



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:58 PM UTC

PDB ID : 5BCA / pdb\_00005bca  
Title : BETA-AMYLASE FROM BACILLUS CEREUS VAR. MYCOIDES  
Authors : Oyama, T.; Kusunoki, M.; Kishimoto, Y.; Takasaki, Y.; Nitta, Y.  
Deposited on : 1999-03-12  
Resolution : 2.20 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

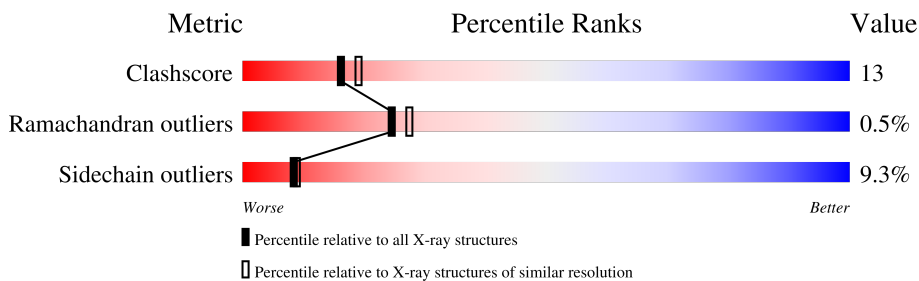
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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  $\geq 3$ , 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	516	59% (green), 32% (yellow), 8% (orange/red), . (grey)
1	B	516	54% (green), 34% (yellow), 9% (orange/red), . (grey)
1	C	516	57% (green), 35% (yellow), 8% (orange/red), . (grey)
1	D	516	55% (green), 37% (yellow), 7% (orange/red), . (grey)

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17232 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 PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	4119	2645	676	781	17	0	0	0
1	B	516	4119	2645	676	781	17	0	0	0
1	C	516	4119	2645	676	781	17	0	0	0
1	D	516	4119	2645	676	781	17	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total 206	O 206	0	0
3	B	170	Total 170	O 170	0	0
3	C	191	Total 191	O 191	0	0
3	D	185	Total 185	O 185	0	0

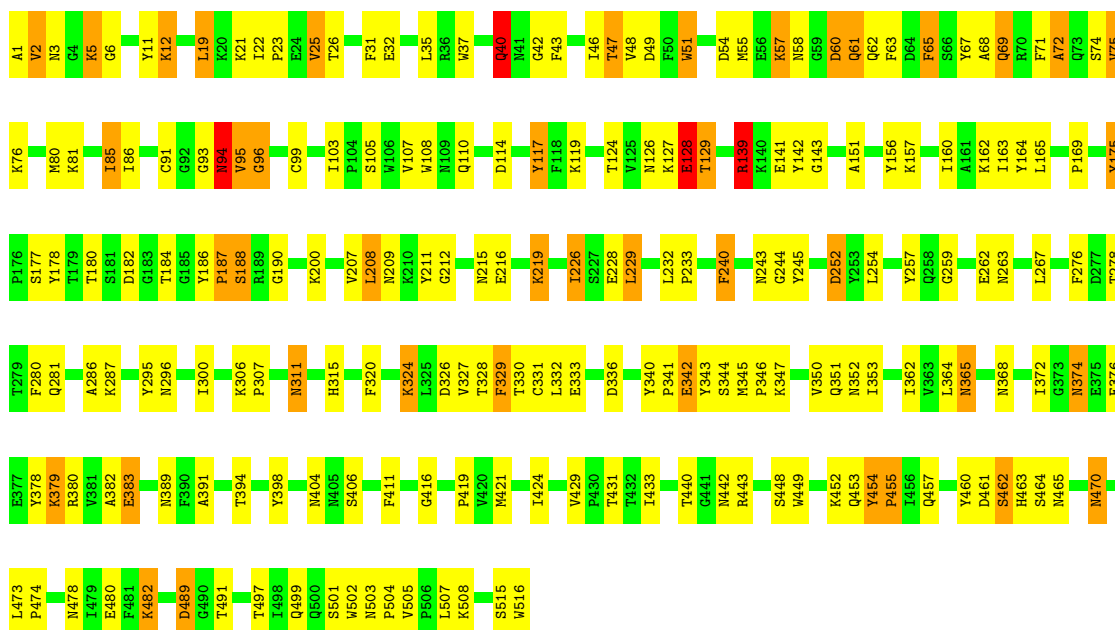
### 3 Residue-property plots [i](#)

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

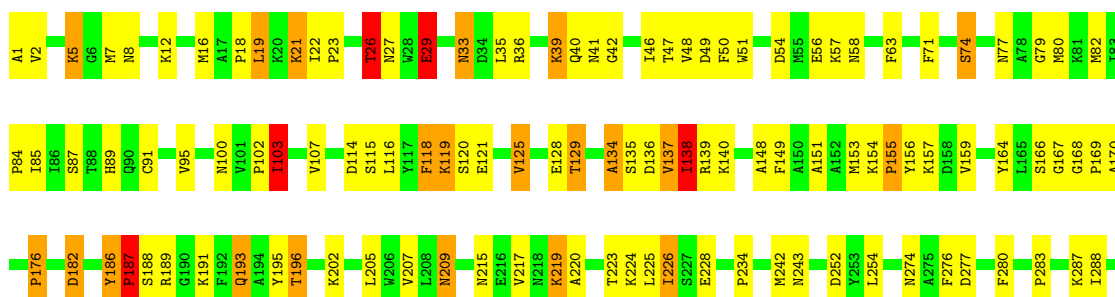
- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)

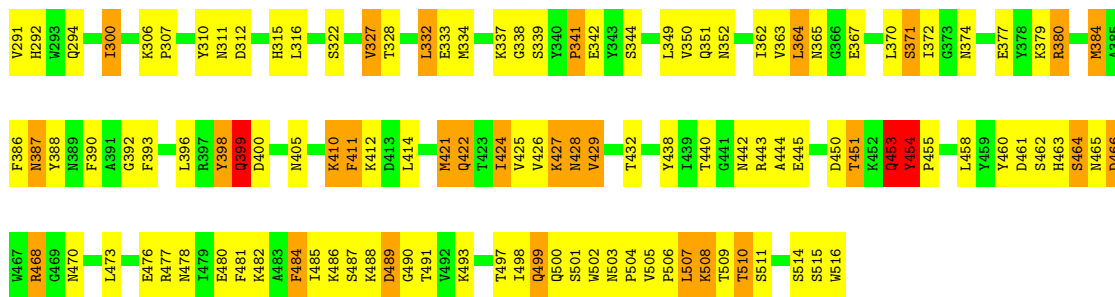
Chain A: 



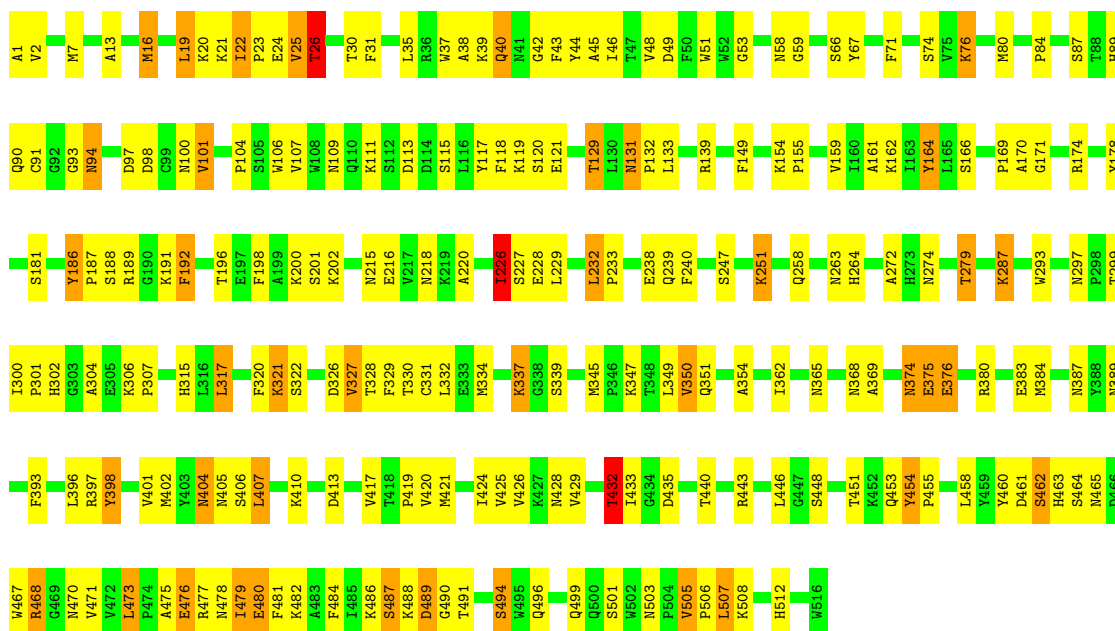
- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)

Chain B: 

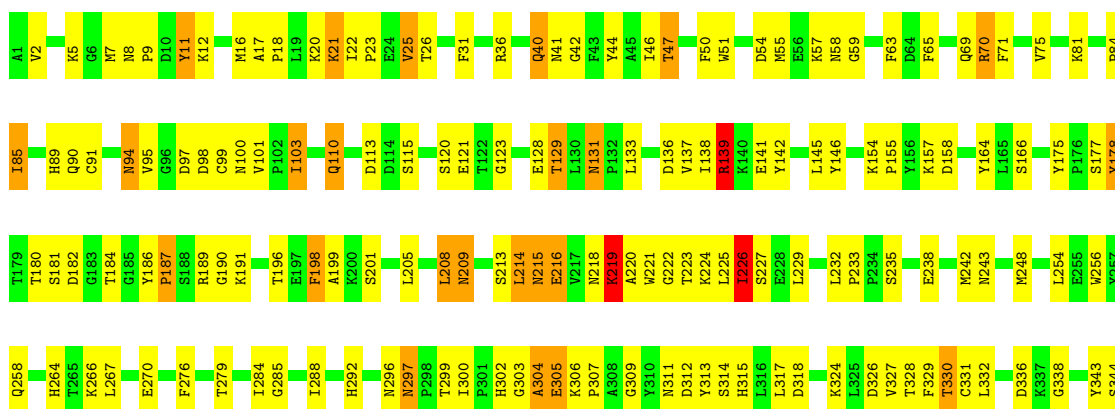


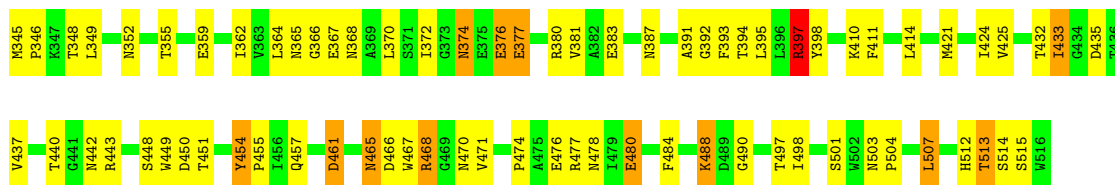


● Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)



● Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.90Å 112.90Å 146.20Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	74.0 (8.00-2.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.186 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.95	1/4234 (0.0%)	2.00	123/5751 (2.1%)
1	B	0.91	0/4234	2.01	146/5751 (2.5%)
1	C	0.95	1/4234 (0.0%)	2.03	142/5751 (2.5%)
1	D	0.95	1/4234 (0.0%)	2.03	126/5751 (2.2%)
All	All	0.94	3/16936 (0.0%)	2.02	537/23004 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLY	CA-C	6.00	1.58	1.52
1	C	272	ALA	C-N	-5.80	1.26	1.33
1	D	392	GLY	N-CA	-5.11	1.40	1.45

All (537) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	380	ARG	CD-NE-CZ	17.08	148.31	124.40
1	B	166	SER	CA-C-O	-11.86	107.15	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	ASN	CA-C-O	-11.64	108.08	121.47
1	D	395	LEU	CA-C-O	-11.41	108.15	120.36
1	C	380	ARG	CD-NE-CZ	11.30	140.22	124.40
1	D	70	ARG	CD-NE-CZ	11.14	140.00	124.40
1	D	209	ASN	CA-CB-CG	-10.98	101.62	112.60
1	B	380	ARG	NE-CZ-NH2	-10.67	109.60	119.20
1	A	43	PHE	CA-CB-CG	10.08	123.88	113.80
1	A	96	GLY	N-CA-C	-9.98	101.80	114.37
1	B	137	VAL	CA-C-O	-9.81	110.45	120.85
1	B	139	ARG	CD-NE-CZ	9.69	137.96	124.40
1	A	62	GLN	OE1-CD-NE2	9.67	132.27	122.60
1	B	46	ILE	CA-C-O	-9.44	110.48	120.48
1	B	274	ASN	CA-CB-CG	9.40	122.00	112.60
1	B	480	GLU	CB-CG-CD	9.40	128.58	112.60
1	D	47	THR	CA-C-O	-9.37	110.78	120.71
1	C	272	ALA	CA-C-N	9.29	132.72	120.28
1	C	272	ALA	C-N-CA	9.29	132.72	120.28
1	D	387	ASN	CA-CB-CG	-9.24	103.36	112.60
1	D	41	ASN	CA-CB-CG	-9.23	103.37	112.60
1	D	466	ASP	CA-CB-CG	9.21	121.81	112.60
1	D	284	ILE	CA-C-N	-9.20	111.73	121.48
1	D	284	ILE	C-N-CA	-9.20	111.73	121.48
1	B	466	ASP	CA-CB-CG	9.08	121.68	112.60
1	C	100	ASN	OD1-CG-ND2	8.98	131.58	122.60
1	B	380	ARG	CD-NE-CZ	8.67	136.53	124.40
1	B	352	ASN	N-CA-CB	-8.64	97.42	110.12
1	A	151	ALA	CA-C-O	-8.60	111.35	120.55
1	C	16	MET	CA-CB-CG	8.57	131.24	114.10
1	C	315	HIS	CA-CB-CG	-8.55	105.25	113.80
1	C	43	PHE	CA-C-N	8.55	135.19	120.58
1	C	43	PHE	C-N-CA	8.55	135.19	120.58
1	A	470	ASN	CA-CB-CG	-8.50	104.10	112.60
1	C	43	PHE	O-C-N	-8.44	113.06	123.01
1	D	90	GLN	OE1-CD-NE2	-8.23	114.37	122.60
1	C	432	THR	N-CA-CB	8.21	123.37	111.05
1	A	329	PHE	CA-CB-CG	-8.18	105.62	113.80
1	C	174	ARG	NE-CZ-NH2	8.12	126.51	119.20
1	C	440	THR	CA-C-O	-8.04	112.50	121.51
1	C	301	PRO	CA-C-O	-8.01	112.66	121.23
1	A	419	PRO	CA-C-O	-8.00	111.88	121.48
1	C	71	PHE	CA-CB-CG	7.97	121.77	113.80
1	D	478	ASN	OD1-CG-ND2	-7.90	114.70	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	GLY	CA-C-O	-7.90	112.41	121.49
1	A	85	ILE	CA-C-O	-7.88	112.09	120.53
1	B	151	ALA	CA-C-O	-7.87	112.08	120.42
1	C	192	PHE	CA-CB-CG	-7.86	105.94	113.80
1	A	326	ASP	CA-CB-CG	7.86	120.46	112.60
1	C	484	PHE	CA-CB-CG	7.86	121.66	113.80
1	C	304	ALA	N-CA-CB	7.77	120.93	110.59
1	B	85	ILE	O-C-N	-7.76	115.03	123.18
1	D	94	ASN	CA-CB-CG	-7.74	104.86	112.60
1	C	178	TYR	CA-CB-CG	7.72	127.81	113.90
1	A	151	ALA	O-C-N	7.70	131.49	122.17
1	B	41	ASN	CA-CB-CG	-7.69	104.91	112.60
1	B	19	LEU	CA-C-O	7.63	128.77	119.31
1	B	438	TYR	CA-C-O	-7.62	113.10	121.33
1	B	217	VAL	N-CA-C	-7.58	103.47	110.82
1	A	263	ASN	CA-C-N	7.53	130.22	120.44
1	A	263	ASN	C-N-CA	7.53	130.22	120.44
1	D	397	ARG	CD-NE-CZ	7.48	134.88	124.40
1	A	296	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	C	196	THR	N-CA-C	-7.38	100.58	110.55
1	D	454	TYR	N-CA-C	7.38	126.11	109.81
1	D	514	SER	CA-C-O	7.37	129.73	121.40
1	D	209	ASN	OD1-CG-ND2	7.34	129.94	122.60
1	D	136	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	129	THR	CA-C-O	-7.33	113.60	121.38
1	A	175	TYR	CA-C-O	7.32	127.19	120.60
1	B	352	ASN	N-CA-C	7.32	119.26	111.28
1	B	277	ASP	CA-CB-CG	-7.28	105.32	112.60
1	D	103	ILE	N-CA-CB	-7.26	101.04	111.21
1	B	405	ASN	CA-CB-CG	7.23	119.83	112.60
1	A	276	PHE	N-CA-C	7.20	122.34	112.90
1	D	264	HIS	CA-CB-CG	7.20	121.00	113.80
1	C	380	ARG	NE-CZ-NH2	-7.19	112.73	119.20
1	C	161	ALA	CA-C-O	7.18	128.00	119.60
1	D	387	ASN	OD1-CG-ND2	7.17	129.77	122.60
1	A	31	PHE	CA-C-O	7.14	128.12	120.55
1	B	243	ASN	CA-CB-CG	-7.11	105.50	112.60
1	B	57	LYS	N-CA-C	7.08	118.65	111.07
1	B	499	GLN	OE1-CD-NE2	7.06	129.66	122.60
1	D	75	VAL	CA-C-O	7.06	128.34	120.85
1	C	274	ASN	CA-C-O	-7.05	113.42	120.82
1	B	33	ASN	CA-CB-CG	-7.02	105.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	393	PHE	CA-CB-CG	-7.01	106.79	113.80
1	C	76	LYS	CA-CB-CG	7.00	128.11	114.10
1	C	475	ALA	CA-C-O	-7.00	113.88	121.44
1	D	440	THR	CA-C-O	-7.00	113.77	121.33
1	B	182	ASP	N-CA-C	-6.99	104.49	113.16
1	B	48	VAL	CA-C-O	-6.99	113.07	120.76
1	C	159	VAL	O-C-N	6.97	129.69	122.09
1	B	138	ILE	CB-CA-C	-6.94	103.09	111.97
1	C	131	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	B	470	ASN	OD1-CG-ND2	6.87	129.47	122.60
1	D	288	ILE	O-C-N	-6.87	115.97	123.18
1	B	365	ASN	CA-CB-CG	-6.82	105.78	112.60
1	B	58	ASN	CA-CB-CG	-6.81	105.79	112.60
1	D	302	HIS	CA-CB-CG	-6.80	107.00	113.80
1	D	139	ARG	CB-CG-CD	6.79	126.92	111.30
1	C	251	LYS	O-C-N	6.78	129.06	122.07
1	D	164	TYR	CA-C-O	-6.75	113.53	121.16
1	D	474	PRO	O-C-N	-6.73	117.95	122.73
1	C	98	ASP	CA-CB-CG	-6.72	105.88	112.60
1	C	274	ASN	N-CA-CB	6.71	119.75	110.01
1	A	208	LEU	CA-C-O	6.71	127.68	119.97
1	B	77	ASN	CA-CB-CG	6.70	119.30	112.60
1	B	387	ASN	CA-C-O	-6.70	111.80	118.97
1	D	131	ASN	OD1-CG-ND2	6.70	129.30	122.60
1	D	442	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	D	270	GLU	CB-CG-CD	6.67	123.94	112.60
1	C	389	ASN	OD1-CG-ND2	6.67	129.27	122.60
1	B	424	ILE	CA-C-N	-6.61	114.48	123.14
1	B	424	ILE	C-N-CA	-6.61	114.48	123.14
1	C	189	ARG	CA-C-N	-6.61	115.50	122.30
1	C	189	ARG	C-N-CA	-6.61	115.50	122.30
1	C	470	ASN	CA-CB-CG	-6.60	106.00	112.60
1	B	215	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	B	125	VAL	CA-C-O	-6.58	113.21	120.84
1	D	46	ILE	O-C-N	-6.58	116.43	123.14
1	C	365	ASN	CA-CB-CG	-6.57	106.03	112.60
1	D	71	PHE	N-CA-C	-6.55	104.06	111.14
1	C	1	ALA	CA-C-N	6.55	129.52	120.49
1	C	1	ALA	C-N-CA	6.55	129.52	120.49
1	A	105	SER	CA-C-O	-6.53	112.72	120.10
1	A	12	LYS	CA-C-O	-6.52	113.69	120.99
1	D	70	ARG	NE-CZ-NH2	6.49	125.04	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	GLN	CA-C-O	-6.49	113.52	120.92
1	C	477	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	D	139	ARG	CD-NE-CZ	-6.47	115.34	124.40
1	D	57	LYS	N-CA-C	6.47	118.02	110.97
1	D	457	GLN	N-CA-C	6.47	120.83	109.96
1	B	26	THR	CB-CA-C	-6.45	100.48	114.10
1	C	174	ARG	O-C-N	-6.44	116.34	123.04
1	C	189	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	A	94	ASN	CA-C-O	-6.43	113.18	120.32
1	C	201	SER	CB-CA-C	-6.42	100.81	110.88
1	D	279	THR	N-CA-CB	-6.41	100.69	109.98
1	A	365	ASN	CA-C-O	-6.40	113.64	121.06
1	D	368	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	A	243	ASN	OD1-CG-ND2	6.39	128.99	122.60
1	D	141	GLU	N-CA-C	6.38	119.05	111.33
1	A	6	GLY	CA-C-N	6.38	130.38	120.75
1	A	6	GLY	C-N-CA	6.38	130.38	120.75
1	B	135	SER	CA-C-N	6.38	128.82	120.28
1	B	135	SER	C-N-CA	6.38	128.82	120.28
1	D	368	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	48	VAL	O-C-N	-6.36	115.71	123.09
1	D	58	ASN	CA-CB-CG	-6.35	106.25	112.60
1	D	352	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	295	TYR	N-CA-C	6.33	117.86	110.97
1	D	484	PHE	CA-CB-CG	6.32	120.12	113.80
1	D	318	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	272	ALA	O-C-N	-6.32	115.27	122.09
1	B	292	HIS	CA-CB-CG	-6.31	107.49	113.80
1	A	311	ASN	CA-C-O	6.31	126.93	119.67
1	B	74	SER	CA-C-O	6.30	127.10	120.42
1	B	129	THR	CA-C-O	-6.28	114.19	121.10
1	C	389	ASN	CA-CB-CG	-6.27	106.33	112.60
1	C	429	VAL	CA-C-O	-6.27	115.11	119.19
1	A	497	THR	CA-C-N	-6.25	115.04	123.10
1	A	497	THR	C-N-CA	-6.25	115.04	123.10
1	B	100	ASN	CA-CB-CG	6.24	118.84	112.60
1	A	389	ASN	N-CA-CB	-6.23	102.72	112.13
1	C	396	LEU	CA-C-O	-6.22	114.07	120.54
1	A	215	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	25	VAL	N-CA-C	6.21	117.15	111.81
1	C	22	ILE	CA-C-N	6.19	125.89	119.82
1	C	22	ILE	C-N-CA	6.19	125.89	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ASN	CA-C-O	-6.18	113.64	120.69
1	A	315	HIS	CA-C-O	-6.18	113.38	120.24
1	B	18	PRO	CA-C-O	-6.18	113.42	122.31
1	A	31	PHE	CA-CB-CG	6.17	119.97	113.80
1	C	24	GLU	CA-C-O	6.17	127.07	119.79
1	C	26	THR	N-CA-CB	6.17	120.91	110.49
1	C	37	TRP	O-C-N	6.15	128.49	122.09
1	D	468	ARG	CA-C-O	-6.15	114.86	121.38
1	D	137	VAL	CA-CB-CG1	6.15	120.85	110.40
1	C	149	PHE	N-CA-C	-6.15	104.49	112.23
1	D	326	ASP	CA-C-O	-6.15	114.86	121.56
1	D	164	TYR	CA-CB-CG	6.14	124.95	113.90
1	C	480	GLU	CA-C-O	-6.14	114.07	120.70
1	D	304	ALA	CA-C-N	6.13	128.41	120.44
1	D	304	ALA	C-N-CA	6.13	128.41	120.44
1	B	440	THR	CA-C-O	-6.12	114.68	121.23
1	D	512	HIS	CA-CB-CG	6.12	119.92	113.80
1	D	303	GLY	N-CA-C	6.12	121.19	114.40
1	A	60	ASP	CA-CB-CG	-6.11	106.49	112.60
1	D	435	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	42	GLY	CA-C-O	-6.11	112.24	119.02
1	B	118	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	26	THR	N-CA-CB	6.10	120.44	110.55
1	C	383	GLU	N-CA-C	6.10	117.60	111.07
1	C	13	ALA	CA-C-O	-6.10	114.25	120.71
1	A	71	PHE	CA-C-O	-6.09	114.38	120.90
1	D	433	ILE	O-C-N	6.09	130.18	122.57
1	C	189	ARG	CD-NE-CZ	6.08	132.91	124.40
1	A	276	PHE	CA-CB-CG	-6.07	107.73	113.80
1	C	337	LYS	CB-CA-C	6.07	120.42	110.83
1	B	87	SER	N-CA-C	6.07	119.40	108.17
1	A	406	SER	O-C-N	6.07	128.34	122.03
1	B	128	GLU	CA-CB-CG	6.05	126.20	114.10
1	D	44	TYR	N-CA-C	-6.05	106.54	114.04
1	C	232	LEU	CA-C-N	6.04	126.61	120.38
1	C	232	LEU	C-N-CA	6.04	126.61	120.38
1	B	19	LEU	O-C-N	-6.04	114.12	122.46
1	D	145	LEU	CA-C-O	6.04	127.16	120.82
1	B	451	THR	N-CA-CB	6.03	119.52	110.65
1	C	131	ASN	CA-CB-CG	6.03	118.63	112.60
1	D	36	ARG	NE-CZ-NH2	-6.03	113.78	119.20
1	C	505	VAL	CA-C-O	6.02	125.04	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ASN	O-C-N	6.01	130.07	123.04
1	C	227	SER	CA-C-O	-6.01	114.61	121.40
1	C	118	PHE	CA-CB-CG	6.00	119.80	113.80
1	A	416	GLY	CA-C-N	-6.00	113.82	122.45
1	A	416	GLY	C-N-CA	-6.00	113.82	122.45
1	C	443	ARG	CG-CD-NE	5.98	125.16	112.00
1	B	370	LEU	CA-C-O	-5.97	114.45	121.44
1	B	280	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	411	PHE	CA-CB-CG	-5.97	107.83	113.80
1	B	49	ASP	N-CA-CB	5.96	119.88	110.23
1	C	321	LYS	CA-C-O	5.95	127.07	120.82
1	C	293	TRP	O-C-N	-5.94	116.02	122.79
1	C	279	THR	CA-CB-OG1	5.93	118.50	109.60
1	C	299	THR	CA-C-O	-5.92	112.73	119.41
1	B	16	MET	CA-C-N	-5.91	112.46	121.92
1	B	16	MET	C-N-CA	-5.91	112.46	121.92
1	D	85	ILE	CA-C-O	-5.91	113.98	120.72
1	D	113	ASP	CA-CB-CG	5.91	118.51	112.60
1	C	350	VAL	N-CA-CB	5.89	117.05	110.51
1	A	336	ASP	CA-C-O	-5.88	115.15	121.56
1	C	181	SER	CA-CB-OG	-5.88	99.33	111.10
1	C	240	PHE	O-C-N	5.88	128.35	122.12
1	D	189	ARG	CD-NE-CZ	5.88	132.63	124.40
1	D	470	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	D	477	ARG	CA-C-O	-5.87	114.25	121.11
1	B	29	GLU	CB-CG-CD	5.86	122.56	112.60
1	D	258	GLN	N-CA-C	-5.86	104.97	111.71
1	B	429	VAL	CA-C-O	5.85	123.47	119.20
1	C	304	ALA	N-CA-C	-5.85	106.69	113.88
1	C	393	PHE	CA-CB-CG	-5.83	107.97	113.80
1	D	84	PRO	CA-C-N	-5.83	115.58	123.10
1	D	84	PRO	C-N-CA	-5.83	115.58	123.10
1	D	196	THR	N-CA-C	-5.83	103.24	110.41
1	A	117	TYR	CB-CA-C	5.82	122.98	111.22
1	C	186	TYR	O-C-N	5.82	126.48	121.30
1	C	368	ASN	O-C-N	-5.82	116.21	122.85
1	D	414	LEU	CA-C-O	-5.81	113.79	120.24
1	D	214	LEU	N-CA-C	-5.81	104.30	111.33
1	A	286	ALA	CA-C-O	-5.81	115.06	121.33
1	D	276	PHE	N-CA-C	5.80	120.63	113.50
1	B	458	LEU	N-CA-CB	5.80	119.60	110.56
1	A	68	ALA	O-C-N	-5.79	115.84	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLU	N-CA-C	5.79	118.37	111.71
1	B	399	GLN	CB-CG-CD	5.79	122.44	112.60
1	B	115	SER	N-CA-C	5.78	118.52	111.82
1	C	301	PRO	O-C-N	5.77	129.65	123.01
1	D	99	CYS	CA-C-O	-5.77	115.05	121.51
1	C	405	ASN	CA-CB-CG	-5.76	106.84	112.60
1	B	8	ASN	CA-C-N	5.76	125.43	119.56
1	B	8	ASN	C-N-CA	5.76	125.43	119.56
1	D	129	THR	CA-C-O	-5.76	112.28	120.51
1	A	19	LEU	N-CA-CB	5.75	118.83	110.26
1	B	327	VAL	CB-CA-C	-5.75	102.07	110.81
1	A	209	ASN	CA-C-O	5.75	126.62	120.70
1	A	252	ASP	CA-C-O	-5.75	114.33	120.42
1	A	65	PHE	CA-CB-CG	-5.75	108.06	113.80
1	A	394	THR	CA-C-O	-5.74	114.50	120.70
1	D	166	SER	CA-C-O	-5.74	114.57	120.54
1	D	199	ALA	O-C-N	-5.74	116.12	122.09
1	A	352	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	315	HIS	O-C-N	5.73	129.68	122.23
1	B	399	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	C	218	ASN	CB-CG-ND2	-5.73	107.81	116.40
1	A	69	GLN	O-C-N	-5.72	116.05	122.12
1	C	413	ASP	N-CA-CB	-5.72	101.78	110.07
1	D	471	VAL	O-C-N	-5.72	117.31	123.14
1	A	455	PRO	CB-CA-C	5.71	118.48	111.12
1	B	387	ASN	O-C-N	5.70	129.38	122.48
1	A	245	TYR	N-CA-C	5.70	118.26	111.71
1	C	45	ALA	N-CA-C	5.69	116.91	108.60
1	C	264	HIS	CA-CB-CG	5.69	119.49	113.80
1	B	451	THR	N-CA-C	-5.68	106.34	113.72
1	B	2	VAL	CA-C-O	5.67	127.60	121.36
1	A	49	ASP	CA-C-N	-5.67	115.06	123.11
1	A	49	ASP	C-N-CA	-5.67	115.06	123.11
1	A	345	MET	O-C-N	-5.67	116.30	121.34
1	B	396	LEU	CA-C-N	5.67	131.90	121.70
1	B	396	LEU	C-N-CA	5.67	131.90	121.70
1	C	215	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	B	291	VAL	CB-CA-C	5.65	119.12	112.68
1	C	120	SER	CA-C-O	5.65	128.26	121.88
1	D	300	ILE	CA-C-O	5.65	127.52	119.95
1	B	149	PHE	CA-C-O	-5.64	114.90	120.82
1	C	159	VAL	N-CA-C	-5.64	107.24	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	327	VAL	N-CA-C	5.64	116.43	108.36
1	D	433	ILE	CA-C-O	-5.64	113.73	120.78
1	D	42	GLY	CA-C-O	-5.64	112.75	119.06
1	C	458	LEU	N-CA-CB	5.63	119.52	110.85
1	A	362	ILE	CA-C-O	-5.63	114.55	120.57
1	B	411	PHE	CA-CB-CG	-5.63	108.17	113.80
1	D	226	ILE	N-CA-CB	5.63	117.39	110.64
1	D	480	GLU	CB-CG-CD	-5.62	103.04	112.60
1	B	367	GLU	CA-C-O	-5.62	114.54	121.06
1	C	512	HIS	CA-C-O	5.61	126.29	120.40
1	B	209	ASN	N-CA-C	-5.61	106.44	113.28
1	B	58	ASN	CA-C-O	-5.60	112.36	119.31
1	B	189	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	D	36	ARG	NH1-CZ-NH2	5.59	126.56	119.30
1	A	61	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	B	291	VAL	N-CA-CB	-5.58	106.65	112.06
1	B	334	MET	N-CA-C	5.58	118.71	110.46
1	C	46	ILE	O-C-N	-5.58	117.02	122.93
1	B	364	LEU	N-CA-C	5.57	117.98	108.90
1	A	54	ASP	N-CA-C	-5.57	106.16	113.12
1	D	198	PHE	CA-CB-CG	-5.57	108.23	113.80
1	C	129	THR	N-CA-C	-5.56	100.61	109.07
1	A	117	TYR	CA-C-O	5.55	128.32	121.60
1	A	142	TYR	CA-CB-CG	5.55	123.89	113.90
1	C	66	SER	N-CA-C	5.55	117.41	111.36
1	D	467	TRP	CA-C-O	-5.55	114.33	120.38
1	B	339	SER	N-CA-C	5.54	118.29	110.14
1	A	32	GLU	CA-C-O	-5.54	114.67	120.55
1	B	21	LYS	CB-CA-C	5.54	119.73	109.54
1	A	505	VAL	N-CA-C	-5.53	103.88	109.02
1	C	164	TYR	CA-C-O	-5.53	114.85	120.71
1	D	364	LEU	N-CA-CB	-5.53	101.38	110.68
1	B	148	ALA	CA-C-O	5.53	126.28	120.42
1	B	294	GLN	CA-C-N	5.53	127.62	120.44
1	B	294	GLN	C-N-CA	5.53	127.62	120.44
1	A	143	GLY	N-CA-C	-5.52	106.10	112.73
1	A	60	ASP	N-CA-CB	-5.52	100.79	109.51
1	C	263	ASN	CA-CB-CG	-5.52	107.08	112.60
1	D	123	GLY	N-CA-C	5.51	122.96	115.30
1	C	387	ASN	CB-CG-ND2	5.50	124.65	116.40
1	C	470	ASN	OD1-CG-ND2	5.50	128.10	122.60
1	C	339	SER	N-CA-CB	-5.49	102.39	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASN	CA-CB-CG	-5.49	107.11	112.60
1	B	226	ILE	N-CA-C	5.48	115.68	110.42
1	A	368	ASN	N-CA-C	-5.47	103.16	110.55
1	D	54	ASP	CA-CB-CG	5.47	118.08	112.60
1	C	350	VAL	CB-CA-C	-5.47	104.88	111.88
1	D	352	ASN	CB-CA-C	5.47	120.15	110.85
1	B	283	PRO	O-C-N	-5.47	116.41	123.03
1	B	410	LYS	N-CA-C	-5.47	105.23	111.14
1	B	16	MET	CA-C-O	-5.46	114.82	121.05
1	B	116	LEU	CA-C-N	-5.46	112.50	123.09
1	B	116	LEU	C-N-CA	-5.46	112.50	123.09
1	C	317	LEU	CA-C-O	-5.45	113.70	119.97
1	A	58	ASN	CA-C-O	-5.45	112.55	119.31
1	C	435	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	304	ALA	N-CA-C	-5.45	107.18	113.88
1	A	501	SER	CA-CB-OG	-5.44	100.21	111.10
1	C	446	LEU	N-CA-CB	-5.43	102.23	110.92
1	A	209	ASN	N-CA-CB	-5.42	102.20	110.07
1	B	234	PRO	N-CA-C	5.42	119.38	111.03
1	C	468	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	D	501	SER	O-C-N	-5.41	116.63	123.17
1	A	457	GLN	CA-C-O	-5.41	114.70	120.92
1	D	328	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	229	LEU	CA-C-O	-5.39	113.77	119.97
1	B	166	SER	CA-C-N	-5.39	113.12	122.83
1	B	166	SER	C-N-CA	-5.39	113.12	122.83
1	A	443	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	B	442	ASN	CA-C-N	-5.38	113.42	123.05
1	B	442	ASN	C-N-CA	-5.38	113.42	123.05
1	D	299	THR	CA-CB-OG1	5.38	117.67	109.60
1	C	74	SER	CA-C-O	-5.38	114.72	120.42
1	B	46	ILE	O-C-N	5.37	128.82	123.18
1	A	162	LYS	CA-C-O	-5.37	115.19	121.10
1	B	207	VAL	O-C-N	5.37	127.17	121.91
1	B	327	VAL	CA-C-N	-5.37	114.88	122.94
1	B	327	VAL	C-N-CA	-5.37	114.88	122.94
1	C	429	VAL	CB-CA-C	-5.37	104.84	110.53
1	B	398	TYR	N-CA-CB	-5.37	101.42	110.49
1	D	381	VAL	O-C-N	5.37	127.31	121.94
1	C	329	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	442	ASN	N-CA-C	5.36	117.21	111.36
1	B	193	GLN	OE1-CD-NE2	-5.36	117.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	SER	CA-C-O	-5.36	115.38	121.00
1	B	384	MET	O-C-N	5.36	128.26	122.15
1	D	110	GLN	CG-CD-NE2	-5.35	108.37	116.40
1	A	440	THR	CA-C-O	-5.35	115.00	120.99
1	B	56	GLU	CA-C-O	5.34	127.76	121.78
1	A	406	SER	CB-CA-C	-5.33	102.75	110.96
1	B	393	PHE	CA-CB-CG	-5.33	108.47	113.80
1	C	113	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	463	HIS	N-CA-C	-5.33	104.90	111.40
1	D	12	LYS	CB-CG-CD	5.32	123.54	111.30
1	C	226	ILE	CA-C-O	-5.32	114.10	119.20
1	A	207	VAL	CA-CB-CG1	5.31	119.43	110.40
1	B	155	PRO	CB-CA-C	-5.31	103.93	111.68
1	C	401	VAL	CB-CA-C	-5.31	104.16	111.65
1	B	196	THR	N-CA-C	-5.31	103.53	110.53
1	D	461	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	40	GLN	CA-C-O	5.30	126.09	120.10
1	A	165	LEU	CA-C-O	-5.30	115.17	121.16
1	B	414	LEU	CA-C-O	-5.30	113.53	120.00
1	C	354	ALA	O-C-N	-5.30	116.58	122.09
1	B	129	THR	O-C-N	-5.29	118.22	123.46
1	B	193	GLN	CA-CB-CG	5.29	124.69	114.10
1	D	309	GLY	CA-C-O	-5.29	113.10	118.97
1	A	75	VAL	N-CA-C	-5.28	104.81	110.36
1	C	58	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	B	497	THR	CA-C-N	-5.28	116.64	123.19
1	B	497	THR	C-N-CA	-5.28	116.64	123.19
1	D	208	LEU	CA-C-O	5.28	126.36	120.82
1	A	86	ILE	CA-C-O	5.26	127.36	120.78
1	B	187	PRO	N-CA-CB	-5.26	96.81	102.60
1	D	330	THR	CA-CB-OG1	-5.26	101.71	109.60
1	B	166	SER	O-C-N	5.26	129.18	123.13
1	C	117	TYR	O-C-N	5.26	130.00	122.74
1	C	494	SER	CA-C-O	-5.26	115.68	121.31
1	A	324	LYS	CA-CB-CG	-5.26	103.59	114.10
1	B	344	SER	CA-C-O	-5.26	114.74	120.36
1	C	238	GLU	N-CA-C	-5.25	104.99	111.40
1	A	57	LYS	N-CA-C	5.25	116.69	110.97
1	D	437	VAL	O-C-N	-5.25	117.36	122.93
1	C	345	MET	CA-C-N	5.25	125.05	119.28
1	C	345	MET	C-N-CA	5.25	125.05	119.28
1	B	119	LYS	CA-C-O	5.24	126.14	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	ASN	CB-CA-C	-5.24	102.65	110.88
1	B	337	LYS	O-C-N	5.24	126.92	121.79
1	C	42	GLY	CA-C-O	-5.24	113.20	119.07
1	C	159	VAL	CA-C-O	-5.24	115.20	119.97
1	A	47	THR	CA-C-O	-5.24	114.90	120.92
1	C	44	TYR	N-CA-CB	-5.23	102.41	110.20
1	B	186	TYR	CA-C-O	5.22	125.09	120.02
1	D	190	GLY	CA-C-O	-5.22	113.74	121.58
1	D	410	LYS	CA-C-O	5.21	126.08	120.55
1	D	513	THR	CA-CB-CG2	-5.21	101.64	110.50
1	A	374	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	345	MET	CA-C-N	5.21	124.53	118.85
1	A	345	MET	C-N-CA	5.21	124.53	118.85
1	D	470	ASN	CB-CG-ND2	5.21	124.21	116.40
1	B	103	ILE	CA-C-O	-5.20	115.19	119.76
1	A	32	GLU	O-C-N	5.20	127.63	122.12
1	C	487	SER	CA-C-O	-5.20	115.50	121.47
1	B	49	ASP	CB-CA-C	-5.19	100.97	109.53
1	C	476	GLU	CA-C-N	-5.19	113.79	122.92
1	C	476	GLU	C-N-CA	-5.19	113.79	122.92
1	B	453	GLN	OE1-CD-NE2	5.18	127.78	122.60
1	C	404	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	D	180	THR	CA-C-O	5.18	126.27	120.82
1	D	243	ASN	CA-CB-CG	-5.18	107.42	112.60
1	C	164	TYR	N-CA-CB	-5.18	102.35	110.69
1	A	51	TRP	N-CA-C	5.18	117.72	109.96
1	C	216	GLU	O-C-N	5.17	128.05	122.15
1	C	428	ASN	CA-CB-CG	-5.17	107.43	112.60
1	D	59	GLY	CA-C-O	-5.17	116.72	121.63
1	A	95	VAL	CA-C-O	5.16	126.74	121.58
1	B	252	ASP	O-C-N	5.16	127.66	122.09
1	C	258	GLN	CA-C-N	5.16	126.63	120.13
1	C	258	GLN	C-N-CA	5.16	126.63	120.13
1	A	99	CYS	CA-C-O	5.15	127.56	121.58
1	B	387	ASN	N-CA-CB	5.15	117.83	110.67
1	A	160	ILE	O-C-N	5.14	129.76	122.97
1	D	279	THR	N-CA-C	5.14	116.74	111.03
1	C	189	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	C	87	SER	CA-C-O	-5.13	115.83	121.58
1	A	72	ALA	O-C-N	-5.13	116.68	122.12
1	C	218	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	A	240	PHE	CA-CB-CG	-5.12	108.68	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ASN	CA-CB-CG	5.12	117.72	112.60
1	C	279	THR	CB-CA-C	-5.12	102.19	110.79
1	B	71	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	139	ARG	CA-C-O	-5.11	115.13	120.55
1	B	454	TYR	CA-C-N	5.11	125.05	119.78
1	B	454	TYR	C-N-CA	5.11	125.05	119.78
1	C	67	TYR	N-CA-C	-5.11	105.62	111.14
1	C	448	SER	N-CA-CB	-5.11	104.23	111.84
1	B	27	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	C	424	ILE	CA-C-N	-5.11	116.45	123.14
1	C	424	ILE	C-N-CA	-5.11	116.45	123.14
1	C	350	VAL	O-C-N	5.11	127.05	121.94
1	B	300	ILE	CB-CG1-CD1	5.10	124.51	113.80
1	A	128	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	259	GLY	CA-C-N	5.10	128.52	120.47
1	A	259	GLY	C-N-CA	5.10	128.52	120.47
1	D	256	TRP	CA-CB-CG	5.10	123.28	113.60
1	A	162	LYS	CA-CB-CG	5.09	124.28	114.10
1	D	11	TYR	O-C-N	-5.09	116.76	122.97
1	C	425	VAL	CA-C-N	-5.09	115.76	122.98
1	C	425	VAL	C-N-CA	-5.09	115.76	122.98
1	A	489	ASP	N-CA-C	5.09	119.36	113.20
1	D	457	GLN	O-C-N	-5.09	117.26	123.16
1	D	71	PHE	CA-CB-CG	5.08	118.88	113.80
1	D	216	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	365	ASN	CA-CB-CG	-5.08	107.52	112.60
1	B	316	LEU	N-CA-C	-5.08	105.63	111.07
1	D	81	LYS	N-CA-CB	5.08	119.77	111.08
1	A	188	SER	CA-C-O	-5.08	116.20	121.99
1	A	383	GLU	CB-CG-CD	5.08	121.23	112.60
1	A	81	LYS	CA-C-O	-5.07	115.69	121.58
1	B	316	LEU	CA-C-O	-5.07	115.49	120.82
1	C	26	THR	CB-CA-C	-5.07	100.33	110.42
1	B	209	ASN	CB-CA-C	5.07	119.45	109.72
1	C	139	ARG	CD-NE-CZ	5.07	131.50	124.40
1	B	42	GLY	CA-C-O	-5.07	113.39	119.01
1	C	287	LYS	N-CA-C	5.07	117.75	109.59
1	B	490	GLY	N-CA-C	-5.06	107.71	116.01
1	D	465	ASN	O-C-N	-5.06	117.16	123.33
1	A	200	LYS	N-CA-C	5.06	116.80	111.28
1	B	170	ALA	CA-C-O	5.06	126.29	120.32
1	B	140	LYS	CA-C-O	-5.05	115.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	MET	CB-CA-C	-5.05	104.64	111.11
1	B	102	PRO	CA-C-N	5.05	129.87	119.72
1	B	102	PRO	C-N-CA	5.05	129.87	119.72
1	D	451	THR	CA-C-O	5.05	125.33	119.32
1	C	94	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	C	201	SER	CA-CB-OG	-5.04	101.01	111.10
1	A	151	ALA	N-CA-C	-5.04	105.26	111.40
1	A	262	GLU	N-CA-C	-5.03	105.79	111.28
1	A	379	LYS	CA-C-N	5.03	126.98	120.44
1	A	379	LYS	C-N-CA	5.03	126.98	120.44
1	D	89	HIS	CA-C-O	-5.03	115.74	121.68
1	D	178	TYR	CA-C-O	-5.03	115.08	120.46
1	B	363	VAL	CA-C-O	5.03	126.97	121.13
1	A	404	ASN	CA-CB-CG	-5.02	107.58	112.60
1	C	432	THR	CB-CA-C	-5.02	100.80	110.24
1	B	103	ILE	N-CA-CB	-5.02	104.16	110.33
1	B	444	ALA	N-CA-CB	-5.02	102.50	110.28
1	B	63	PHE	O-C-N	5.02	128.68	123.06
1	C	133	LEU	N-CA-C	-5.02	106.00	111.82
1	B	107	VAL	N-CA-C	5.01	115.73	110.62
1	A	364	LEU	N-CA-CB	-5.01	102.51	111.08
1	B	46	ILE	N-CA-C	-5.01	101.16	108.17
1	D	411	PHE	O-C-N	5.01	127.23	122.07
1	D	421	MET	CA-C-O	5.01	126.20	120.54
1	D	450	ASP	O-C-N	-5.01	116.71	122.87
1	A	69	GLN	CA-C-O	5.00	125.85	120.55
1	B	484	PHE	CA-CB-CG	5.00	118.80	113.80
1	A	257	TYR	CA-CB-CG	5.00	122.90	113.90
1	B	338	GLY	CA-C-O	-5.00	113.46	119.06
1	D	69	GLN	CA-C-N	5.00	129.18	120.68
1	D	69	GLN	C-N-CA	5.00	129.18	120.68

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ALA	Mainchain
1	B	134	ALA	Mainchain
1	B	276	PHE	Mainchain
1	C	220	ALA	Mainchain
1	D	146	TYR	Mainchain
1	D	50	PHE	Mainchain

## 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	4119	0	3984	88	0
1	B	4119	0	3984	123	0
1	C	4119	0	3984	108	0
1	D	4119	0	3984	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	206	0	0	6	0
3	B	170	0	0	3	0
3	C	191	0	0	7	0
3	D	185	0	0	9	0
All	All	17232	0	15936	425	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 13.

All (425) 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:129:THR:HG21	1:B:169:PRO:HD3	1.36	1.05
1:A:489:ASP:OD1	1:A:491:THR:HG23	1.54	1.05
1:B:422:GLN:NE2	1:B:510:THR:H	1.54	1.04
1:C:164:TYR:HH	1:C:328:THR:HG1	1.04	1.02
1:D:226:ILE:HD12	1:D:227:SER:H	1.24	0.99
1:B:21:LYS:NZ	1:B:54:ASP:OD2	1.96	0.97
1:B:489:ASP:OD1	1:B:491:THR:OG1	1.84	0.95
1:B:422:GLN:HE22	1:B:510:THR:H	1.10	0.92
1:C:84:PRO:HD2	1:C:162:LYS:O	1.71	0.90
1:C:489:ASP:OD2	1:C:491:THR:HG23	1.79	0.82
1:A:216:GLU:OE2	1:A:219:LYS:NZ	2.14	0.80
1:D:63:PHE:HB3	1:D:65:PHE:CE2	2.17	0.80
1:A:489:ASP:OD1	1:A:491:THR:CG2	2.30	0.79
1:B:422:GLN:HE22	1:B:510:THR:N	1.81	0.78
1:B:312:ASP:CG	1:B:315:HIS:HD2	1.93	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:ASN:OD1	1:C:376:GLU:N	2.18	0.77
1:B:485:ILE:HG13	1:B:516:TRP:CH2	2.19	0.77
1:D:182:ASP:O	1:D:191:LYS:NZ	2.17	0.77
1:B:427:LYS:O	1:B:515:SER:HA	1.85	0.76
1:A:211:TYR:OH	1:A:252:ASP:OD2	2.03	0.76
1:B:351:GLN:HG3	1:B:384:MET:HE1	1.68	0.76
1:C:479:ILE:HD12	1:C:481:PHE:CD1	2.21	0.76
1:A:51:TRP:CZ2	1:A:91:CYS:SG	2.79	0.75
1:C:287:LYS:HG2	1:C:328:THR:HB	1.68	0.75
1:C:154:LYS:HG3	1:C:279:THR:HG21	1.68	0.75
1:C:200:LYS:NZ	3:C:773:HOH:O	2.18	0.74
1:A:51:TRP:CZ3	1:A:91:CYS:HB2	2.22	0.74
1:C:247:SER:HB2	3:C:662:HOH:O	1.85	0.74
1:D:226:ILE:HD12	1:D:227:SER:N	2.00	0.73
1:D:218:ASN:ND2	1:D:225:LEU:H	1.87	0.73
1:D:16:MET:CG	1:D:397:ARG:NH1	2.51	0.73
1:D:218:ASN:CG	1:D:225:LEU:H	1.97	0.73
1:C:479:ILE:HD12	1:C:481:PHE:HD1	1.55	0.72
1:D:383:GLU:HB2	3:D:755:HOH:O	1.89	0.72
1:D:94:ASN:HB2	1:D:97:ASP:OD2	1.89	0.71
1:A:365:ASN:HB3	3:A:630:HOH:O	1.90	0.71
1:C:482:LYS:HE2	1:C:496:GLN:O	1.91	0.71
1:C:26:THR:HG21	1:C:30:THR:CG2	2.20	0.70
1:D:16:MET:HG2	1:D:397:ARG:NH1	2.06	0.70
1:A:182:ASP:O	1:A:184:THR:HG23	1.92	0.70
1:B:482:LYS:HG2	1:B:499:GLN:HA	1.71	0.70
1:B:476:GLU:HG3	1:B:507:LEU:HD22	1.73	0.69
1:B:485:ILE:HG13	1:B:516:TRP:HH2	1.57	0.69
1:B:300:ILE:O	1:B:300:ILE:HG13	1.91	0.69
1:B:129:THR:HG21	1:B:169:PRO:CD	2.19	0.69
1:C:320:PHE:CD2	1:C:327:VAL:HG22	2.29	0.68
1:C:476:GLU:CG	1:C:507:LEU:HD22	2.24	0.68
1:C:202:LYS:NZ	3:C:727:HOH:O	2.26	0.67
1:B:242:MET:HG2	1:B:300:ILE:HG22	1.77	0.67
1:A:462:SER:O	1:A:465:ASN:N	2.27	0.67
1:B:33:ASN:OD1	1:B:36:ARG:NH1	2.26	0.67
1:D:26:THR:HG21	3:D:757:HOH:O	1.93	0.67
1:A:454:TYR:N	1:A:455:PRO:CD	2.58	0.67
1:C:49:ASP:OD2	3:C:722:HOH:O	2.13	0.67
1:A:460:TYR:OH	1:A:465:ASN:OD1	2.01	0.66
1:B:427:LYS:N	1:B:514:SER:O	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:PHE:CZ	1:C:35:LEU:HD11	2.31	0.66
1:A:320:PHE:CD2	1:A:327:VAL:HG22	2.31	0.65
1:C:111:LYS:HD2	3:C:732:HOH:O	1.95	0.65
1:C:460:TYR:OH	1:C:465:ASN:HA	1.97	0.65
1:A:461:ASP:O	1:A:465:ASN:N	2.30	0.65
1:D:16:MET:CE	1:D:397:ARG:HH12	2.10	0.65
1:A:280:PHE:O	1:A:281:GLN:HB2	1.97	0.64
1:C:347:LYS:O	1:C:351:GLN:HG3	1.98	0.64
1:D:305:GLU:OE1	3:D:644:HOH:O	2.15	0.64
1:B:429:VAL:HG22	1:B:516:TRP:CE3	2.33	0.64
1:D:336:ASP:OD2	1:D:348:THR:OG1	2.16	0.64
1:C:26:THR:HG21	1:C:30:THR:HG22	1.80	0.64
1:B:421:MET:O	1:B:422:GLN:HG2	1.98	0.64
1:C:420:VAL:HG22	1:C:421:MET:N	2.12	0.63
1:B:487:SER:OG	1:B:489:ASP:OD2	2.15	0.63
1:D:327:VAL:HG23	1:D:362:ILE:HG21	1.79	0.63
1:B:341:PRO:HD2	1:B:342:GLU:OE1	1.99	0.62
1:A:232:LEU:HB3	1:A:233:PRO:HD2	1.82	0.62
1:C:31:PHE:CE2	1:C:35:LEU:HD11	2.35	0.62
1:C:226:ILE:HD13	1:C:226:ILE:H	1.64	0.62
1:A:454:TYR:N	1:A:455:PRO:HD2	2.14	0.62
1:B:398:TYR:HB3	1:B:399:GLN:OE1	2.00	0.62
1:B:421:MET:C	1:B:422:GLN:HG2	2.25	0.62
1:C:489:ASP:OD2	1:C:491:THR:CG2	2.48	0.62
1:C:38:ALA:HB2	1:C:402:MET:HE1	1.82	0.61
1:B:454:TYR:N	1:B:455:PRO:HD2	2.15	0.61
1:B:312:ASP:OD2	1:B:315:HIS:HD2	1.84	0.61
1:B:422:GLN:NE2	1:B:510:THR:N	2.38	0.61
1:D:365:ASN:HB3	3:D:628:HOH:O	2.01	0.61
1:C:398:TYR:O	1:C:402:MET:HB2	2.00	0.60
1:B:461:ASP:CG	1:B:464:SER:HB2	2.27	0.60
1:B:312:ASP:OD2	1:B:315:HIS:CD2	2.55	0.60
1:A:95:VAL:HG12	1:A:96:GLY:N	2.16	0.60
1:D:254:LEU:HD13	1:D:311:ASN:ND2	2.16	0.60
1:A:95:VAL:CG1	1:A:96:GLY:N	2.65	0.60
1:D:22:ILE:N	1:D:23:PRO:HD2	2.17	0.59
1:D:218:ASN:HD21	1:D:225:LEU:H	1.49	0.59
1:A:126:ASN:OD1	1:A:128:GLU:HG2	2.01	0.59
1:B:454:TYR:N	1:B:455:PRO:CD	2.65	0.59
1:C:420:VAL:CG2	1:C:421:MET:N	2.65	0.59
1:B:461:ASP:O	1:B:465:ASN:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:CD	1:A:219:LYS:NZ	2.60	0.59
1:D:16:MET:HG3	1:D:397:ARG:NH1	2.17	0.59
1:B:1:ALA:HA	1:B:387:ASN:OD1	2.02	0.59
1:B:425:VAL:HG22	1:B:468:ARG:HB3	1.84	0.59
1:C:487:SER:O	1:C:488:LYS:C	2.45	0.59
1:C:89:HIS:ND1	1:C:166:SER:OG	2.31	0.58
1:B:372:ILE:HG23	1:B:377:GLU:HB2	1.84	0.58
1:A:51:TRP:CH2	1:A:91:CYS:HB2	2.38	0.58
1:C:200:LYS:HE3	1:C:232:LEU:HD22	1.84	0.58
1:A:306:LYS:HB2	1:A:307:PRO:HD3	1.86	0.58
1:C:115:SER:HB2	1:C:198:PHE:CD2	2.38	0.58
1:D:488:LYS:HD2	1:D:488:LYS:C	2.29	0.58
1:A:502:TRP:C	1:A:503:ASN:HD22	2.12	0.58
1:C:22:ILE:HB	1:C:23:PRO:HD3	1.85	0.58
1:C:26:THR:CG2	1:C:30:THR:HG21	2.33	0.58
1:B:485:ILE:CG1	1:B:516:TRP:CH2	2.86	0.58
1:B:1:ALA:HB3	1:B:5:LYS:O	2.04	0.58
1:A:129:THR:HG21	1:A:169:PRO:HD3	1.87	0.57
1:C:302:HIS:HA	3:C:613:HOH:O	2.04	0.57
1:A:344:SER:OG	1:A:346:PRO:HD3	2.04	0.57
1:B:176:PRO:O	1:B:193:GLN:NE2	2.36	0.57
1:C:374:ASN:OD1	1:C:376:GLU:HB2	2.05	0.57
1:B:89:HIS:HA	1:B:103:ILE:HD11	1.87	0.57
1:C:454:TYR:N	1:C:455:PRO:CD	2.67	0.57
1:C:129:THR:HG21	1:C:169:PRO:HD3	1.87	0.57
1:D:218:ASN:HD21	1:D:225:LEU:N	2.03	0.57
1:B:156:TYR:O	1:B:159:VAL:HG22	2.04	0.57
1:B:176:PRO:C	1:B:193:GLN:HE21	2.12	0.57
1:D:184:THR:HG21	1:D:191:LYS:HG3	1.87	0.57
1:B:450:ASP:OD2	1:B:453:GLN:N	2.32	0.56
1:A:330:THR:O	1:A:331:CYS:HB2	2.02	0.56
1:B:476:GLU:CG	1:B:507:LEU:HD22	2.35	0.56
1:C:90:GLN:HE21	1:C:93:GLY:HA3	1.71	0.56
1:C:460:TYR:CZ	1:C:465:ASN:HA	2.40	0.56
1:A:347:LYS:O	1:A:351:GLN:HG3	2.06	0.56
1:C:121:GLU:OE2	1:C:191:LYS:HA	2.05	0.56
1:B:39:LYS:HD3	1:B:80:MET:SD	2.46	0.56
1:B:129:THR:CG2	1:B:169:PRO:HD3	2.23	0.56
1:B:485:ILE:HD11	1:B:516:TRP:CZ2	2.40	0.56
1:D:488:LYS:HD2	1:D:488:LYS:O	2.05	0.56
1:B:327:VAL:HG23	1:B:362:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LEU:HB3	1:C:233:PRO:HD2	1.88	0.56
1:D:355:THR:O	1:D:359:GLU:HB2	2.06	0.56
1:C:19:LEU:HD13	1:C:397:ARG:NH1	2.20	0.55
1:A:473:LEU:HB3	1:A:474:PRO:HD2	1.88	0.55
1:B:287:LYS:HG2	1:B:328:THR:HB	1.89	0.55
1:A:95:VAL:CG1	1:A:96:GLY:H	2.19	0.55
1:D:296:ASN:OD1	1:D:343:TYR:HB3	2.06	0.55
1:A:372:ILE:HG21	1:A:378:TYR:CD1	2.41	0.55
1:C:26:THR:HG21	1:C:30:THR:HG21	1.86	0.55
1:A:306:LYS:N	1:A:307:PRO:CD	2.69	0.55
1:A:254:LEU:HD13	1:A:311:ASN:ND2	2.22	0.55
1:C:35:LEU:HB3	1:C:80:MET:HG3	1.89	0.55
1:B:364:LEU:HD21	1:B:390:PHE:CZ	2.42	0.55
1:C:454:TYR:N	1:C:455:PRO:HD2	2.22	0.54
1:A:156:TYR:O	1:A:157:LYS:C	2.47	0.54
1:A:482:LYS:HE2	3:A:785:HOH:O	2.07	0.54
1:D:443:ARG:HA	3:D:694:HOH:O	2.07	0.54
1:B:478:ASN:HB3	1:B:503:ASN:ND2	2.23	0.54
1:D:424:ILE:O	1:D:468:ARG:HA	2.08	0.54
1:A:462:SER:O	1:A:463:HIS:C	2.51	0.54
1:C:375:GLU:OE1	1:C:410:LYS:HE3	2.08	0.54
1:C:374:ASN:OD1	1:C:376:GLU:CB	2.56	0.54
1:C:476:GLU:HG2	1:C:507:LEU:HD22	1.88	0.54
1:D:329:PHE:O	1:D:366:GLY:HA2	2.08	0.53
1:A:421:MET:SD	1:A:470:ASN:HB3	2.48	0.53
1:D:488:LYS:C	1:D:490:GLY:H	2.16	0.53
1:A:164:TYR:CE1	1:A:287:LYS:HE2	2.43	0.53
1:C:90:GLN:NE2	1:C:93:GLY:HA3	2.22	0.53
1:C:476:GLU:CG	1:C:507:LEU:CD2	2.87	0.53
1:D:232:LEU:HB3	1:D:233:PRO:HD2	1.91	0.53
1:B:164:TYR:OH	1:B:328:THR:OG1	2.22	0.53
1:D:367:GLU:HG2	1:D:394:THR:HB	1.91	0.53
1:C:488:LYS:O	1:C:490:GLY:N	2.42	0.53
1:D:47:THR:CG2	1:D:85:ILE:HD11	2.39	0.53
1:C:461:ASP:O	1:C:465:ASN:N	2.42	0.53
1:B:485:ILE:HD11	1:B:516:TRP:CH2	2.44	0.53
1:D:22:ILE:N	1:D:23:PRO:CD	2.72	0.53
1:D:115:SER:HA	3:D:633:HOH:O	2.09	0.52
1:D:425:VAL:HB	1:D:513:THR:HG23	1.91	0.52
1:C:460:TYR:CE1	1:C:465:ASN:HA	2.45	0.52
1:C:351:GLN:HG2	1:C:384:MET:HE1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:O	1:C:97:ASP:HB2	2.08	0.52
1:D:11:TYR:HA	1:D:391:ALA:O	2.09	0.52
1:B:488:LYS:O	1:B:489:ASP:C	2.52	0.52
1:B:485:ILE:CD1	1:B:516:TRP:CZ2	2.93	0.52
1:C:20:LYS:HD2	1:C:25:VAL:CG2	2.40	0.52
1:D:115:SER:HB3	1:D:198:PHE:CG	2.45	0.52
1:A:51:TRP:CH2	1:A:91:CYS:SG	3.02	0.51
1:A:216:GLU:CD	1:A:219:LYS:HZ1	2.18	0.51
1:C:115:SER:HB2	1:C:198:PHE:CE2	2.44	0.51
1:C:471:VAL:HG12	1:C:473:LEU:HD13	1.91	0.51
1:D:17:ALA:HB1	1:D:18:PRO:HD2	1.92	0.51
1:D:218:ASN:OD1	1:D:225:LEU:N	2.40	0.51
1:A:114:ASP:HB2	1:A:117:TYR:CZ	2.45	0.51
1:D:17:ALA:HB1	1:D:18:PRO:CD	2.40	0.51
1:C:404:ASN:ND2	1:C:407:LEU:HD22	2.25	0.51
1:D:306:LYS:N	1:D:307:PRO:CD	2.73	0.51
1:C:104:PRO:HB2	1:C:107:VAL:HG23	1.93	0.51
1:D:94:ASN:O	1:D:95:VAL:C	2.53	0.51
1:C:330:THR:O	1:C:331:CYS:HB2	2.11	0.51
1:D:497:THR:HG22	1:D:498:ILE:HG13	1.93	0.51
1:A:103:ILE:HD11	1:A:108:TRP:CZ2	2.46	0.51
1:D:238:GLU:O	1:D:242:MET:HG3	2.11	0.51
1:A:329:PHE:CE1	1:A:353:ILE:HG13	2.46	0.50
1:B:478:ASN:HB3	1:B:503:ASN:HD22	1.76	0.50
1:C:59:GLY:HA2	1:C:106:TRP:CD1	2.45	0.50
1:D:47:THR:HG22	1:D:85:ILE:HD11	1.92	0.50
1:B:51:TRP:CZ2	1:B:91:CYS:SG	3.05	0.50
1:B:22:ILE:N	1:B:23:PRO:CD	2.74	0.50
1:B:89:HIS:CA	1:B:103:ILE:HD11	2.42	0.50
1:C:226:ILE:HD13	1:C:226:ILE:N	2.26	0.50
1:B:333:GLU:O	1:B:380:ARG:HD2	2.12	0.49
1:A:372:ILE:HG21	1:A:378:TYR:CE1	2.48	0.49
1:C:479:ILE:CD1	1:C:481:PHE:CD1	2.95	0.49
1:D:55:MET:O	1:D:63:PHE:HA	2.12	0.49
1:A:35:LEU:HB3	1:A:80:MET:HG3	1.95	0.49
1:A:93:GLY:C	1:A:94:ASN:ND2	2.71	0.49
1:B:450:ASP:OD2	1:B:453:GLN:HG2	2.12	0.49
1:C:426:VAL:N	1:C:467:TRP:O	2.36	0.49
1:A:190:GLY:HA3	3:A:775:HOH:O	2.13	0.49
1:B:460:TYR:CE2	1:B:462:SER:HA	2.48	0.49
1:A:69:GLN:HG2	1:A:156:TYR:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:CD	1:A:228:GLU:H	2.21	0.48
1:A:287:LYS:HG2	1:A:328:THR:HB	1.93	0.48
1:D:312:ASP:O	1:D:313:TYR:C	2.52	0.48
1:B:451:THR:HG22	1:B:484:PHE:CE1	2.48	0.48
1:B:453:GLN:C	1:B:455:PRO:HD2	2.37	0.48
1:C:19:LEU:HD13	1:C:397:ARG:CZ	2.44	0.48
1:D:292:HIS:HB2	1:D:346:PRO:HD3	1.96	0.48
1:D:330:THR:OG1	1:D:331:CYS:N	2.44	0.48
1:A:51:TRP:CE3	1:A:91:CYS:HB2	2.49	0.48
1:A:347:LYS:HE2	3:A:776:HOH:O	2.13	0.48
1:C:51:TRP:CZ2	1:C:91:CYS:SG	3.06	0.48
1:B:489:ASP:CG	1:B:491:THR:OG1	2.53	0.48
1:D:488:LYS:C	1:D:490:GLY:N	2.70	0.48
1:B:485:ILE:CD1	1:B:516:TRP:CH2	2.98	0.47
1:B:371:SER:HB3	1:B:400:ASP:OD2	2.14	0.47
1:B:118:PHE:O	1:B:125:VAL:HA	2.14	0.47
1:D:115:SER:HB2	1:D:198:PHE:CD2	2.48	0.47
1:B:412:LYS:O	1:B:477:ARG:NH2	2.40	0.47
1:B:47:THR:HG21	3:B:680:HOH:O	2.15	0.47
1:B:487:SER:OG	1:B:489:ASP:CG	2.57	0.47
1:C:104:PRO:O	1:C:107:VAL:HG23	2.15	0.47
1:D:16:MET:HE3	1:D:397:ARG:HH12	1.79	0.47
1:B:427:LYS:HE3	1:B:427:LYS:HB3	1.64	0.47
1:C:109:ASN:ND2	3:D:789:HOH:O	2.47	0.47
1:A:376:GLU:O	1:A:379:LYS:HB2	2.15	0.47
1:A:503:ASN:HA	1:A:504:PRO:HA	1.60	0.47
1:D:47:THR:HG22	1:D:85:ILE:CD1	2.45	0.47
1:A:240:PHE:HA	1:A:244:GLY:HA3	1.96	0.47
1:B:306:LYS:N	1:B:307:PRO:CD	2.78	0.47
1:C:7:MET:HE2	1:C:419:PRO:HB3	1.97	0.47
1:C:26:THR:CG2	1:C:30:THR:CG2	2.90	0.47
1:B:7:MET:HE3	1:B:386:PHE:CD1	2.50	0.46
1:C:476:GLU:HG3	1:C:507:LEU:HD22	1.93	0.46
1:D:20:LYS:HE3	1:D:25:VAL:HG22	1.96	0.46
1:D:432:THR:O	1:D:433:ILE:C	2.58	0.46
1:B:411:PHE:CD1	1:B:411:PHE:C	2.94	0.46
1:D:266:LYS:NZ	3:D:762:HOH:O	2.34	0.46
1:D:138:ILE:HD12	1:D:142:TYR:CZ	2.51	0.46
1:B:120:SER:HB2	1:B:182:ASP:OD2	2.15	0.46
1:B:351:GLN:HG2	1:B:388:TYR:CZ	2.50	0.46
1:B:451:THR:HG22	1:B:484:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:LEU:HD21	1:D:226:ILE:O	2.15	0.46
1:D:312:ASP:OD1	1:D:314:SER:CB	2.64	0.46
1:D:461:ASP:O	1:D:465:ASN:N	2.45	0.46
1:A:448:SER:O	1:A:449:TRP:HB2	2.15	0.46
1:B:453:GLN:HE21	1:B:453:GLN:HB3	1.43	0.46
1:C:505:VAL:HG13	1:C:506:PRO:HD2	1.97	0.46
1:D:115:SER:CB	1:D:198:PHE:CD2	2.98	0.46
1:D:476:GLU:HG3	1:D:507:LEU:HD22	1.98	0.46
1:B:39:LYS:HE2	1:B:79:GLY:O	2.16	0.46
1:C:326:ASP:OD2	3:C:776:HOH:O	2.20	0.46
1:B:429:VAL:HG22	1:B:516:TRP:HE3	1.80	0.46
1:B:443:ARG:HB3	1:B:445:GLU:OE1	2.15	0.46
1:D:139:ARG:HH11	1:D:139:ARG:HD3	1.56	0.46
1:A:178:TYR:HA	1:A:184:THR:OG1	2.16	0.46
1:B:21:LYS:NZ	1:B:54:ASP:CG	2.72	0.46
1:B:477:ARG:O	1:B:505:VAL:HG23	2.15	0.46
1:C:334:MET:HE3	1:C:369:ALA:HB3	1.98	0.46
1:C:478:ASN:OD1	1:C:503:ASN:HA	2.15	0.46
1:D:21:LYS:C	1:D:23:PRO:HD2	2.42	0.46
1:D:327:VAL:CG2	1:D:362:ILE:HG21	2.45	0.46
1:A:110:GLN:OE1	3:A:786:HOH:O	2.21	0.45
1:B:136:ASP:OD1	1:B:137:VAL:N	2.49	0.45
1:C:327:VAL:HG23	1:C:362:ILE:HG21	1.97	0.45
1:D:63:PHE:CB	1:D:65:PHE:CE2	2.93	0.45
1:A:119:LYS:HA	1:A:124:THR:O	2.17	0.45
1:D:186:TYR:HA	1:D:187:PRO:HA	1.75	0.45
1:D:219:LYS:HB3	1:D:220:ALA:H	1.65	0.45
1:A:175:TYR:O	1:A:177:SER:N	2.45	0.45
1:B:426:VAL:HA	1:B:514:SER:O	2.15	0.45
1:C:7:MET:HE1	1:C:417:VAL:CG2	2.47	0.45
1:C:232:LEU:HB3	1:C:233:PRO:CD	2.46	0.45
1:B:505:VAL:HA	1:B:506:PRO:HD3	1.81	0.45
1:D:208:LEU:O	1:D:209:ASN:C	2.58	0.45
1:D:503:ASN:HA	1:D:504:PRO:HA	1.65	0.45
1:A:453:GLN:C	1:A:455:PRO:HD2	2.42	0.45
1:C:115:SER:CB	1:C:198:PHE:CD2	2.99	0.45
1:D:184:THR:CG2	1:D:191:LYS:HG3	2.46	0.45
1:D:201:SER:O	1:D:205:LEU:HD23	2.16	0.45
1:D:120:SER:O	1:D:121:GLU:C	2.59	0.45
1:A:47:THR:HG22	1:A:85:ILE:HD11	1.99	0.44
1:A:51:TRP:CH2	1:A:91:CYS:CB	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ASN:HA	1:B:504:PRO:HA	1.72	0.44
1:C:7:MET:HE1	1:C:417:VAL:HG23	1.99	0.44
1:A:60:ASP:O	1:A:61:GLN:HB2	2.17	0.44
1:B:50:PHE:HE2	1:B:84:PRO:HB3	1.82	0.44
1:C:375:GLU:CB	1:C:410:LYS:HD2	2.48	0.44
1:C:432:THR:O	1:C:433:ILE:C	2.59	0.44
1:D:214:LEU:O	1:D:215:ASN:C	2.59	0.44
1:C:40:GLN:HE21	1:C:40:GLN:HB2	1.69	0.44
1:C:350:VAL:CG1	1:C:384:MET:HE2	2.48	0.44
1:B:327:VAL:HG23	1:B:362:ILE:CG2	2.48	0.44
1:D:221:TRP:O	1:D:223:THR:HG23	2.18	0.44
1:D:128:GLU:O	1:D:129:THR:HB	2.17	0.44
1:A:346:PRO:O	1:A:350:VAL:HG23	2.18	0.44
1:B:332:LEU:HD22	1:B:350:VAL:HG11	1.99	0.44
1:B:153:MET:C	1:B:155:PRO:HD2	2.43	0.44
1:B:182:ASP:O	1:B:191:LYS:NZ	2.33	0.44
1:B:242:MET:CG	1:B:300:ILE:HG22	2.47	0.44
1:C:297:ASN:OD1	1:C:297:ASN:C	2.61	0.44
1:B:120:SER:CB	1:B:182:ASP:OD2	2.67	0.43
1:B:453:GLN:HG2	1:B:453:GLN:H	1.75	0.43
1:D:8:ASN:HA	1:D:9:PRO:HD2	1.83	0.43
1:D:115:SER:CB	1:D:198:PHE:CG	3.01	0.43
1:A:342:GLU:O	1:A:343:TYR:C	2.61	0.43
1:B:312:ASP:CG	1:B:315:HIS:CD2	2.84	0.43
1:D:305:GLU:HG2	1:D:313:TYR:OH	2.18	0.43
1:A:108:TRP:CZ2	1:A:127:LYS:HB3	2.53	0.43
1:B:399:GLN:H	1:B:399:GLN:CD	2.22	0.43
1:C:186:TYR:HA	1:C:187:PRO:HA	1.71	0.43
1:A:22:ILE:HB	1:A:23:PRO:HD3	1.99	0.43
1:A:63:PHE:HB3	1:A:65:PHE:CE2	2.54	0.43
1:A:515:SER:O	1:A:516:TRP:C	2.60	0.43
1:C:488:LYS:C	1:C:490:GLY:H	2.27	0.43
1:A:74:SER:O	1:A:75:VAL:C	2.59	0.43
1:A:21:LYS:HG2	1:A:67:TYR:CZ	2.53	0.43
1:A:340:TYR:CE1	1:A:341:PRO:HB3	2.53	0.43
1:C:451:THR:O	1:C:486:LYS:CE	2.67	0.43
1:D:448:SER:O	1:D:449:TRP:HB2	2.19	0.43
1:A:2:VAL:O	1:A:3:ASN:HB2	2.19	0.43
1:A:55:MET:O	1:A:63:PHE:HA	2.19	0.43
1:C:453:GLN:C	1:C:455:PRO:HD2	2.43	0.43
1:B:134:ALA:O	1:B:138:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:O	1:C:97:ASP:CB	2.67	0.43
1:D:51:TRP:CZ2	1:D:91:CYS:SG	3.12	0.43
1:A:93:GLY:C	1:A:94:ASN:HD22	2.27	0.43
1:D:16:MET:HG3	1:D:397:ARG:HH11	1.82	0.43
1:D:175:TYR:O	1:D:177:SER:N	2.50	0.43
1:B:35:LEU:HB3	1:B:80:MET:HG3	2.00	0.43
1:B:119:LYS:HE3	3:B:689:HOH:O	2.19	0.43
1:B:427:LYS:O	1:B:428:ASN:HB2	2.19	0.43
1:D:313:TYR:O	1:D:317:LEU:HG	2.19	0.43
1:D:372:ILE:HG23	1:D:377:GLU:HG3	2.01	0.43
1:B:50:PHE:HZ	1:B:82:MET:HE1	1.84	0.42
1:B:154:LYS:HB3	1:B:155:PRO:HD3	2.01	0.42
1:D:16:MET:HE2	1:D:397:ARG:HH12	1.82	0.42
1:B:121:GLU:HG2	1:B:195:TYR:CE1	2.54	0.42
1:D:226:ILE:CD1	1:D:227:SER:H	2.13	0.42
1:B:114:ASP:CG	1:B:196:THR:HB	2.44	0.42
1:C:154:LYS:N	1:C:155:PRO:CD	2.81	0.42
1:C:306:LYS:HB2	1:C:307:PRO:HD3	2.02	0.42
1:B:186:TYR:HA	1:B:187:PRO:HA	1.64	0.42
1:C:121:GLU:OE2	1:C:192:PHE:N	2.50	0.42
1:B:461:ASP:OD2	1:B:464:SER:HB2	2.19	0.42
1:C:53:GLY:HA3	1:C:101:VAL:HG12	2.00	0.42
1:C:375:GLU:HB2	1:C:410:LYS:HD2	2.02	0.42
1:C:321:LYS:HA	1:C:321:LYS:HD2	1.81	0.42
1:D:219:LYS:O	1:D:222:GLY:N	2.43	0.42
1:B:167:GLY:N	3:B:635:HOH:O	2.47	0.42
1:B:500:GLN:O	1:B:501:SER:HB3	2.20	0.42
1:C:505:VAL:HA	1:C:506:PRO:HD3	1.80	0.42
1:A:11:TYR:HA	1:A:391:ALA:O	2.20	0.42
1:B:23:PRO:HA	1:B:26:THR:O	2.20	0.42
1:B:219:LYS:HG3	1:B:220:ALA:N	2.34	0.42
1:B:288:ILE:HG23	1:B:310:TYR:CZ	2.55	0.42
1:C:317:LEU:O	1:C:320:PHE:HB2	2.20	0.41
1:D:226:ILE:H	1:D:226:ILE:HG13	1.64	0.41
1:D:443:ARG:HH11	1:D:443:ARG:HD2	1.75	0.41
1:A:37:TRP:O	1:A:40:GLN:HB2	2.20	0.41
1:A:429:VAL:HG12	1:A:431:THR:HG23	2.02	0.41
1:D:154:LYS:N	1:D:155:PRO:CD	2.83	0.41
1:D:248:MET:HE3	1:D:248:MET:O	2.21	0.41
1:A:1:ALA:HB3	1:A:5:LYS:O	2.21	0.41
1:A:94:ASN:ND2	1:A:94:ASN:N	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TYR:HA	1:A:341:PRO:HA	1.82	0.41
1:B:21:LYS:HZ1	1:B:54:ASP:CG	2.28	0.41
1:B:153:MET:O	1:B:154:LYS:C	2.63	0.41
1:C:169:PRO:C	1:C:171:GLY:N	2.77	0.41
1:D:22:ILE:HD12	1:D:31:PHE:CD1	2.56	0.41
1:B:12:LYS:O	1:B:392:GLY:HA2	2.21	0.41
1:C:131:ASN:HA	1:C:132:PRO:HD2	1.82	0.41
1:D:221:TRP:O	1:D:222:GLY:C	2.63	0.41
1:D:40:GLN:HE21	1:D:40:GLN:HB2	1.74	0.41
1:D:218:ASN:ND2	1:D:225:LEU:N	2.60	0.41
1:B:460:TYR:CD1	1:B:466:ASP:O	2.73	0.41
1:B:487:SER:OG	1:B:489:ASP:OD1	2.38	0.41
1:D:131:ASN:C	1:D:133:LEU:N	2.77	0.41
1:A:226:ILE:HG22	3:A:784:HOH:O	2.20	0.41
1:A:382:ALA:O	1:A:383:GLU:C	2.63	0.41
1:C:462:SER:C	1:C:464:SER:N	2.78	0.41
1:C:482:LYS:HG3	1:C:499:GLN:HA	2.03	0.41
1:D:139:ARG:HB2	1:D:267:LEU:HD11	2.02	0.41
1:C:109:ASN:OD1	1:D:40:GLN:NE2	2.54	0.41
1:D:297:ASN:HB2	1:D:343:TYR:CD2	2.56	0.41
1:D:454:TYR:N	1:D:455:PRO:CD	2.83	0.41
1:A:139:ARG:HB2	1:A:267:LEU:HD11	2.02	0.40
1:A:186:TYR:HA	1:A:187:PRO:HA	1.80	0.40
1:B:464:SER:HB3	1:B:466:ASP:CG	2.46	0.40
1:B:508:LYS:O	1:B:509:THR:C	2.64	0.40
1:C:21:LYS:O	1:C:22:ILE:C	2.64	0.40
1:C:462:SER:O	1:C:463:HIS:C	2.64	0.40
1:D:297:ASN:OD1	1:D:297:ASN:C	2.64	0.40
1:D:304:ALA:C	1:D:307:PRO:HD2	2.46	0.40
1:A:333:GLU:O	1:A:380:ARG:NH1	2.55	0.40
1:B:168:GLY:HA3	1:B:169:PRO:HD2	1.83	0.40
1:D:306:LYS:HB2	1:D:307:PRO:HD3	2.02	0.40
1:D:338:GLY:N	3:D:717:HOH:O	2.54	0.40
1:B:460:TYR:HA	1:B:466:ASP:O	2.20	0.40
1:D:374:ASN:HD21	1:D:376:GLU:HB2	1.87	0.40
1:A:107:VAL:O	1:A:110:GLN:HB2	2.22	0.40
1:A:208:LEU:O	1:A:212:GLY:N	2.45	0.40
1:B:29:GLU:O	1:B:33:ASN:ND2	2.54	0.40
1:B:254:LEU:HD13	1:B:311:ASN:ND2	2.36	0.40
1:B:424:ILE:O	1:B:468:ARG:HA	2.21	0.40
1:C:169:PRO:C	1:C:171:GLY:H	2.29	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/516 (100%)	486 (95%)	26 (5%)	2 (0%)	30	34
1	B	514/516 (100%)	490 (95%)	22 (4%)	2 (0%)	30	34
1	C	514/516 (100%)	486 (95%)	24 (5%)	4 (1%)	16	16
1	D	514/516 (100%)	475 (92%)	37 (7%)	2 (0%)	30	34
All	All	2056/2064 (100%)	1937 (94%)	109 (5%)	10 (0%)	24	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	TYR
1	B	428	ASN
1	C	489	ASP
1	D	219	LYS
1	C	170	ALA
1	D	398	TYR
1	C	398	TYR
1	C	454	TYR
1	A	454	TYR
1	B	454	TYR

### 5.3.2 Protein sidechains [i](#)

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	440/440 (100%)	405 (92%)	35 (8%)	11	13
1	B	440/440 (100%)	390 (89%)	50 (11%)	5	5
1	C	440/440 (100%)	403 (92%)	37 (8%)	10	11
1	D	440/440 (100%)	398 (90%)	42 (10%)	8	8
All	All	1760/1760 (100%)	1596 (91%)	164 (9%)	8	9

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	5	LYS
1	A	12	LYS
1	A	19	LEU
1	A	25	VAL
1	A	26	THR
1	A	40	GLN
1	A	46	ILE
1	A	57	LYS
1	A	76	LYS
1	A	94	ASN
1	A	128	GLU
1	A	139	ARG
1	A	163	ILE
1	A	180	THR
1	A	187	PRO
1	A	188	SER
1	A	219	LYS
1	A	226	ILE
1	A	229	LEU
1	A	278	THR
1	A	300	ILE
1	A	324	LYS
1	A	332	LEU
1	A	342	GLU
1	A	374	ASN
1	A	424	ILE
1	A	433	ILE
1	A	452	LYS
1	A	462	SER
1	A	464	SER
1	A	480	GLU
1	A	482	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	507	LEU
1	A	508	LYS
1	B	5	LYS
1	B	19	LEU
1	B	26	THR
1	B	29	GLU
1	B	39	LYS
1	B	40	GLN
1	B	74	SER
1	B	95	VAL
1	B	103	ILE
1	B	138	ILE
1	B	157	LYS
1	B	176	PRO
1	B	187	PRO
1	B	188	SER
1	B	202	LYS
1	B	205	LEU
1	B	209	ASN
1	B	219	LYS
1	B	223	THR
1	B	224	LYS
1	B	225	LEU
1	B	226	ILE
1	B	228	GLU
1	B	322	SER
1	B	332	LEU
1	B	341	PRO
1	B	349	LEU
1	B	371	SER
1	B	374	ASN
1	B	379	LYS
1	B	399	GLN
1	B	410	LYS
1	B	421	MET
1	B	422	GLN
1	B	427	LYS
1	B	432	THR
1	B	453	GLN
1	B	464	SER
1	B	468	ARG
1	B	473	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	481	PHE
1	B	486	LYS
1	B	489	ASP
1	B	493	LYS
1	B	498	ILE
1	B	502	TRP
1	B	507	LEU
1	B	508	LYS
1	B	510	THR
1	B	511	SER
1	C	2	VAL
1	C	16	MET
1	C	19	LEU
1	C	25	VAL
1	C	26	THR
1	C	39	LYS
1	C	40	GLN
1	C	48	VAL
1	C	76	LYS
1	C	101	VAL
1	C	119	LYS
1	C	188	SER
1	C	226	ILE
1	C	228	GLU
1	C	229	LEU
1	C	239	GLN
1	C	251	LYS
1	C	300	ILE
1	C	322	SER
1	C	332	LEU
1	C	337	LYS
1	C	349	LEU
1	C	374	ASN
1	C	375	GLU
1	C	376	GLU
1	C	406	SER
1	C	407	LEU
1	C	432	THR
1	C	462	SER
1	C	468	ARG
1	C	473	LEU
1	C	479	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	480	GLU
1	C	494	SER
1	C	501	SER
1	C	507	LEU
1	C	508	LYS
1	D	2	VAL
1	D	5	LYS
1	D	7	MET
1	D	21	LYS
1	D	25	VAL
1	D	40	GLN
1	D	70	ARG
1	D	98	ASP
1	D	100	ASN
1	D	101	VAL
1	D	103	ILE
1	D	110	GLN
1	D	139	ARG
1	D	157	LYS
1	D	158	ASP
1	D	178	TYR
1	D	181	SER
1	D	187	PRO
1	D	213	SER
1	D	215	ASN
1	D	216	GLU
1	D	219	LYS
1	D	224	LYS
1	D	226	ILE
1	D	229	LEU
1	D	235	SER
1	D	297	ASN
1	D	305	GLU
1	D	315	HIS
1	D	324	LYS
1	D	332	LEU
1	D	344	SER
1	D	349	LEU
1	D	370	LEU
1	D	374	ASN
1	D	376	GLU
1	D	377	GLU

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Mol	Chain	Res	Type
1	D	397	ARG
1	D	480	GLU
1	D	488	LYS
1	D	507	LEU
1	D	515	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	94	ASN
1	A	243	ASN
1	A	311	ASN
1	A	351	GLN
1	A	352	ASN
1	A	365	ASN
1	A	389	ASN
1	A	470	ASN
1	A	503	ASN
1	B	58	ASN
1	B	73	GLN
1	B	77	ASN
1	B	215	ASN
1	B	243	ASN
1	B	315	HIS
1	B	374	ASN
1	B	422	GLN
1	B	453	GLN
1	B	463	HIS
1	B	470	ASN
1	B	499	GLN
1	B	503	ASN
1	C	40	GLN
1	C	351	GLN
1	C	352	ASN
1	C	405	ASN
1	C	453	GLN
1	C	463	HIS
1	C	503	ASN
1	D	40	GLN
1	D	90	GLN
1	D	100	ASN

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Mol	Chain	Res	Type
1	D	209	ASN
1	D	215	ASN
1	D	292	HIS
1	D	311	ASN
1	D	352	ASN
1	D	365	ASN
1	D	374	ASN
1	D	389	ASN
1	D	463	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.