



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:14 PM GMT

PDB ID : 5BCA  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

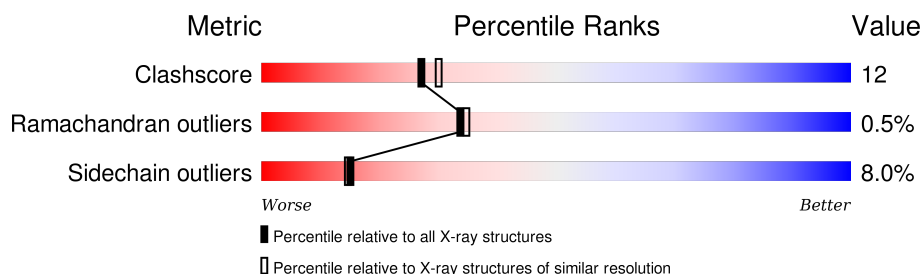
# 1 Overall quality at a glance

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	516	
1	B	516	
1	C	516	
1	D	516	

## 2 Entry composition

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
1	A	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	B	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	C	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	D	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

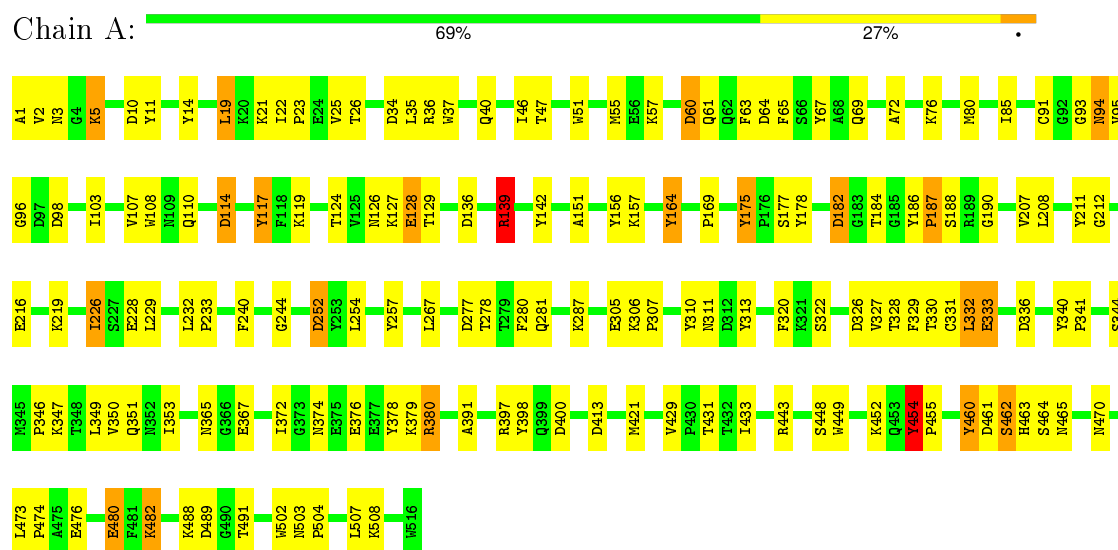
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total	O	0	0
			206	206		
3	B	170	Total	O	0	0
			170	170		
3	C	191	Total	O	0	0
			191	191		
3	D	185	Total	O	0	0
			185	185		

### 3 Residue-property plots

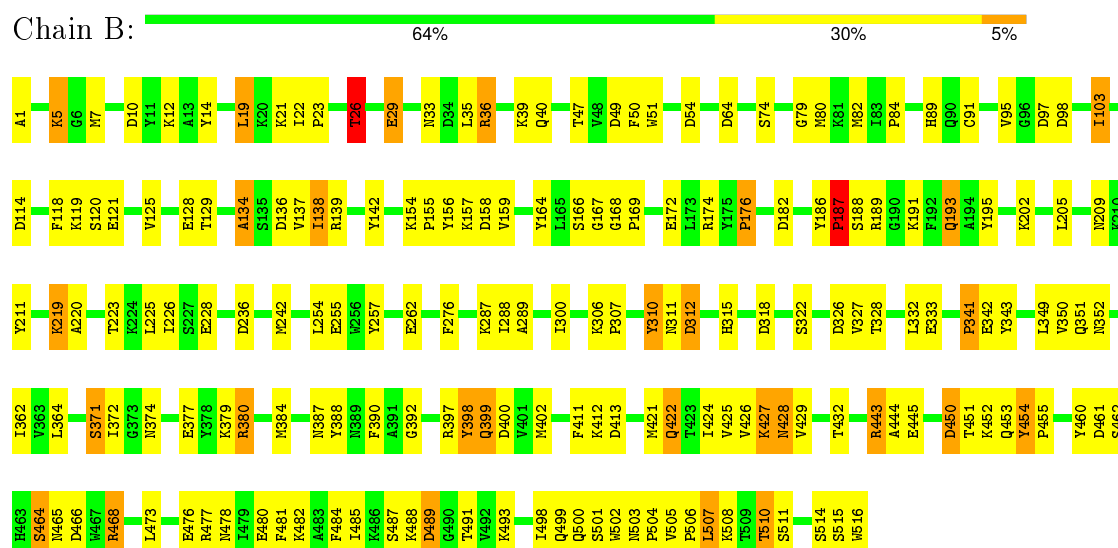
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

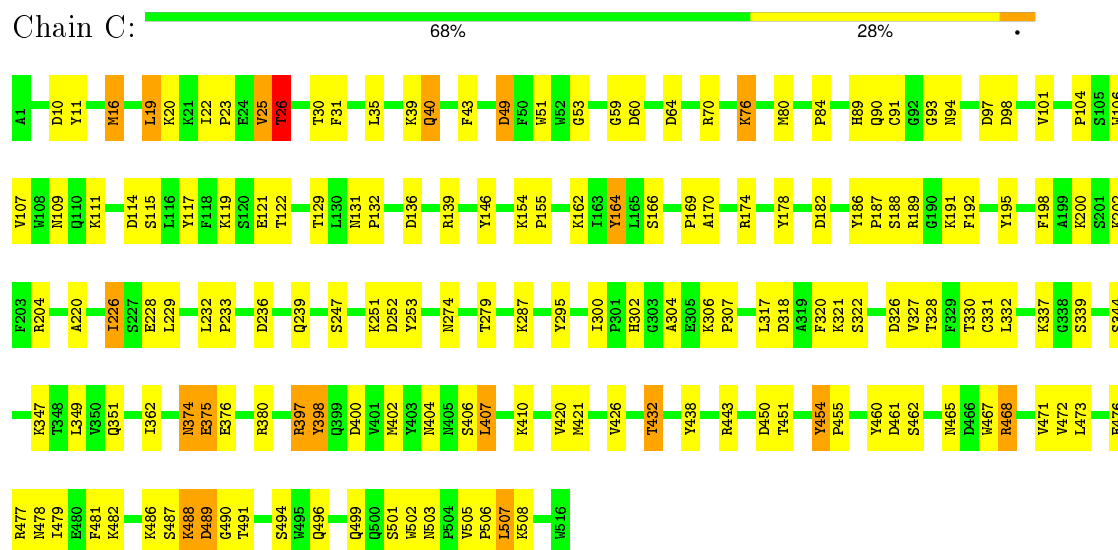
- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)



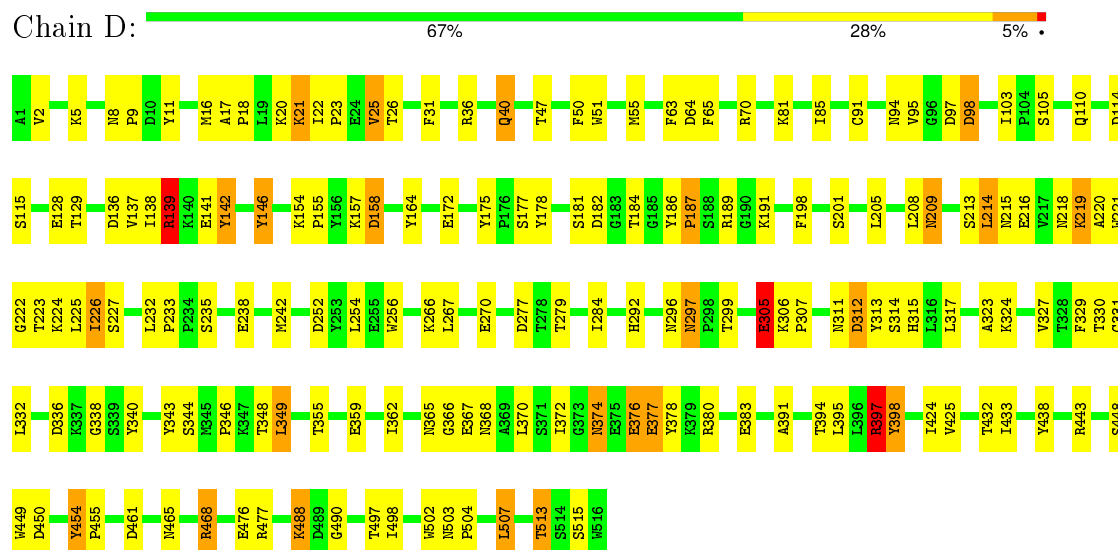
- Molecule 1: PROTEIN (1,4-ALPHA-D-GLUCAN MALTOHYDROLASE.)



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



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



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.90 Å   112.90 Å   146.20 Å 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.	Xtriage
Total number of atoms	17232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.74	0/4234	1.59	46/5751 (0.8%)
1	B	0.71	0/4234	1.61	52/5751 (0.9%)
1	C	0.74	0/4234	1.66	60/5751 (1.0%)
1	D	0.74	0/4234	1.63	54/5751 (0.9%)
All	All	0.73	0/16936	1.62	212/23004 (0.9%)

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

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

There are no bond length outliers.

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	ARG	NE-CZ-NH2	-21.41	109.60	120.30
1	D	380	ARG	CD-NE-CZ	17.65	148.31	123.60
1	C	189	ARG	NE-CZ-NH1	15.27	127.94	120.30
1	C	380	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	B	189	ARG	NE-CZ-NH1	13.59	127.10	120.30
1	D	36	ARG	NE-CZ-NH2	-13.05	113.78	120.30
1	C	174	ARG	NE-CZ-NH2	12.41	126.51	120.30
1	C	450	ASP	CB-CG-OD2	12.25	129.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	TYR	CB-CG-CD1	12.12	128.27	121.00
1	C	139	ARG	NE-CZ-NH1	12.11	126.36	120.30
1	A	443	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	C	380	ARG	CD-NE-CZ	11.88	140.22	123.60
1	D	70	ARG	CD-NE-CZ	11.71	140.00	123.60
1	D	146	TYR	CB-CG-CD2	-11.57	114.06	121.00
1	C	189	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	B	380	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	454	TYR	CB-CG-CD2	-10.58	114.65	121.00
1	C	16	MET	CA-CB-CG	10.55	131.24	113.30
1	A	380	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	C	443	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	B	139	ARG	CD-NE-CZ	10.26	137.96	123.60
1	A	60	ASP	CB-CG-OD2	10.16	127.44	118.30
1	C	70	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	B	443	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	A	413	ASP	CB-CG-OD1	10.03	127.33	118.30
1	B	36	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	C	178	TYR	CB-CG-CD2	9.91	126.94	121.00
1	A	252	ASP	CB-CG-OD1	9.80	127.12	118.30
1	C	178	TYR	CB-CG-CD1	-9.53	115.28	121.00
1	D	70	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	C	477	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	C	236	ASP	CB-CG-OD1	9.30	126.67	118.30
1	C	136	ASP	CB-CG-OD1	9.24	126.62	118.30
1	B	380	ARG	CD-NE-CZ	9.24	136.53	123.60
1	B	174	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	C	443	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	380	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	36	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	B	114	ASP	CB-CG-OD1	8.49	125.94	118.30
1	C	468	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	D	136	ASP	CB-CG-OD1	8.36	125.83	118.30
1	A	454	TYR	CB-CG-CD1	8.31	125.98	121.00
1	A	310	TYR	CB-CG-CD1	8.14	125.89	121.00
1	B	139	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	D	450	ASP	CB-CG-OD2	8.10	125.59	118.30
1	C	49	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	D	397	ARG	CD-NE-CZ	8.05	134.88	123.60
1	B	14	TYR	CB-CG-CD2	-8.02	116.19	121.00
1	B	257	TYR	CB-CG-CD1	-8.02	116.19	121.00
1	C	146	TYR	CB-CG-CD2	-7.95	116.23	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ASP	CB-CG-OD1	7.92	125.42	118.30
1	B	36	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	B	158	ASP	CB-CG-OD1	7.88	125.40	118.30
1	A	34	ASP	CB-CG-OD2	7.86	125.38	118.30
1	D	305	GLU	OE1-CD-OE2	7.81	132.67	123.30
1	C	304	ALA	N-CA-CB	7.74	120.93	110.10
1	D	513	THR	CA-CB-CG2	-7.69	101.64	112.40
1	B	443	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	C	182	ASP	CB-CG-OD1	7.65	125.19	118.30
1	C	178	TYR	CA-CB-CG	7.58	127.81	113.40
1	B	310	TYR	CB-CG-CD1	7.54	125.52	121.00
1	C	70	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	310	TYR	CB-CG-CD2	-7.34	116.60	121.00
1	B	352	ASN	N-CA-CB	-7.32	97.42	110.60
1	B	318	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	97	ASP	CB-CG-OD2	7.29	124.87	118.30
1	D	98	ASP	CB-CG-OD1	7.29	124.86	118.30
1	D	340	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	D	270	GLU	OE1-CD-OE2	-7.25	114.60	123.30
1	C	60	ASP	CB-CG-OD2	7.18	124.77	118.30
1	A	305	GLU	OE1-CD-OE2	-7.12	114.75	123.30
1	D	141	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	B	312	ASP	CB-CG-OD2	-7.11	111.91	118.30
1	C	332	LEU	CA-CB-CG	7.08	131.60	115.30
1	A	114	ASP	CB-CG-OD1	6.94	124.54	118.30
1	C	11	TYR	CB-CG-CD1	6.93	125.16	121.00
1	A	413	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	432	THR	N-CA-CB	6.88	123.37	110.30
1	D	312	ASP	CB-CG-OD1	6.86	124.47	118.30
1	D	158	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	136	ASP	CB-CG-OD1	6.75	124.38	118.30
1	D	114	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	B	257	TYR	CB-CG-CD2	6.73	125.04	121.00
1	C	76	LYS	CA-CB-CG	6.69	128.11	113.40
1	C	189	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	139	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	137	VAL	CA-CB-CG1	6.63	120.85	110.90
1	D	378	TYR	CB-CG-CD1	6.62	124.97	121.00
1	D	142	TYR	CB-CG-CD1	6.61	124.97	121.00
1	B	236	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	146	TYR	CB-CG-CD1	6.57	124.94	121.00
1	C	253	TYR	CB-CG-CD2	-6.52	117.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	ARG	NH1-CZ-NH2	6.51	126.56	119.40
1	D	349	LEU	CA-CB-CG	6.46	130.15	115.30
1	D	189	ARG	CD-NE-CZ	6.45	132.63	123.60
1	C	443	ARG	CG-CD-NE	6.36	125.16	111.80
1	B	450	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C	64	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	98	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	C	98	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	A	117	TYR	CB-CA-C	6.29	122.98	110.40
1	A	310	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	D	114	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	182	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	378	TYR	CB-CG-CD2	-6.19	117.29	121.00
1	B	166	SER	CA-C-O	-6.17	107.15	120.10
1	D	252	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	10	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	236	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	D	332	LEU	CA-CB-CG	6.09	129.30	115.30
1	D	164	TYR	CA-CB-CG	6.08	124.95	113.40
1	A	397	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	D	64	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	480	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	A	36	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	43	PHE	O-C-N	-6.03	113.06	122.70
1	B	413	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	277	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	333	GLU	OE1-CD-OE2	-5.97	116.13	123.30
1	C	139	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
1	D	477	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	139	ARG	CD-NE-CZ	-5.90	115.34	123.60
1	A	175	TYR	CB-CG-CD2	5.89	124.54	121.00
1	A	460	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	D	139	ARG	CB-CG-CD	5.89	126.92	111.60
1	A	349	LEU	CA-CB-CG	5.88	128.82	115.30
1	C	10	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	64	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	367	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	B	128	GLU	CA-CB-CG	5.82	126.20	113.40
1	A	400	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	211	TYR	CB-CG-CD1	5.79	124.47	121.00
1	B	172	GLU	OE1-CD-OE2	-5.79	116.36	123.30
1	A	313	TYR	CB-CG-CD1	5.78	124.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	400	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	262	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	C	295	TYR	CB-CG-CD2	-5.76	117.55	121.00
1	B	14	TYR	CB-CG-CD1	5.75	124.45	121.00
1	B	326	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	D	368	ASN	CA-C-O	-5.72	108.08	120.10
1	D	395	LEU	CA-C-O	-5.69	108.15	120.10
1	A	207	VAL	CA-CB-CG1	5.69	119.43	110.90
1	B	343	TYR	CB-CG-CD2	5.68	124.41	121.00
1	D	214	LEU	CA-CB-CG	5.65	128.29	115.30
1	C	139	ARG	CD-NE-CZ	5.64	131.50	123.60
1	D	454	TYR	N-CA-C	5.60	126.11	111.00
1	A	60	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	C	26	THR	N-CA-CB	5.59	120.91	110.30
1	A	332	LEU	CA-CB-CG	5.58	128.14	115.30
1	C	438	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	C	252	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	189	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	11	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	D	340	TYR	CB-CG-CD1	5.52	124.31	121.00
1	A	142	TYR	CA-CB-CG	5.52	123.89	113.40
1	B	402	MET	CG-SD-CE	5.52	109.03	100.20
1	D	299	THR	CA-CB-CG2	-5.50	104.71	112.40
1	C	174	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	151	ALA	O-C-N	5.49	131.49	122.70
1	D	277	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	139	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	142	TYR	CB-CG-CD1	5.47	124.28	121.00
1	B	10	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	60	ASP	N-CA-CB	-5.45	100.79	110.60
1	A	19	LEU	CA-CB-CG	5.45	127.82	115.30
1	B	444	ALA	N-CA-CB	-5.43	102.50	110.10
1	C	339	SER	N-CA-CB	-5.41	102.39	110.50
1	C	43	PHE	C-N-CA	5.40	135.19	121.70
1	C	344	SER	N-CA-CB	-5.38	102.43	110.50
1	B	19	LEU	O-C-N	-5.36	114.12	122.70
1	D	209	ASN	CA-CB-CG	-5.35	101.62	113.40
1	D	98	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	C	49	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	398	TYR	CB-CG-CD1	5.34	124.20	121.00
1	B	26	THR	N-CA-CB	5.33	120.44	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	GLU	CB-CG-CD	5.32	128.58	114.20
1	C	204	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	B	289	ALA	CB-CA-C	-5.29	102.16	110.10
1	B	187	PRO	N-CA-CB	-5.26	96.81	102.60
1	C	25	VAL	CA-CB-CG2	-5.23	103.05	110.90
1	D	477	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	182	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	A	64	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	323	ALA	CB-CA-C	-5.22	102.27	110.10
1	D	438	TYR	CB-CG-CD2	5.21	124.12	121.00
1	C	117	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	D	468	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	14	TYR	CB-CG-CD1	5.17	124.10	121.00
1	C	195	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	B	174	ARG	CG-CD-NE	5.16	122.63	111.80
1	B	49	ASP	N-CA-CB	5.16	119.88	110.60
1	A	476	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	C	114	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	193	GLN	CA-CB-CG	5.13	124.69	113.40
1	B	255	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	B	398	TYR	N-CA-CB	-5.10	101.42	110.60
1	D	81	LYS	N-CA-CB	5.09	119.77	110.60
1	D	172	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	C	122	THR	CA-CB-CG2	-5.09	105.27	112.40
1	A	336	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	274	ASN	N-CA-CB	5.08	119.75	110.60
1	C	318	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	279	THR	N-CA-CB	-5.06	100.69	110.30
1	C	477	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	256	TRP	CA-CB-CG	5.04	123.28	113.70
1	D	284	ILE	C-N-CA	-5.03	111.73	122.30
1	C	337	LYS	CB-CA-C	5.01	120.42	110.40
1	D	397	ARG	CG-CD-NE	5.01	122.33	111.80
1	D	158	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	A	164	TYR	CB-CG-CD1	5.00	124.00	121.00
1	A	257	TYR	CA-CB-CG	5.00	122.90	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ALA	Mainchain

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Mol	Chain	Res	Type	Group
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 ⓘ

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	83	0
1	B	4119	0	3984	115	0
1	C	4119	0	3984	92	0
1	D	4119	0	3984	100	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	6	0
3	D	185	0	0	9	0
All	All	17232	0	15936	389	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 12.

All (389) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:D:182:ASP:O	1:D:191:LYS:NZ	2.17	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: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:B:312:ASP:CG	1:B:315:HIS:HD2	1.93	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:485:ILE:HG13	1:B:516:TRP:HH2	1.57	0.69
1:B:476:GLU:HG3	1:B:507:LEU:HD22	1.73	0.69
1:B:300:ILE:HG13	1:B:300:ILE:O	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:D:218:ASN:CG	1:D:225:LEU:H	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:THR:HG21	3:D:757:HOH:O	1.93	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: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:B:427:LYS:N	1:B:514:SER:O	2.26	0.66
1:A:460:TYR:OH	1:A:465:ASN:OD1	2.01	0.66
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:D:16:MET:CE	1:D:397:ARG:HH12	2.10	0.65
1:A:461:ASP:O	1:A:465:ASN:N	2.30	0.65
1:A:280:PHE:O	1:A:281:GLN:HB2	1.97	0.64
1:D:305:GLU:OE1	3:D:644:HOH:O	2.15	0.64
1:C:347:LYS:O	1:C:351:GLN:HG3	1.98	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:H	1:C:226:ILE:HD13	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:C:489:ASP:OD2	1:C:491:THR:CG2	2.48	0.62
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:312:ASP:OD2	1:B:315:HIS:CD2	2.55	0.60
1:D:254:LEU:HD13	1:D:311:ASN:ND2	2.16	0.60
1:A:95:VAL:HG12	1:A:96:GLY:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:16:MET:HG3	1:D:397:ARG:NH1	2.17	0.59
1:B:425:VAL:HG22	1:B:468:ARG:HB3	1.84	0.59
1:B:1:ALA:HA	1:B:387:ASN:OD1	2.02	0.59
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:C:26:THR:CG2	1:C:30:THR:HG21	2.33	0.58
1:C:22:ILE:HB	1:C:23:PRO:HD3	1.85	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:B:421:MET:C	1:B:422:GLN:HG2	2.25	0.57
1:C:302:HIS:HA	3:C:613:HOH:O	2.04	0.57
1:C:374:ASN:OD1	1:C:376:GLU:HB2	2.05	0.57
1:B:176:PRO:O	1:B:193:GLN:NE2	2.36	0.57
1:A:344:SER:OG	1:A:346:PRO:HD3	2.04	0.57
1:C:454:TYR:N	1:C:455:PRO:CD	2.67	0.57
1:B:89:HIS:HA	1:B:103:ILE:HD11	1.87	0.57
1:D:218:ASN:HD21	1:D:225:LEU:N	2.03	0.57
1:C:129:THR:HG21	1:C:169:PRO:HD3	1.87	0.57
1:D:184:THR:HG21	1:D:191:LYS:HG3	1.87	0.57
1:B:156:TYR:O	1:B:159:VAL:HG22	2.04	0.57
1:B:450:ASP:OD2	1:B:453:GLN:N	2.32	0.56
1:B:476:GLU:CG	1:B:507:LEU:HD22	2.35	0.56
1:A:330:THR:O	1:A:331:CYS:HB2	2.02	0.56
1:C:460:TYR:CZ	1:C:465:ASN:HA	2.40	0.56
1:C:90:GLN:HE21	1:C:93:GLY:HA3	1.71	0.56
1:C:121:GLU:OE2	1:C:191:LYS:HA	2.05	0.56
1:A:347:LYS:O	1:A:351:GLN:HG3	2.06	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:B:39:LYS:HD3	1:B:80:MET:SD	2.46	0.56
1:D:488:LYS:O	1:D:488:LYS:HD2	2.05	0.56
1:B:461:ASP:CG	1:B:464:SER:HB2	2.27	0.56
1:C:232:LEU:HB3	1:C:233:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:VAL:HG23	1:B:362:ILE:HG21	1.87	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:C:35:LEU:HB3	1:C:80:MET:HG3	1.89	0.55
1:A:254:LEU:HD13	1:A:311:ASN:ND2	2.22	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:D:443:ARG:HA	3:D:694:HOH:O	2.07	0.54
1:A:482:LYS:HE2	3:A:785:HOH:O	2.07	0.54
1:A:216:GLU:CD	1:A:219:LYS:NZ	2.60	0.54
1:B:478:ASN:HB3	1:B:503:ASN:ND2	2.23	0.54
1:C:487:SER:O	1:C:488:LYS:C	2.45	0.54
1:D:424:ILE:O	1:D:468:ARG:HA	2.08	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:C:476:GLU:CG	1:C:507:LEU:CD2	2.87	0.53
1:C:90:GLN:NE2	1:C:93:GLY:HA3	2.22	0.53
1:A:164:TYR:CE1	1:A:287:LYS:HE2	2.43	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:A:502:TRP:C	1:A:503:ASN:HD22	2.12	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:425:VAL:HB	1:D:513:THR:HG23	1.91	0.52
1:D:115:SER:HA	3:D:633:HOH:O	2.09	0.52
1:C:460:TYR:CE1	1:C:465:ASN:HA	2.45	0.52
1:D:488:LYS:C	1:D:488:LYS:HD2	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:O	1:A:157:LYS:C	2.47	0.52
1:C:89:HIS:ND1	1:C:166:SER:OG	2.31	0.52
1:B:176:PRO:C	1:B:193:GLN:HE21	2.12	0.52
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:485:ILE:CD1	1:B:516:TRP:CZ2	2.93	0.52
1:D:115:SER:HB3	1:D:198:PHE:CG	2.45	0.52
1:C:20:LYS:HD2	1:C:25:VAL:CG2	2.40	0.52
1:A:51:TRP:CH2	1:A:91:CYS:SG	3.02	0.51
1:C:115:SER:HB2	1:C:198:PHE:CE2	2.44	0.51
1:D:218:ASN:OD1	1:D:225:LEU:N	2.40	0.51
1:D:17:ALA:HB1	1:D:18:PRO:HD2	1.92	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:CD	2.40	0.51
1:A:114:ASP:HB2	1:A:117:TYR:CZ	2.45	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:497:THR:HG22	1:D:498:ILE:HG13	1.93	0.51
1:C:330:THR:O	1:C:331:CYS:HB2	2.11	0.51
1:D:238:GLU:O	1:D:242:MET:HG3	2.11	0.51
1:A:103:ILE:HD11	1:A:108:TRP:CZ2	2.46	0.51
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:A:329:PHE:CE1	1:A:353:ILE:HG13	2.46	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:C:226:ILE:HD13	1:C:226:ILE:N	2.26	0.50
1:B:89:HIS:CA	1:B:103:ILE:HD11	2.42	0.50
1:B:333:GLU:O	1:B:380:ARG:HD2	2.12	0.49
1:C:479:ILE:CD1	1:C:481:PHE:CD1	2.95	0.49
1:A:372:ILE:HG21	1:A:378:TYR:CE1	2.48	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:462:SER:O	1:A:463:HIS:C	2.51	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:D:488:LYS:C	1:D:490:GLY:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HG2	1:A:328:THR:HB	1.93	0.48
1:A:69:GLN:HG2	1:A:156:TYR:HE2	1.78	0.48
1:C:19:LEU:HD13	1:C:397:ARG:CZ	2.44	0.48
1:B:451:THR:HG22	1:B:484:PHE:CE1	2.48	0.48
1:D:330:THR:OG1	1:D:331:CYS:N	2.44	0.48
1:D:292:HIS:HB2	1:D:346:PRO:HD3	1.96	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: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:488:LYS:O	1:B:489:ASP:C	2.52	0.47
1:C:104:PRO:O	1:C:107:VAL:HG23	2.15	0.47
1:B:47:THR:HG21	3:B:680:HOH:O	2.15	0.47
1:B:427:LYS:HB3	1:B:427:LYS:HE3	1.64	0.47
1:C:109:ASN:ND2	3:D:789:HOH:O	2.47	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:376:GLU:O	1:A:379:LYS:HB2	2.15	0.47
1:C:26:THR:CG2	1:C:30:THR:CG2	2.90	0.47
1:B:306:LYS:N	1:B:307:PRO:CD	2.78	0.47
1:A:240:PHE:HA	1:A:244:GLY:HA3	1.96	0.47
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:266:LYS:NZ	3:D:762:HOH:O	2.34	0.46
1:D:94:ASN:O	1:D:95:VAL:C	2.53	0.46
1:D:138:ILE:HD12	1:D:142:TYR:CZ	2.51	0.46
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:B:451:THR:HG22	1:B:484:PHE:CZ	2.50	0.46
1:B:351:GLN:HG2	1:B:388:TYR:CZ	2.50	0.46
1:B:120:SER:HB2	1:B:182:ASP:OD2	2.15	0.46
1:D:461:ASP:O	1:D:465:ASN:N	2.45	0.46
1:B:453:GLN:HB3	1:B:453:GLN:HE21	1.43	0.46
1:A:448:SER:O	1:A:449:TRP:HB2	2.15	0.46
1:D:115:SER:CB	1:D:198:PHE:CD2	2.98	0.46
1:C:505:VAL:HG13	1:C:506:PRO:HD2	1.97	0.46
1:D:476:GLU:HG3	1:D:507:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:16:MET:HE2	1:D:397:ARG:HH12	1.79	0.46
1:D:139:ARG:HD3	1:D:139:ARG:HH11	1.56	0.46
1:B:443:ARG:HB3	1:B:445:GLU:OE1	2.15	0.46
1:A:178:TYR:HA	1:A:184:THR:OG1	2.16	0.46
1:D:327:VAL:CG2	1:D:362:ILE:HG21	2.45	0.46
1:B:477:ARG:O	1:B:505:VAL:HG23	2.15	0.46
1:C:478:ASN:OD1	1:C:503:ASN:HA	2.15	0.46
1:D:63:PHE:CB	1:D:65:PHE:CE2	2.93	0.45
1:C:327:VAL:HG23	1:C:362:ILE:HG21	1.97	0.45
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: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:A:216:GLU:CD	1:A:219:LYS:HZ1	2.19	0.45
1:D:219:LYS:HB3	1:D:220:ALA:H	1.65	0.45
1:B:426:VAL:HA	1:B:514:SER:O	2.15	0.45
1:C:232:LEU:HB3	1:C:233:PRO:CD	2.46	0.45
1:A:175:TYR:O	1:A:177:SER:N	2.45	0.45
1:B:505:VAL:HA	1:B:506:PRO:HD3	1.81	0.45
1:D:503:ASN:HA	1:D:504:PRO:HA	1.65	0.45
1:D:184:THR:CG2	1:D:191:LYS:HG3	2.46	0.45
1:C:115:SER:CB	1:C:198:PHE:CD2	2.99	0.45
1:D:201:SER:O	1:D:205:LEU:HD23	2.16	0.45
1:A:51:TRP:CH2	1:A:91:CYS:CB	3.00	0.44
1:A:47:THR:HG22	1:A:85:ILE:HD11	1.99	0.44
1:D:488:LYS:C	1:D:490:GLY:N	2.70	0.44
1:B:503:ASN:HA	1:B:504:PRO:HA	1.72	0.44
1:A:93:GLY:C	1:A:94:ASN:ND2	2.71	0.44
1:C:375:GLU:CB	1:C:410:LYS:HD2	2.48	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:40:GLN:HE21	1:C:40:GLN:HB2	1.69	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:312:ASP:O	1:D:313:TYR:C	2.52	0.44
1:D:128:GLU:O	1:D:129:THR:HB	2.17	0.44
1:B:453:GLN:C	1:B:455:PRO:HD2	2.37	0.44
1:A:346:PRO:O	1:A:350:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD22	1:B:350:VAL:HG11	1.99	0.44
1:A:228:GLU:H	1:A:228:GLU:CD	2.21	0.44
1:B:242:MET:CG	1:B:300:ILE:HG22	2.47	0.44
1:B:182:ASP:O	1:B:191:LYS:NZ	2.33	0.44
1:D:16:MET:HE3	1:D:397:ARG:HH12	1.82	0.44
1:B:453:GLN:HG2	1:B:453:GLN:H	1.75	0.43
1:D:115:SER:CB	1:D:198:PHE:CG	3.01	0.43
1:B:120:SER:CB	1:B:182:ASP:OD2	2.67	0.43
1:D:8:ASN:HA	1:D:9:PRO:HD2	1.83	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: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:21:LYS:HG2	1:A:67:TYR:CZ	2.53	0.43
1:D:448:SER:O	1:D:449:TRP:HB2	2.19	0.43
1:C:451:THR:O	1:C:486:LYS:CE	2.67	0.43
1:A:340:TYR:CE1	1:A:341:PRO:HB3	2.53	0.43
1:B:489:ASP:CG	1:B:491:THR:OG1	2.53	0.43
1:A:55:MET:O	1:A:63:PHE:HA	2.19	0.43
1:A:2:VAL:O	1:A:3:ASN:HB2	2.19	0.43
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:B:134:ALA:O	1:B:138:ILE:HG13	2.18	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: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: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:D:372:ILE:HG23	1:D:377:GLU:HG3	2.01	0.43
1:B:154:LYS:HB3	1:B:155:PRO:HD3	2.01	0.42
1:D:226:ILE:CD1	1:D:227:SER:H	2.13	0.42
1:B:121:GLU:HG2	1:B:195:TYR:CE1	2.54	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:487:SER:OG	1:B:489:ASP:CG	2.57	0.42
1:C:121:GLU:OE2	1:C:192:PHE:N	2.50	0.42
1:B:186:TYR:HA	1:B:187:PRO:HA	1.64	0.42
1:B:461:ASP:OD2	1:B:464:SER:HB2	2.19	0.42
1:C:375:GLU:HB2	1:C:410:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLY:HA3	1:C:101:VAL:HG12	2.00	0.42
1:D:219:LYS:O	1:D:222:GLY:N	2.43	0.42
1:B:50:PHE:HZ	1:B:82:MET:HE1	1.85	0.42
1:C:321:LYS:HD2	1:C:321:LYS:HA	1.81	0.42
1:C:505:VAL:HA	1:C:506:PRO:HD3	1.80	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:D:432:THR:O	1:D:433:ILE:C	2.58	0.42
1:B:23:PRO:HA	1:B:26:THR:O	2.20	0.42
1:B:288:ILE:HG23	1:B:310:TYR:CZ	2.55	0.42
1:A:11:TYR:HA	1:A:391:ALA:O	2.20	0.42
1:B:219:LYS:HG3	1:B:220:ALA:N	2.34	0.42
1:D:226:ILE:HG13	1:D:226:ILE:H	1.64	0.41
1:C:317:LEU:O	1:C:320:PHE:HB2	2.20	0.41
1:C:421:MET:HE2	1:C:472:VAL:HG22	2.02	0.41
1:D:443:ARG:HH11	1:D:443:ARG:HD2	1.75	0.41
1:B:411:PHE:C	1:B:411:PHE:CD1	2.94	0.41
1:A:37:TRP:O	1:A:40:GLN:HB2	2.20	0.41
1:A:178:TYR:HA	1:A:184:THR:HG1	1.86	0.41
1:D:154:LYS:N	1:D:155:PRO:CD	2.83	0.41
1:A:429:VAL:HG12	1:A:431:THR:HG23	2.02	0.41
1:D:22:ILE:HD12	1:D:31:PHE:CD1	2.56	0.41
1:A:94:ASN:N	1:A:94:ASN:ND2	2.66	0.41
1:A:340:TYR:HA	1:A:341:PRO:HA	1.82	0.41
1:A:1:ALA:HB3	1:A:5:LYS:O	2.21	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:218:ASN:ND2	1:D:225:LEU:N	2.60	0.41
1:D:40:GLN:HE21	1:D:40:GLN:HB2	1.74	0.41
1:B:21:LYS:NZ	1:B:54:ASP:CG	2.72	0.41
1:B:487:SER:OG	1:B:489:ASP:OD1	2.38	0.41
1:D:21:LYS:C	1:D:23:PRO:HD2	2.42	0.41
1:B:460:TYR:CD1	1:B:466:ASP:O	2.73	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:B:7:MET:HB2	1:B:7:MET:HE3	1.93	0.41
1:A:226:ILE:HG22	3:A:784:HOH:O	2.20	0.41
1:D:297:ASN:HB2	1:D:343:TYR:CD2	2.56	0.41
1:C:109:ASN:OD1	1:D:40:GLN:NE2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:HA	1:A:187:PRO:HA	1.80	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:A:333:GLU:O	1:A:380:ARG:NH1	2.55	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:B:29:GLU:O	1:B:33:ASN:ND2	2.54	0.40
1:B:424:ILE:O	1:B:468:ARG:HA	2.21	0.40
1:A:107:VAL:O	1:A:110:GLN:HB2	2.22	0.40
1:B:350:VAL:HG12	1:B:384:MET:HE3	2.03	0.40
1:B:254:LEU:HD13	1:B:311:ASN:ND2	2.36	0.40
1:A:208:LEU:O	1:A:212:GLY:N	2.45	0.40
1:D:208:LEU:O	1:D:209:ASN:C	2.58	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%)	39	42
1	B	514/516 (100%)	490 (95%)	22 (4%)	2 (0%)	39	42
1	C	514/516 (100%)	486 (95%)	24 (5%)	4 (1%)	24	22
1	D	514/516 (100%)	475 (92%)	37 (7%)	2 (0%)	39	42
All	All	2056/2064 (100%)	1937 (94%)	109 (5%)	10 (0%)	34	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	TYR

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Mol	Chain	Res	Type
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 ⓘ

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%)	412 (94%)	28 (6%)	22	24
1	B	440/440 (100%)	395 (90%)	45 (10%)	9	8
1	C	440/440 (100%)	409 (93%)	31 (7%)	19	19
1	D	440/440 (100%)	404 (92%)	36 (8%)	14	13
All	All	1760/1760 (100%)	1620 (92%)	140 (8%)	15	15

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	19	LEU
1	A	25	VAL
1	A	26	THR
1	A	46	ILE
1	A	57	LYS
1	A	76	LYS
1	A	94	ASN
1	A	98	ASP
1	A	128	GLU
1	A	139	ARG
1	A	187	PRO

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Mol	Chain	Res	Type
1	A	188	SER
1	A	226	ILE
1	A	229	LEU
1	A	278	THR
1	A	322	SER
1	A	332	LEU
1	A	374	ASN
1	A	433	ILE
1	A	452	LYS
1	A	462	SER
1	A	464	SER
1	A	480	GLU
1	A	482	LYS
1	A	488	LYS
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	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	225	LEU
1	B	226	ILE
1	B	228	GLU
1	B	322	SER
1	B	341	PRO
1	B	349	LEU
1	B	371	SER
1	B	374	ASN

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Mol	Chain	Res	Type
1	B	379	LYS
1	B	397	ARG
1	B	399	GLN
1	B	422	GLN
1	B	427	LYS
1	B	432	THR
1	B	452	LYS
1	B	464	SER
1	B	468	ARG
1	B	473	LEU
1	B	481	PHE
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	16	MET
1	C	19	LEU
1	C	26	THR
1	C	39	LYS
1	C	40	GLN
1	C	76	LYS
1	C	119	LYS
1	C	164	TYR
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	349	LEU
1	C	374	ASN
1	C	375	GLU
1	C	397	ARG
1	C	406	SER
1	C	407	LEU
1	C	432	THR

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Mol	Chain	Res	Type
1	C	462	SER
1	C	468	ARG
1	C	488	LYS
1	C	494	SER
1	C	501	SER
1	C	502	TRP
1	C	507	LEU
1	C	508	LYS
1	D	2	VAL
1	D	5	LYS
1	D	21	LYS
1	D	25	VAL
1	D	40	GLN
1	D	98	ASP
1	D	103	ILE
1	D	105	SER
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	224	LYS
1	D	226	ILE
1	D	235	SER
1	D	297	ASN
1	D	305	GLU
1	D	315	HIS
1	D	324	LYS
1	D	344	SER
1	D	349	LEU
1	D	370	LEU
1	D	374	ASN
1	D	376	GLU
1	D	377	GLU
1	D	397	ARG
1	D	488	LYS
1	D	502	TRP

*Continued on next page...*

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Mol	Chain	Res	Type
1	D	507	LEU
1	D	515	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	94	ASN
1	A	110	GLN
1	A	215	ASN
1	A	351	GLN
1	A	365	ASN
1	A	503	ASN
1	B	58	ASN
1	B	215	ASN
1	B	243	ASN
1	B	311	ASN
1	B	315	HIS
1	B	422	GLN
1	B	453	GLN
1	B	463	HIS
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	58	ASN
1	D	215	ASN
1	D	292	HIS
1	D	311	ASN
1	D	351	GLN
1	D	352	ASN
1	D	374	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.