217:THR:HB	1:B:218:PRO:CD	2.44	0.47
1:B:569:ASN:H	1:B:569:ASN:ND2	2.13	0.47
1:B:172:LEU:C	1:B:172:LEU:HD23	2.40	0.47
1:A:414:ILE:HB	1:A:729:LEU:HB2	1.97	0.46
1:C:54:LYS:H	1:C:54:LYS:HG2	1.61	0.46
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.96	0.46
1:A:343:MET:HE2	1:A:343:MET:HA	1.96	0.46
1:C:406:ARG:NH2	1:C:730:TYR:O	2.47	0.46
1:A:427:ASP:HB3	1:A:430:ILE:HG13	1.97	0.46
1:B:339:ILE:HD12	1:B:414:ILE:HG23	1.97	0.46
1:C:209:THR:N	1:C:210:PRO:CD	2.79	0.46
1:C:312:GLU:O	1:C:316:LEU:HG	2.16	0.46
1:C:519:ASN:HD22	1:C:519:ASN:HA	1.59	0.46
1:A:217:THR:HB	1:A:218:PRO:CD	2.45	0.46
1:B:450:ASN:HB2	1:B:454:ASP:OD2	2.15	0.46
1:B:180:LEU:CD1	1:B:488:ALA:HB1	2.45	0.46
1:B:294:GLN:HG2	1:B:298:ARG:HD3	1.98	0.46
1:B:698:ASN:HD22	1:B:733:ASN:ND2	2.13	0.46
1:C:138:ASP:O	1:C:141:MET:HB2	2.15	0.46
1:C:257:ASN:HB2	1:C:435:GLN:OE1	2.15	0.46
1:A:489:LEU:HB3	1:A:513:LEU:HD22	1.98	0.46
1:C:254:ILE:HG22	1:C:256:ILE:HG13	1.98	0.46
1:A:9:LYS:HE2	1:A:55:THR:HG21	1.97	0.46
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.97	0.46
1:B:313:VAL:HG13	1:B:314:GLU:N	2.31	0.46
1:B:403:MET:HE2	1:B:718:LEU:HB2	1.98	0.46
1:B:592:ASN:O	1:B:593:GLU:C	2.59	0.46
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.97	0.46
1:C:1:MET:HA	1:C:3:GLN:NE2	2.31	0.46
1:C:414:ILE:HB	1:C:729:LEU:HB2	1.98	0.46
1:C:626:SER:CB	1:C:633:ASN:HD22	2.29	0.46
1:B:1:MET:HA	1:B:3:GLN:HE21	1.80	0.46
1:B:221:GLN:NE2	1:B:250:GLN:OE1	2.49	0.46
1:B:404:GLN:HG3	2:E:361:ILE:HD11	1.98	0.45
1:C:240:THR:O	1:C:244:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:CG1	1:A:55:THR:HG22	2.46	0.45
1:A:83:ARG:CG	1:A:141:MET:HG3	2.42	0.45
1:C:522:TYR:CD1	1:C:657:PRO:HB2	2.50	0.45
1:A:519:ASN:HD22	1:A:519:ASN:HA	1.59	0.45
1:A:633:ASN:O	1:A:634:GLY:C	2.59	0.45
1:C:353:ILE:HG13	1:C:395:ALA:HB2	1.98	0.45
1:C:669:LEU:HD11	1:C:698:ASN:CG	2.41	0.45
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.99	0.45
1:C:221:GLN:NE2	1:C:250:GLN:OE1	2.49	0.45
1:A:17:ILE:HD12	1:A:19:LEU:HD23	1.97	0.45
1:A:487:ARG:NH2	1:A:561:GLU:OE1	2.42	0.45
1:A:21:LYS:O	1:A:25:VAL:HG23	2.17	0.45
1:C:475:LEU:O	1:C:478:LEU:HB2	2.16	0.45
1:B:411:ARG:NE	1:B:731:TYR:HE1	2.15	0.45
1:B:633:ASN:O	1:B:634:GLY:C	2.58	0.45
1:C:450:ASN:HB2	1:C:454:ASP:OD2	2.17	0.45
1:A:8:THR:O	1:A:54:LYS:HA	2.17	0.45
1:A:313:VAL:HG13	1:A:314:GLU:N	2.32	0.45
1:A:565:CYS:SG	1:A:568:PHE:HB2	2.57	0.45
1:C:180:LEU:HD13	1:C:488:ALA:HB1	1.98	0.45
1:C:263:ALA:HB3	1:C:357:SER:HB2	1.99	0.45
1:C:309:TRP:O	1:C:310:HIS:C	2.59	0.45
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.51	0.44
1:C:548:GLN:HE21	1:C:548:GLN:CA	2.28	0.44
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.97	0.44
1:A:406:ARG:NH2	1:A:730:TYR:O	2.46	0.44
1:B:548:GLN:HB2	1:B:688:PHE:HB3	1.99	0.44
1:A:279:ILE:H	1:A:279:ILE:HG12	1.65	0.44
1:C:620:MET:HB2	1:C:621:PRO:CD	2.45	0.44
1:B:585:LYS:HD2	1:B:585:LYS:H	1.82	0.44
1:C:117:ASN:ND2	1:C:117:ASN:H	2.16	0.44
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.99	0.44
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.98	0.44
1:C:348:LEU:HD11	2:F:375:LEU:HD21	2.00	0.44
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.98	0.44
1:C:585:LYS:HD2	1:C:585:LYS:H	1.82	0.44
1:B:698:ASN:HD22	1:B:733:ASN:HD22	1.64	0.44
1:C:203:PHE:HB3	1:C:629:SER:HB3	1.99	0.44
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.00	0.44
1:B:737:GLY:O	1:B:738:ALA:HB3	2.18	0.44
1:A:192:TYR:O	1:A:193:VAL:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:O	1:A:244:ILE:HG13	2.18	0.44
1:A:321:ASN:O	1:A:329:ARG:NE	2.50	0.44
1:A:426:PHE:O	1:A:428:PRO:HD3	2.18	0.44
1:A:698:ASN:HD22	1:A:733:ASN:ND2	2.15	0.44
1:B:343:MET:HE2	1:B:343:MET:HA	2.00	0.44
1:A:122:ASP:O	1:A:189:ARG:NH2	2.51	0.44
1:C:151:LEU:HA	1:C:155:TYR:HB2	2.00	0.44
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.99	0.43
1:A:365:TYR:O	1:A:368:PHE:HB3	2.18	0.43
1:B:256:ILE:O	1:B:304:LEU:HA	2.18	0.43
1:B:260:ARG:HG2	1:B:260:ARG:NH1	2.21	0.43
1:C:227:LEU:HB3	1:C:435:GLN:NE2	2.32	0.43
1:A:207:LEU:HD13	1:A:212:MET:HE3	2.00	0.43
1:A:406:ARG:HG3	1:A:412:ILE:O	2.18	0.43
1:B:227:LEU:HD11	1:B:437:ASN:HB3	1.98	0.43
1:C:592:ASN:O	1:C:593:GLU:C	2.60	0.43
1:A:150:GLN:NE2	1:A:627:GLN:NE2	2.64	0.43
1:A:560:LYS:HA	2:P:1:TYR:N	2.34	0.43
1:A:258:ALA:HB1	1:A:261:ILE:HD12	1.99	0.43
1:B:1:MET:HA	1:B:3:GLN:NE2	2.33	0.43
1:C:520:PHE:HB3	1:C:635:ILE:HA	2.00	0.43
1:A:369:PHE:CG	1:A:434:ARG:HG2	2.54	0.43
1:B:227:LEU:HB3	1:B:435:GLN:NE2	2.34	0.43
1:B:262:ARG:HD2	1:B:274:PHE:HB2	2.00	0.43
1:C:404:GLN:HG3	2:F:361:ILE:HD11	2.00	0.43
1:C:18:ASN:HD22	1:C:21:LYS:HE3	1.84	0.43
1:C:106:VAL:O	1:C:110:VAL:HG23	2.19	0.43
1:A:294:GLN:HG2	1:A:298:ARG:HD3	2.00	0.43
1:A:403:MET:HE2	1:A:718:LEU:HB2	2.00	0.43
1:B:548:GLN:HE21	1:B:548:GLN:CA	2.27	0.43
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.99	0.43
1:A:532:SER:CB	1:A:673:PRO:HD2	2.49	0.42
1:A:734:THR:O	1:A:735:ARG:CB	2.62	0.42
1:B:109:MET:HG3	1:B:115:TYR:CE2	2.54	0.42
1:C:311:LEU:HA	1:C:355:LEU:HB3	2.00	0.42
1:A:171:PHE:HA	1:A:174:ILE:HG22	2.01	0.42
1:C:339:ILE:HG22	1:C:340:ASN:N	2.35	0.42
1:C:569:ASN:H	1:C:569:ASN:ND2	2.16	0.42
1:C:621:PRO:HD3	1:C:694:SER:OG	2.20	0.42
1:B:406:ARG:NH2	1:B:730:TYR:O	2.50	0.42
1:C:403:MET:HE2	1:C:718:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ILE:O	1:C:501:PRO:C	2.62	0.42
1:A:436:SER:OG	1:A:437:ASN:N	2.52	0.42
1:B:187:GLU:HB2	3:B:780:HOH:O	2.19	0.42
1:B:492:LEU:O	1:B:496:GLN:HG2	2.19	0.42
1:C:262:ARG:HD2	1:C:274:PHE:HB2	2.00	0.42
1:C:411:ARG:NE	1:C:731:TYR:HE1	2.17	0.42
1:C:519:ASN:CG	1:C:631:ALA:HB1	2.45	0.42
1:A:150:GLN:NE2	1:A:627:GLN:HE22	2.17	0.42
1:A:328:ASN:HD22	1:A:328:ASN:HA	1.64	0.42
1:C:90:ARG:HG3	1:C:90:ARG:NH1	2.34	0.42
1:C:217:THR:OG1	1:C:219:THR:HG22	2.19	0.42
1:C:519:ASN:HD22	1:C:632:THR:H	1.68	0.42
1:C:704:PHE:CD2	1:C:710:PRO:HD3	2.54	0.42
1:A:329:ARG:HG3	1:A:331:ARG:HH12	1.84	0.42
1:B:285:PHE:O	1:B:288:ALA:HB3	2.19	0.42
1:B:723:LYS:NZ	2:E:374:GLN:O	2.44	0.42
1:C:279:ILE:HD13	1:C:319:LEU:HD21	2.00	0.42
1:A:520:PHE:HB3	1:A:635:ILE:HA	2.02	0.42
1:A:676:ASP:O	1:A:677:GLY:C	2.62	0.42
1:A:185:PRO:O	1:A:186:ARG:C	2.63	0.42
1:A:548:GLN:HE21	1:A:548:GLN:CA	2.27	0.42
1:B:106:VAL:O	1:B:110:VAL:HG23	2.20	0.42
1:B:207:LEU:HD13	1:B:212:MET:HE3	2.02	0.42
1:B:555:SER:HB3	1:B:611:LEU:HD22	2.01	0.42
1:A:134:PHE:CE2	1:A:194:LYS:HB2	2.54	0.42
1:B:254:ILE:HG22	1:B:256:ILE:HG13	2.02	0.42
1:C:258:ALA:HB3	1:C:304:LEU:HD21	2.01	0.42
1:A:1:MET:HA	1:A:3:GLN:HE21	1.85	0.42
1:C:394:LYS:O	1:C:395:ALA:C	2.63	0.42
1:A:196:PHE:O	1:A:197:TYR:C	2.62	0.41
1:A:519:ASN:CG	1:A:631:ALA:HB1	2.45	0.41
1:B:8:THR:O	1:B:54:LYS:HA	2.20	0.41
1:B:227:LEU:HB2	1:B:460:ALA:HB3	2.02	0.41
1:C:176:VAL:HG11	1:C:212:MET:CE	2.49	0.41
1:A:441:GLN:HG2	1:A:442:ILE:N	2.31	0.41
1:C:217:THR:HB	1:C:218:PRO:HD2	2.01	0.41
1:C:217:THR:CB	1:C:218:PRO:CD	2.98	0.41
1:C:256:ILE:O	1:C:304:LEU:HA	2.20	0.41
1:C:18:ASN:ND2	1:C:21:LYS:HE3	2.35	0.41
1:A:292:CYS:C	1:B:276:THR:HG21	2.45	0.41
1:A:441:GLN:HE21	1:A:620:MET:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:CG	1:B:141:MET:HG3	2.48	0.41
1:B:466:ALA:HA	1:B:516:GLY:O	2.20	0.41
1:B:519:ASN:HD22	1:B:519:ASN:HA	1.46	0.41
1:C:109:MET:HG3	1:C:115:TYR:CE2	2.56	0.41
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.56	0.41
1:A:444:LEU:HA	1:A:445:PRO:HD3	1.85	0.41
1:A:669:LEU:HD11	1:A:698:ASN:CG	2.45	0.41
1:B:629:SER:O	1:B:630:ASN:C	2.64	0.41
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.48	0.41
1:C:406:ARG:HG3	1:C:412:ILE:O	2.21	0.41
1:A:90:ARG:HG3	1:A:90:ARG:HH11	1.85	0.41
1:A:262:ARG:HD2	1:A:274:PHE:HB2	2.03	0.41
1:B:226:VAL:HG12	1:B:461:LEU:HD23	2.02	0.41
1:B:518:ILE:HA	1:B:634:GLY:HA2	2.01	0.41
1:C:226:VAL:HG12	1:C:461:LEU:CD2	2.50	0.41
1:A:7:VAL:HG11	1:A:55:THR:HG22	2.03	0.41
1:A:504:LYS:O	1:A:505:ARG:C	2.64	0.41
1:B:279:ILE:H	1:B:279:ILE:HG12	1.51	0.41
1:A:339:ILE:HG22	1:A:340:ASN:N	2.36	0.41
1:A:339:ILE:HD12	1:A:414:ILE:HG23	2.03	0.41
1:A:475:LEU:O	1:A:478:LEU:HB2	2.21	0.41
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.87	0.41
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.92	0.41
1:B:143:PHE:CZ	1:B:151:LEU:HD11	2.56	0.41
1:B:212:MET:HE2	1:B:212:MET:HA	2.03	0.41
1:B:339:ILE:HG23	1:B:343:MET:HB2	2.02	0.41
1:B:462:CYS:HB3	1:B:464:LEU:HD21	2.02	0.41
1:B:676:ASP:O	1:B:677:GLY:C	2.62	0.41
1:B:704:PHE:CD2	1:B:710:PRO:HD3	2.56	0.41
1:C:222:PHE:HD2	1:C:496:GLN:HB3	1.86	0.41
1:C:686:GLN:CD	1:C:727:LYS:HD2	2.46	0.41
1:C:737:GLY:O	1:C:738:ALA:CB	2.69	0.41
1:B:339:ILE:HG22	1:B:340:ASN:N	2.34	0.41
1:C:8:THR:O	1:C:54:LYS:HA	2.20	0.41
1:C:28:TRP:O	1:C:31:GLU:HB2	2.21	0.41
1:C:321:ASN:O	1:C:329:ARG:NE	2.54	0.40
1:C:441:GLN:HG2	1:C:442:ILE:N	2.32	0.40
1:C:466:ALA:HA	1:C:516:GLY:O	2.21	0.40
1:B:138:ASP:O	1:B:141:MET:HB2	2.21	0.40
1:B:734:THR:O	1:B:735:ARG:CB	2.66	0.40
1:A:99:PRO:HG2	1:A:137:HIS:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:OG1	1:B:284:HIS:HA	2.22	0.40
2:D:370:LEU:O	2:D:371:SER:C	2.63	0.40
1:B:400:SER:HB3	1:B:711:MET:HE3	2.04	0.40
1:B:512:THR:HG22	1:B:615:THR:HG23	2.03	0.40
1:C:97:PHE:O	1:C:99:PRO:HD3	2.21	0.40
1:C:207:LEU:HD13	1:C:212:MET:CE	2.52	0.40
1:C:285:PHE:O	1:C:289:VAL:HG23	2.21	0.40
1:A:281:PHE:O	1:A:282:TYR:C	2.62	0.40
1:A:569:ASN:ND2	1:A:569:ASN:N	2.68	0.40
1:A:737:GLY:O	1:A:738:ALA:CB	2.69	0.40
1:B:28:TRP:O	1:B:31:GLU:HB2	2.21	0.40
1:B:620:MET:HB2	1:B:621:PRO:CD	2.50	0.40
1:C:487:ARG:HH22	1:C:561:GLU:CD	2.28	0.40
1:C:492:LEU:O	1:C:496:GLN:HG2	2.22	0.40
1:A:656:VAL:HA	1:A:657:PRO:HD3	1.93	0.40
1:C:462:CYS:HB3	1:C:464:LEU:HD21	2.02	0.40
1:C:555:SER:HB3	1:C:611:LEU:HD22	2.02	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	736/761 (97%)	675 (92%)	51 (7%)	10 (1%)	9	34
1	B	736/761 (97%)	678 (92%)	46 (6%)	12 (2%)	7	30
1	C	736/761 (97%)	679 (92%)	47 (6%)	10 (1%)	9	34
2	D	16/20 (80%)	13 (81%)	2 (12%)	1 (6%)	1	6
2	E	16/20 (80%)	13 (81%)	1 (6%)	2 (12%)	0	1
2	F	16/20 (80%)	13 (81%)	1 (6%)	2 (12%)	0	1
2	P	2/20 (10%)	0	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2258/2363 (96%)	2071 (92%)	149 (7%)	38 (2%)	7	30

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	735	ARG
1	B	14	THR
1	B	294	GLN
1	B	735	ARG
2	E	371	SER
1	C	294	GLN
1	C	735	ARG
2	P	3	VAL
1	A	5	LEU
1	A	11	ASP
1	A	14	THR
1	A	51	ASP
1	A	216	ARG
2	D	371	SER
1	B	5	LEU
1	B	11	ASP
1	B	216	ARG
1	C	5	LEU
1	C	11	ASP
1	C	14	THR
1	C	51	ASP
1	C	216	ARG
2	F	371	SER
1	B	13	SER
1	B	51	ASP
1	A	15	GLU
1	B	15	GLU
1	C	15	GLU
1	A	13	SER
1	C	13	SER
2	E	359	GLY
1	B	12	GLY
1	A	12	GLY
1	B	300	GLY
1	B	737	GLY
1	C	12	GLY

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Mol	Chain	Res	Type
2	F	359	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	632/651 (97%)	545 (86%)	87 (14%)	3	15
1	B	632/651 (97%)	543 (86%)	89 (14%)	3	15
1	C	632/651 (97%)	544 (86%)	88 (14%)	3	15
2	D	17/19 (90%)	14 (82%)	3 (18%)	2	9
2	E	17/19 (90%)	14 (82%)	3 (18%)	2	9
2	F	17/19 (90%)	13 (76%)	4 (24%)	1	3
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	0
All	All	1950/2029 (96%)	1675 (86%)	275 (14%)	3	15

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLN
1	A	8	THR
1	A	9	LYS
1	A	10	ARG
1	A	14	THR
1	A	16	ARG
1	A	17	ILE
1	A	21	LYS
1	A	31	GLU
1	A	40	GLN
1	A	44	ARG
1	A	48	GLN
1	A	58	ILE
1	A	62	ILE
1	A	64	LYS

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Mol	Chain	Res	Type
1	A	72	ARG
1	A	73	ASP
1	A	96	GLN
1	A	117	ASN
1	A	139	ARG
1	A	141	MET
1	A	149	LYS
1	A	161	VAL
1	A	165	ILE
1	A	168	SER
1	A	174	ILE
1	A	189	ARG
1	A	204	LYS
1	A	206	SER
1	A	225	CYS
1	A	260	ARG
1	A	264	LEU
1	A	279	ILE
1	A	283	LYS
1	A	293	SER
1	A	297	VAL
1	A	298	ARG
1	A	317	LEU
1	A	320	LYS
1	A	323	ARG
1	A	341	LYS
1	A	364	LEU
1	A	380	THR
1	A	384	LYS
1	A	386	ASP
1	A	387	SER
1	A	390	LYS
1	A	393	VAL
1	A	394	LYS
1	A	396	VAL
1	A	400	SER
1	A	408	SER
1	A	409	THR
1	A	424	SER
1	A	430	ILE
1	A	440	LEU
1	A	441	GLN

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Mol	Chain	Res	Type
1	A	465	SER
1	A	474	ASN
1	A	484	LEU
1	A	510	ARG
1	A	512	THR
1	A	519	ASN
1	A	526	LYS
1	A	530	ARG
1	A	542	LYS
1	A	560	LYS
1	A	569	ASN
1	A	570	GLU
1	A	585	LYS
1	A	605	SER
1	A	607	LYS
1	A	616	LEU
1	A	625	SER
1	A	628	ILE
1	A	629	SER
1	A	639	ARG
1	A	644	ILE
1	A	645	LYS
1	A	647	SER
1	A	648	LYS
1	A	652	LEU
1	A	696	ASN
1	A	708	LYS
1	A	709	VAL
1	A	736	ASP
2	D	361	ILE
2	D	362	ASP
2	D	372	ASN
1	B	1	MET
1	B	3	GLN
1	B	8	THR
1	B	9	LYS
1	B	10	ARG
1	B	14	THR
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	31	GLU

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Mol	Chain	Res	Type
1	B	40	GLN
1	B	48	GLN
1	B	56	SER
1	B	58	ILE
1	B	62	ILE
1	B	64	LYS
1	B	72	ARG
1	B	73	ASP
1	B	96	GLN
1	B	117	ASN
1	B	139	ARG
1	B	141	MET
1	B	149	LYS
1	B	161	VAL
1	B	165	ILE
1	B	168	SER
1	B	174	ILE
1	B	189	ARG
1	B	204	LYS
1	B	206	SER
1	B	225	CYS
1	B	260	ARG
1	B	264	LEU
1	B	274	PHE
1	B	279	ILE
1	B	283	LYS
1	B	293	SER
1	B	297	VAL
1	B	298	ARG
1	B	317	LEU
1	B	320	LYS
1	B	323	ARG
1	B	341	LYS
1	B	353	ILE
1	B	364	LEU
1	B	380	THR
1	B	384	LYS
1	B	386	ASP
1	B	387	SER
1	B	390	LYS
1	B	393	VAL
1	B	394	LYS

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Mol	Chain	Res	Type
1	B	396	VAL
1	B	400	SER
1	B	408	SER
1	B	409	THR
1	B	424	SER
1	B	430	ILE
1	B	440	LEU
1	B	441	GLN
1	B	465	SER
1	B	474	ASN
1	B	484	LEU
1	B	510	ARG
1	B	512	THR
1	B	519	ASN
1	B	526	LYS
1	B	530	ARG
1	B	542	LYS
1	B	560	LYS
1	B	570	GLU
1	B	585	LYS
1	B	605	SER
1	B	607	LYS
1	B	616	LEU
1	B	623	GLU
1	B	625	SER
1	B	628	ILE
1	B	629	SER
1	B	639	ARG
1	B	644	ILE
1	B	645	LYS
1	B	647	SER
1	B	648	LYS
1	B	652	LEU
1	B	696	ASN
1	B	708	LYS
1	B	709	VAL
1	B	736	ASP
2	E	361	ILE
2	E	362	ASP
2	E	372	ASN
1	C	1	MET
1	C	3	GLN

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Mol	Chain	Res	Type
1	C	8	THR
1	C	9	LYS
1	C	10	ARG
1	C	14	THR
1	C	16	ARG
1	C	17	ILE
1	C	21	LYS
1	C	31	GLU
1	C	40	GLN
1	C	44	ARG
1	C	48	GLN
1	C	56	SER
1	C	58	ILE
1	C	62	ILE
1	C	64	LYS
1	C	72	ARG
1	C	73	ASP
1	C	96	GLN
1	C	117	ASN
1	C	139	ARG
1	C	141	MET
1	C	149	LYS
1	C	161	VAL
1	C	165	ILE
1	C	168	SER
1	C	174	ILE
1	C	189	ARG
1	C	204	LYS
1	C	206	SER
1	C	225	CYS
1	C	260	ARG
1	C	264	LEU
1	C	274	PHE
1	C	279	ILE
1	C	283	LYS
1	C	293	SER
1	C	297	VAL
1	C	298	ARG
1	C	317	LEU
1	C	320	LYS
1	C	323	ARG
1	C	341	LYS

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Mol	Chain	Res	Type
1	C	353	ILE
1	C	364	LEU
1	C	380	THR
1	C	384	LYS
1	C	386	ASP
1	C	387	SER
1	C	393	VAL
1	C	394	LYS
1	C	396	VAL
1	C	400	SER
1	C	408	SER
1	C	409	THR
1	C	424	SER
1	C	430	ILE
1	C	440	LEU
1	C	441	GLN
1	C	465	SER
1	C	484	LEU
1	C	510	ARG
1	C	512	THR
1	C	519	ASN
1	C	526	LYS
1	C	530	ARG
1	C	542	LYS
1	C	560	LYS
1	C	570	GLU
1	C	585	LYS
1	C	605	SER
1	C	607	LYS
1	C	616	LEU
1	C	625	SER
1	C	628	ILE
1	C	629	SER
1	C	639	ARG
1	C	644	ILE
1	C	645	LYS
1	C	647	SER
1	C	648	LYS
1	C	652	LEU
1	C	692	SER
1	C	696	ASN
1	C	708	LYS

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Mol	Chain	Res	Type
1	C	709	VAL
1	C	736	ASP
2	F	358	VAL
2	F	361	ILE
2	F	362	ASP
2	F	372	ASN
2	P	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	46	HIS
1	A	117	ASN
1	A	130	GLN
1	A	191	GLN
1	A	221	GLN
1	A	328	ASN
1	A	338	GLN
1	A	415	GLN
1	A	453	ASN
1	A	456	ASN
1	A	519	ASN
1	A	548	GLN
1	A	569	ASN
1	A	627	GLN
1	A	633	ASN
1	A	654	GLN
1	A	686	GLN
1	A	696	ASN
1	A	698	ASN
1	A	713	GLN
1	A	733	ASN
2	D	372	ASN
1	B	3	GLN
1	B	18	ASN
1	B	46	HIS
1	B	117	ASN
1	B	130	GLN
1	B	191	GLN
1	B	221	GLN
1	B	328	ASN

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Mol	Chain	Res	Type
1	B	332	HIS
1	B	415	GLN
1	B	453	ASN
1	B	456	ASN
1	B	519	ASN
1	B	548	GLN
1	B	569	ASN
1	B	627	GLN
1	B	633	ASN
1	B	654	GLN
1	B	686	GLN
1	B	696	ASN
1	B	698	ASN
1	B	713	GLN
1	B	733	ASN
2	E	372	ASN
1	C	3	GLN
1	C	18	ASN
1	C	46	HIS
1	C	117	ASN
1	C	130	GLN
1	C	191	GLN
1	C	221	GLN
1	C	328	ASN
1	C	332	HIS
1	C	415	GLN
1	C	453	ASN
1	C	519	ASN
1	C	548	GLN
1	C	569	ASN
1	C	627	GLN
1	C	633	ASN
1	C	654	GLN
1	C	686	GLN
1	C	696	ASN
1	C	698	ASN
1	C	713	GLN
1	C	733	ASN
2	F	372	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.