



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:07 PM GMT

PDB ID : 1CLX  
Title : CATALYTIC CORE OF XYLANASE A  
Authors : Harris, G.W.; Jenkins, J.A.; Connerton, I.; Pickersgill, R.W.  
Deposited on : 1995-08-31  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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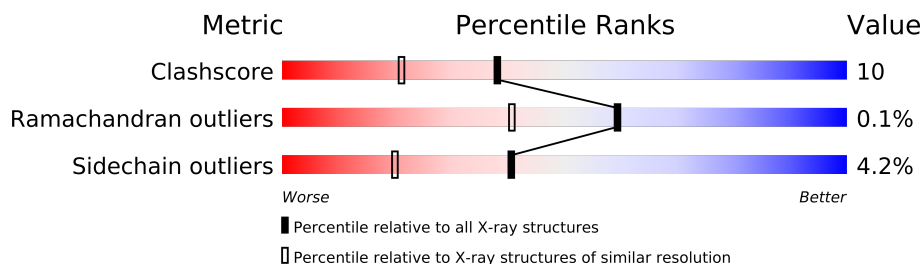
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11908 atoms, of which 0 are hydrogen and 0 are deuterium.

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 XYLANASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			
1	B	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			
1	C	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			
1	D	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			

- 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	272	Total	O	0	0
			272	272		
3	B	278	Total	O	0	0
			278	278		
3	C	276	Total	O	0	0
			276	276		
3	D	282	Total	O	0	0
			282	282		

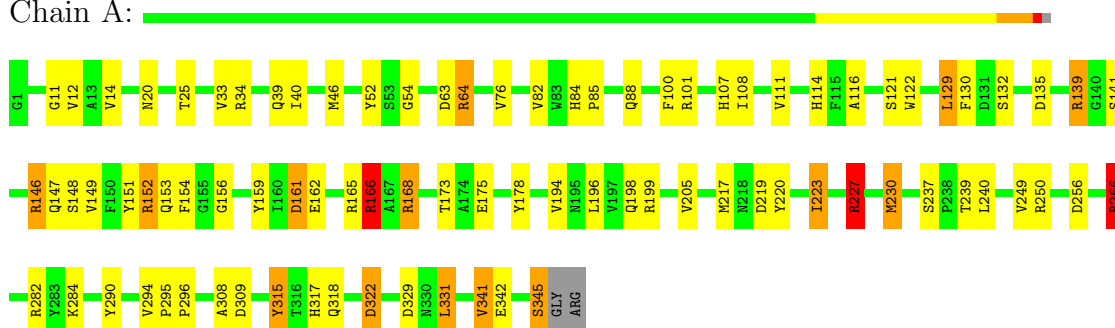
### 3 Residue-property plots

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.

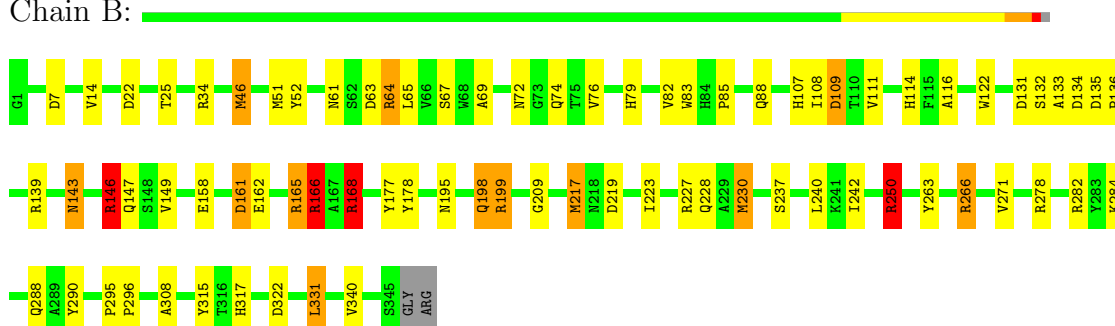
#### • Molecule 1: XYLANASE A

Chain A:



#### • Molecule 1: XYLANASE A

Chain B:



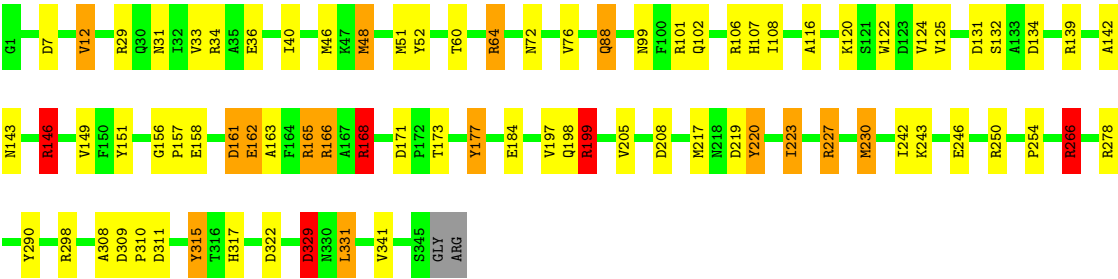
#### • Molecule 1: XYLANASE A

Chain C:



#### • Molecule 1: XYLANASE A

Chain D: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.11Å 97.32Å 151.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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	0.90	0/2766	1.54	39/3769 (1.0%)
1	B	0.92	0/2766	1.48	33/3769 (0.9%)
1	C	0.92	1/2766 (0.0%)	1.49	39/3769 (1.0%)
1	D	0.91	0/2766	1.52	46/3769 (1.2%)
All	All	0.91	1/11064 (0.0%)	1.51	157/15076 (1.0%)

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	8
1	B	0	7
1	C	0	12
1	D	0	8
All	All	0	35

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	313	TRP	NE1-CE2	-5.07	1.30	1.37

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	B	146	ARG	NE-CZ-NH1	15.60	128.10	120.30
1	D	266	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	D	266	ARG	CD-NE-CZ	14.28	143.59	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	ARG	NE-CZ-NH2	-14.24	113.18	120.30
1	A	266	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	D	146	ARG	NE-CZ-NH1	12.50	126.55	120.30
1	C	146	ARG	NE-CZ-NH1	11.23	125.92	120.30
1	C	266	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	C	266	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	146	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	A	168	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	A	34	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	B	266	ARG	NE-CZ-NH2	-9.31	115.65	120.30
1	B	146	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	116	ALA	C-N-CA	-9.13	103.12	122.30
1	A	266	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	C	106	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	D	29	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	B	178	TYR	CB-CG-CD1	-8.93	115.64	121.00
1	A	315	TYR	CB-CG-CD2	-8.85	115.69	121.00
1	B	315	TYR	CB-CG-CD2	-8.65	115.81	121.00
1	A	116	ALA	N-CA-CB	8.32	121.75	110.10
1	B	135	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	101	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	C	299	ARG	NE-CZ-NH1	-7.97	116.32	120.30
1	C	146	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	178	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	D	139	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	C	165	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	282	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	C	165	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	82	VAL	CA-CB-CG2	7.40	122.00	110.90
1	B	116	ALA	C-N-CA	-7.38	106.80	122.30
1	D	12	VAL	CA-CB-CG2	7.34	121.91	110.90
1	D	146	ARG	CD-NE-CZ	7.24	133.73	123.60
1	C	149	VAL	CA-CB-CG1	7.24	121.76	110.90
1	B	199	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	46	MET	CG-SD-CE	7.01	111.41	100.20
1	A	230	MET	CG-SD-CE	6.96	111.34	100.20
1	B	168	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	178	TYR	CB-CG-CD1	-6.91	116.86	121.00
1	D	46	MET	CG-SD-CE	6.90	111.25	100.20
1	C	266	ARG	CD-NE-CZ	6.86	133.20	123.60
1	C	51	MET	CG-SD-CE	6.85	111.16	100.20
1	C	205	VAL	CA-CB-CG2	6.80	121.10	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	C	217	MET	CG-SD-CE	6.55	110.69	100.20
1	D	146	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	165	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	C	123	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	131	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	271	VAL	CA-CB-CG2	6.49	120.63	110.90
1	A	282	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	146	ARG	CD-NE-CZ	6.46	132.64	123.60
1	C	230	MET	CG-SD-CE	6.45	110.52	100.20
1	D	168	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	D	36	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	D	197	VAL	CA-CB-CG2	6.44	120.56	110.90
1	B	266	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	B	76	VAL	CA-CB-CG2	6.40	120.50	110.90
1	D	168	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	230	MET	CG-SD-CE	6.29	110.27	100.20
1	C	119	VAL	CA-CB-CG2	6.28	120.31	110.90
1	D	29	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	194	VAL	CA-CB-CG2	6.25	120.28	110.90
1	C	304	VAL	CA-CB-CG2	6.25	120.28	110.90
1	B	263	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	D	51	MET	CG-SD-CE	6.22	110.15	100.20
1	C	194	VAL	CA-CB-CG2	6.21	120.22	110.90
1	A	227	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	B	250	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	116	ALA	C-N-CA	-6.16	109.36	122.30
1	D	278	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	311	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	116	ALA	N-CA-CB	6.13	118.68	110.10
1	D	298	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	101	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	D	116	ALA	C-N-CA	-6.07	109.56	122.30
1	A	205	VAL	CA-CB-CG2	6.06	119.98	110.90
1	B	14	VAL	CA-CB-CG2	6.04	119.97	110.90
1	D	217	MET	CG-SD-CE	6.03	109.85	100.20
1	D	177	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	A	12	VAL	CA-CB-CG2	6.02	119.93	110.90
1	A	217	MET	CG-SD-CE	6.01	109.81	100.20
1	D	246	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	C	66	VAL	CA-CB-CG2	5.98	119.87	110.90
1	C	145	TYR	CB-CG-CD1	-5.92	117.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	256	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	46	MET	CG-SD-CE	5.88	109.60	100.20
1	B	227	ARG	CD-NE-CZ	-5.85	115.41	123.60
1	A	149	VAL	CA-CB-CG1	5.79	119.58	110.90
1	D	116	ALA	CA-C-N	5.78	127.76	116.20
1	B	109	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	139	ARG	CD-NE-CZ	-5.74	115.56	123.60
1	B	149	VAL	CA-CB-CG1	5.73	119.49	110.90
1	C	299	ARG	CD-NE-CZ	-5.70	115.62	123.60
1	D	76	VAL	CA-CB-CG2	5.70	119.44	110.90
1	A	309	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	46	MET	CG-SD-CE	5.68	109.29	100.20
1	C	331	LEU	CB-CG-CD1	5.67	120.64	111.00
1	B	278	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	116	ALA	O-C-N	-5.66	113.58	123.20
1	D	230	MET	CG-SD-CE	5.65	109.24	100.20
1	D	165	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	D	329	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	22	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	82	VAL	CA-CB-CG2	5.63	119.34	110.90
1	A	111	VAL	CA-CB-CG1	5.54	119.22	110.90
1	A	341	VAL	CA-CB-CG2	5.53	119.20	110.90
1	C	305	TRP	CH2-CZ2-CE2	5.53	122.92	117.40
1	D	177	TYR	CG-CD2-CE2	-5.53	116.88	121.30
1	A	249	VAL	CA-CB-CG2	5.52	119.18	110.90
1	D	171	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	129	LEU	CB-CG-CD2	5.48	120.31	111.00
1	C	220	TYR	CG-CD2-CE2	-5.48	116.92	121.30
1	C	82	VAL	CA-CB-CG2	5.46	119.09	110.90
1	D	315	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	178	TYR	CG-CD1-CE1	-5.44	116.95	121.30
1	C	256	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	168	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	249	VAL	CA-CB-CG2	5.40	119.01	110.90
1	A	34	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	D	106	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	341	VAL	CA-CB-CG2	5.38	118.97	110.90
1	C	48	MET	CG-SD-CE	5.36	108.77	100.20
1	C	220	TYR	CA-CB-CG	-5.33	103.27	113.40
1	C	127	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	B	217	MET	CG-SD-CE	5.29	108.67	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	VAL	CA-CB-CG1	5.29	118.84	110.90
1	D	149	VAL	CA-CB-CG1	5.28	118.83	110.90
1	D	184	GLU	OE1-CD-OE2	-5.28	116.96	123.30
1	A	14	VAL	CA-CB-CG2	5.26	118.80	110.90
1	D	48	MET	CG-SD-CE	5.26	108.62	100.20
1	D	217	MET	CA-CB-CG	-5.25	104.37	113.30
1	B	79	HIS	C-N-CA	5.24	134.80	121.70
1	A	266	ARG	CD-NE-CZ	5.23	130.92	123.60
1	D	116	ALA	CB-CA-C	5.22	117.93	110.10
1	A	135	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	116	ALA	N-CA-CB	5.20	117.39	110.10
1	C	271	VAL	CA-CB-CG2	5.20	118.70	110.90
1	B	340	VAL	CA-CB-CG2	5.20	118.69	110.90
1	D	199	ARG	CD-NE-CZ	-5.15	116.39	123.60
1	D	220	TYR	CA-CB-CG	-5.13	103.65	113.40
1	A	220	TYR	CG-CD2-CE2	-5.12	117.20	121.30
1	B	51	MET	CG-SD-CE	5.09	108.35	100.20
1	A	20	ASN	O-C-N	5.08	130.83	122.70
1	D	223	ILE	CA-CB-CG2	5.08	121.06	110.90
1	B	178	TYR	CD1-CG-CD2	5.06	123.47	117.90
1	A	76	VAL	CA-CB-CG2	5.05	118.48	110.90
1	B	166	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	125	VAL	CA-CB-CG2	5.05	118.48	110.90
1	D	124	VAL	CA-CB-CG2	5.04	118.46	110.90
1	C	341	VAL	CA-CB-CG2	5.02	118.43	110.90
1	C	112	ALA	N-CA-CB	5.02	117.13	110.10
1	D	205	VAL	CA-CB-CG2	5.01	118.42	110.90

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	TRP	Peptide
1	A	146	ARG	Sidechain
1	A	152	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	227	ARG	Sidechain
1	A	250	ARG	Sidechain
1	A	266	ARG	Sidechain
1	A	64	ARG	Sidechain
1	B	122	TRP	Peptide
1	B	146	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	166	ARG	Sidechain
1	B	168	ARG	Sidechain
1	B	250	ARG	Sidechain
1	B	282	ARG	Sidechain
1	B	64	ARG	Sidechain
1	C	106	ARG	Sidechain
1	C	122	TRP	Peptide
1	C	152	ARG	Sidechain
1	C	165	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	168	ARG	Sidechain
1	C	199	ARG	Sidechain
1	C	278	ARG	Sidechain
1	C	298	ARG	Sidechain
1	C	52	TYR	Peptide
1	C	64	ARG	Sidechain
1	C	74	GLN	Peptide
1	D	101	ARG	Sidechain
1	D	122	TRP	Peptide
1	D	165	ARG	Sidechain
1	D	168	ARG	Sidechain
1	D	199	ARG	Sidechain
1	D	227	ARG	Sidechain
1	D	250	ARG	Sidechain
1	D	64	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2699	0	2560	52	6
1	B	2699	0	2560	46	2
1	C	2699	0	2560	61	1
1	D	2699	0	2560	50	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	272	0	0	13	9
3	B	278	0	0	10	3
3	C	276	0	0	16	3
3	D	282	0	0	17	10
All	All	11908	0	10240	209	20

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (209) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:143:ASN:CG	3:C:1031:HOH:O	1.77	1.20
1:C:198:GLN:CG	3:C:1123:HOH:O	1.99	1.09
1:C:198:GLN:HG3	3:C:1123:HOH:O	1.53	1.08
1:C:161:ASP:OD1	1:C:199:ARG:NH2	1.92	1.00
1:C:61:ASN:HD22	1:C:64:ARG:HH12	1.08	0.99
1:B:198:GLN:CG	3:B:846:HOH:O	2.10	0.98
1:D:230:MET:HE2	1:D:242:ILE:HG21	1.45	0.97
1:C:61:ASN:ND2	1:C:64:ARG:HH12	1.63	0.95
1:B:198:GLN:HG2	3:B:846:HOH:O	1.68	0.92
1:A:198:GLN:HG2	3:A:569:HOH:O	1.70	0.92
1:C:61:ASN:HD22	1:C:64:ARG:NH1	1.69	0.91
1:B:7:ASP:OD1	3:B:711:HOH:O	1.88	0.90
1:B:230:MET:HE2	1:B:242:ILE:HG21	1.55	0.89
1:B:317:HIS:HD2	3:B:655:HOH:O	1.56	0.88
1:C:40:ILE:HG22	3:C:1102:HOH:O	1.76	0.85
1:D:308:ALA:HB2	1:D:331:LEU:CD1	2.07	0.84
1:B:198:GLN:HG3	3:B:846:HOH:O	1.74	0.84
1:D:52:TYR:OH	1:D:107:HIS:HD2	1.61	0.82
1:D:161:ASP:OD1	1:D:199:ARG:NH2	2.13	0.82
1:D:120:LYS:NZ	3:D:1367:HOH:O	2.13	0.81
1:B:52:TYR:OH	1:B:107:HIS:HD2	1.65	0.80
1:A:317:HIS:HD2	3:A:378:HOH:O	1.65	0.79
1:D:198:GLN:CG	3:D:1400:HOH:O	2.31	0.79
1:D:219:ASP:HB2	3:D:1225:HOH:O	1.83	0.78
1:A:219:ASP:HB2	3:A:394:HOH:O	1.83	0.78
1:B:61:ASN:HD22	1:B:64:ARG:HH12	1.31	0.77
1:D:40:ILE:HG22	3:D:1379:HOH:O	1.83	0.77
1:D:198:GLN:HG2	3:D:1400:HOH:O	1.83	0.77
1:C:109:ASP:OD1	1:C:166:ARG:HG2	1.85	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:ASP:O	1:B:146:ARG:NH2	2.19	0.76
1:C:258:ASN:OD1	1:C:260:SER:HB2	1.85	0.74
1:C:198:GLN:HG2	3:C:1123:HOH:O	1.70	0.74
1:D:134:ASP:O	1:D:146:ARG:NH2	2.19	0.74
1:A:230:MET:HE1	1:A:290:TYR:HD1	1.53	0.73
1:B:230:MET:CE	1:B:242:ILE:HG21	2.19	0.73
1:B:219:ASP:HB2	3:B:671:HOH:O	1.89	0.73
1:A:40:ILE:HG22	3:A:548:HOH:O	1.87	0.73
1:D:33:VAL:HG13	3:D:1379:HOH:O	1.89	0.72
1:C:52:TYR:OH	1:C:107:HIS:HD2	1.71	0.72
1:A:63:ASP:OD1	1:A:114:HIS:HE1	1.73	0.72
1:C:142:ALA:CB	3:C:1151:HOH:O	2.36	0.72
1:C:266:ARG:HD2	3:C:1245:HOH:O	1.88	0.71
1:B:63:ASP:OD1	1:B:114:HIS:HE1	1.73	0.71
1:A:100:PHE:CB	1:A:153:GLN:HE21	2.03	0.71
1:A:227:ARG:HG3	1:A:227:ARG:NH1	2.06	0.71
1:A:230:MET:CE	1:A:290:TYR:HD1	2.02	0.71
1:C:230:MET:HE2	1:C:242:ILE:HG21	1.73	0.71
1:C:134:ASP:CG	1:C:146:ARG:HH22	1.95	0.68
1:B:168:ARG:HG3	1:B:168:ARG:O	1.94	0.68
1:C:142:ALA:HB2	3:C:1151:HOH:O	1.92	0.68
1:C:134:ASP:OD2	1:C:146:ARG:NH2	2.24	0.68
1:C:63:ASP:OD1	1:C:114:HIS:HE1	1.78	0.67
1:D:230:MET:CE	1:D:242:ILE:HG21	2.23	0.67
1:A:296:PRO:O	3:A:401:HOH:O	2.13	0.66
1:A:161:ASP:O	1:A:165:ARG:HG3	1.96	0.66
1:D:162:GLU:O	1:D:166:ARG:HB2	1.96	0.66
1:C:40:ILE:CG2	3:C:1102:HOH:O	2.39	0.65
1:A:40:ILE:CG2	3:A:548:HOH:O	2.44	0.64
1:B:61:ASN:ND2	1:B:64:ARG:HH12	1.96	0.64
1:A:230:MET:HE1	1:A:290:TYR:CD1	2.32	0.63
1:C:61:ASN:ND2	1:C:64:ARG:NH1	2.36	0.63
1:A:341:VAL:O	1:A:345:SER:OG	2.10	0.63
1:A:317:HIS:HE1	1:A:322:ASP:OD2	1.82	0.63
1:B:109:ASP:OD1	1:B:166:ARG:HG2	1.98	0.62
1:D:52:TYR:OH	1:D:107:HIS:CD2	2.50	0.62
1:D:60:THR:HG21	3:D:1281:HOH:O	2.00	0.62
1:A:129:LEU:HD21	1:A:196:LEU:HD12	1.81	0.62
1:C:309:ASP:N	1:C:310:PRO:HD2	2.15	0.62
1:C:227:ARG:NH1	3:C:949:HOH:O	2.31	0.62
1:B:34:ARG:NH1	1:B:72:ASN:OD1	2.28	0.61
1:A:308:ALA:HB2	1:A:331:LEU:CD1	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:317:HIS:HE1	1:C:322:ASP:OD2	1.83	0.61
1:D:108:ILE:HG21	1:D:166:ARG:HB3	1.82	0.60
1:B:230:MET:HE1	1:B:290:TYR:HD1	1.66	0.60
1:D:33:VAL:CG1	3:D:1379:HOH:O	2.46	0.60
1:C:143:ASN:CB	3:C:1031:HOH:O	2.35	0.60
1:D:108:ILE:HD12	1:D:163:ALA:HA	1.84	0.60
1:B:46:MET:HE2	1:B:65:LEU:HD23	1.82	0.60
1:D:266:ARG:HD2	3:D:968:HOH:O	2.03	0.58
1:A:129:LEU:CD2	1:A:196:LEU:HD12	2.33	0.58
1:D:308:ALA:HB2	1:D:331:LEU:HD11	1.85	0.58
1:C:161:ASP:CG	1:C:199:ARG:HH22	2.00	0.58
1:D:317:HIS:HE1	1:D:322:ASP:OD2	1.87	0.57
1:B:52:TYR:OH	1:B:107:HIS:CD2	2.54	0.57
1:A:52:TYR:OH	1:A:107:HIS:HD2	1.88	0.57
1:B:230:MET:HE1	1:B:290:TYR:CD1	2.39	0.57
1:D:317:HIS:HD2	3:D:1209:HOH:O	1.87	0.56
1:C:230:MET:CE	1:C:290:TYR:HD1	2.19	0.56
1:C:230:MET:HE1	1:C:290:TYR:HD1	1.70	0.56
1:B:161:ASP:OD1	1:B:199:ARG:NH2	2.38	0.56
1:D:34:ARG:NH1	1:D:72:ASN:OD1	2.38	0.56
1:D:317:HIS:CD2	3:D:1209:HOH:O	2.58	0.55
1:B:131:ASP:OD1	1:B:133:ALA:HB3	2.07	0.55
1:A:100:PHE:HB2	1:A:153:GLN:HE21	1.72	0.55
1:A:108:ILE:HG21	1:A:166:ARG:HB3	1.89	0.54
1:A:317:HIS:CD2	3:A:378:HOH:O	2.48	0.54
1:D:162:GLU:HG3	1:D:162:GLU:O	2.08	0.54
1:B:108:ILE:HG21	1:B:166:ARG:HB3	1.90	0.54
1:C:130:PHE:CD2	1:C:141:SER:HB2	2.43	0.54
1:A:230:MET:CE	1:A:290:TYR:CD1	2.86	0.53
1:B:136:PRO:HD2	3:B:753:HOH:O	2.09	0.53
1:C:230:MET:HE1	1:C:290:TYR:CD1	2.43	0.53
1:C:52:TYR:OH	1:C:107:HIS:CD2	2.59	0.53
1:D:48:MET:HG3	1:D:88:GLN:HE22	1.73	0.53
1:C:116:ALA:O	1:C:171:ASP:OD2	2.26	0.53
1:C:278:ARG:O	1:C:278:ARG:HD2	2.08	0.52
1:A:284:LYS:HE3	1:A:342:GLU:CB	2.40	0.52
1:D:198:GLN:HG3	3:D:1400:HOH:O	2.02	0.52
1:C:134:ASP:O	1:C:146:ARG:NH2	2.43	0.52
1:A:161:ASP:OD1	1:A:199:ARG:NH2	2.36	0.52
3:A:414:HOH:O	1:B:266:ARG:HD2	2.09	0.52
1:C:142:ALA:HB1	3:C:1151:HOH:O	2.03	0.51
1:D:308:ALA:CB	1:D:331:LEU:CD1	2.86	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:102:GLN:HG2	1:D:102:GLN:O	2.10	0.51
1:D:157:PRO:HD2	1:D:158:GLU:OE2	2.10	0.51
1:C:237:SER:HB3	1:C:240:LEU:HB2	1.92	0.51
1:C:143:ASN:OD1	3:C:1031:HOH:O	2.05	0.50
1:C:67:SER:O	1:C:71:GLN:HG3	2.11	0.50
1:A:198:GLN:CG	3:A:569:HOH:O	2.42	0.50
1:C:168:ARG:O	1:C:168:ARG:HG3	2.11	0.49
1:C:13:ALA:HA	1:C:41:THR:O	2.13	0.49
1:D:309:ASP:HB2	1:D:310:PRO:HD3	1.95	0.49
1:B:317:HIS:HE1	1:B:322:ASP:OD2	1.96	0.49
1:C:33:VAL:CG1	3:C:1102:HOH:O	2.60	0.48
1:C:31:ASN:OD1	1:C:34:ARG:NH2	2.41	0.48
1:A:284:LYS:HE3	1:A:342:GLU:HB3	1.94	0.48
1:D:7:ASP:OD1	1:D:7:ASP:N	2.46	0.48
1:A:266:ARG:O	1:A:266:ARG:HG3	2.14	0.48
1:B:308:ALA:HB2	1:B:331:LEU:CD1	2.44	0.48
1:A:84:HIS:N	1:A:85:PRO:CD	2.77	0.47
1:D:230:MET:HE1	1:D:290:TYR:HD1	1.79	0.47
1:C:162:GLU:O	1:C:162:GLU:HG3	2.14	0.47
1:B:69:ALA:HB1	1:B:74:GLN:HB2	1.97	0.47
1:C:293:VAL:O	1:C:295:PRO:HD3	2.15	0.46
1:C:46:MET:HE3	1:C:65:LEU:HD23	1.97	0.46
1:C:143:ASN:HB2	3:C:1031:HOH:O	2.09	0.46
1:D:230:MET:HE1	1:D:290:TYR:CD1	2.50	0.46
1:A:227:ARG:HG3	1:A:227:ARG:HH11	1.79	0.46
1:A:100:PHE:CB	1:A:153:GLN:NE2	2.76	0.46
1:C:334:LYS:HB3	1:C:335:PRO:HD2	1.97	0.46
1:D:40:ILE:CG2	3:D:1379:HOH:O	2.55	0.46
1:B:217:MET:HG2	1:B:250:ARG:HB2	1.97	0.46
1:B:284:LYS:O	1:B:288:GLN:HG3	2.16	0.46
1:C:69:ALA:HB1	1:C:74:GLN:HB2	1.96	0.46
1:D:230:MET:CE	1:D:290:TYR:HD1	2.28	0.46
1:A:130:PHE:CD2	1:A:141:SER:HB2	2.50	0.46
1:C:205:VAL:HG13	1:C:206:PRO:HD2	1.97	0.46
1:D:134:ASP:CG	1:D:146:ARG:HH22	2.20	0.45
1:C:83:TRP:CZ2	1:C:85:PRO:HG2	2.51	0.45
1:B:131:ASP:HB3	1:B:134:ASP:HB3	1.98	0.45
1:B:161:ASP:O	1:B:165:ARG:HG3	2.16	0.45
1:A:121:SER:HB3	1:A:175:GLU:HB2	1.99	0.45
1:C:223:ILE:HD12	3:C:950:HOH:O	2.16	0.45
1:A:52:TYR:OH	1:A:107:HIS:CD2	2.69	0.45
1:A:139:ARG:HB2	1:A:147:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:64:ARG:HG3	3:D:1356:HOH:O	2.16	0.45
1:D:315:TYR:OH	1:D:329:ASP:OD2	2.22	0.45
1:B:228:GLN:CG	3:B:842:HOH:O	2.65	0.44
1:B:134:ASP:CG	1:B:146:ARG:HH22	2.20	0.44
1:A:84:HIS:N	1:A:85:PRO:HD3	2.32	0.44
1:A:154:PHE:CG	1:A:159:TYR:HB3	2.52	0.44
1:D:108:ILE:CD1	1:D:163:ALA:HA	2.46	0.44
1:A:230:MET:HE3	1:A:290:TYR:HD1	1.80	0.44
1:B:308:ALA:HB2	1:B:331:LEU:HD12	2.00	0.44
1:C:171:ASP:OD1	1:C:173:THR:OG1	2.33	0.44
1:D:168:ARG:NH2	1:D:208:ASP:OD2	2.46	0.44
1:C:220:TYR:C	1:C:220:TYR:CD2	2.90	0.43
1:C:213:GLN:O	1:C:214:MET:HB2	2.18	0.43
1:A:294:VAL:HA	1:A:295:PRO:HD3	1.86	0.43
1:D:220:TYR:C	1:D:220:TYR:CD1	2.91	0.43
1:A:33:VAL:CG1	3:A:548:HOH:O	2.66	0.43
1:D:177:TYR:CE2	1:D:243:LYS:HB2	2.54	0.43
1:B:237:SER:HB3	1:B:240:LEU:HB2	2.00	0.43
1:B:83:TRP:CZ2	1:B:85:PRO:HG2	2.54	0.43
1:C:309:ASP:N	1:C:310:PRO:CD	2.82	0.42
1:A:223:ILE:N	1:A:223:ILE:HD12	2.34	0.42
1:A:33:VAL:CG2	3:A:548:HOH:O	2.66	0.42
1:B:139:ARG:HB2	1:B:147:GLN:HB2	2.01	0.42
1:C:240:LEU:HA	1:C:240:LEU:HD12	1.68	0.42
1:B:195:ASN:HD22	1:B:195:ASN:HA	1.68	0.42
1:A:237:SER:HB3	1:A:240:LEU:HB2	2.01	0.42
1:A:148:SER:O	1:A:152:ARG:HG3	2.19	0.42
1:D:99:ASN:ND2	3:D:1442:HOH:O	2.52	0.42
1:C:13:ALA:HB2	1:C:305:TRP:CE3	2.55	0.42
1:C:330:ASN:HB2	1:C:332:GLN:HG2	2.02	0.42
1:B:136:PRO:HD2	1:B:146:ARG:HH21	1.85	0.41
1:B:83:TRP:CD2	1:B:85:PRO:HD2	2.55	0.41
1:D:151:TYR:CZ	1:D:156:GLY:HA2	2.55	0.41
1:B:228:GLN:HG2	3:B:842:HOH:O	2.19	0.41
1:D:254:PRO:HA	3:D:1180:HOH:O	2.19	0.41
1:D:12:VAL:CG1	3:D:1379:HOH:O	2.67	0.41
1:C:284:LYS:HG3	1:C:343:ALA:HB2	2.03	0.41
1:D:168:ARG:HG3	1:D:168:ARG:O	2.20	0.41
1:A:11:GLY:HA2	1:A:39:GLN:O	2.20	0.41
1:B:46:MET:CE	1:B:65:LEU:HD23	2.47	0.41
1:A:295:PRO:HA	1:A:296:PRO:HD3	1.86	0.41
1:A:331:LEU:HD12	1:A:331:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:177:TYR:CE2	1:B:209:GLY:HA3	2.56	0.41
1:A:284:LYS:HE3	1:A:342:GLU:HB2	2.03	0.40
1:B:295:PRO:HA	1:B:296:PRO:HD3	1.95	0.40
1:A:318:GLN:NE2	3:A:737:HOH:O	2.42	0.40
1:A:151:TYR:CZ	1:A:156:GLY:HA2	2.56	0.40
1:A:33:VAL:HG11	3:A:548:HOH:O	2.22	0.40
1:C:284:LYS:HE3	1:C:342:GLU:HB3	2.04	0.40
1:C:89:LEU:HD23	1:C:89:LEU:HA	1.92	0.40
1:B:317:HIS:HB2	3:B:704:HOH:O	2.21	0.40
1:D:31:ASN:OD1	1:D:34:ARG:NH2	2.49	0.40
1:D:142:ALA:O	1:D:143:ASN:HB2	2.21	0.40
1:A:315:TYR:OH	1:A:329:ASP:OD2	2.21	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:622:HOH:O	3:D:1395:HOH:O[2_675]	0.78	1.42
3:A:477:HOH:O	3:A:546:HOH:O[3_646]	0.88	1.32
3:A:507:HOH:O	3:D:1354:HOH:O[3_656]	1.28	0.92
3:B:899:HOH:O	3:D:1286:HOH:O[3_656]	1.40	0.80
3:A:547:HOH:O	3:A:597:HOH:O[3_656]	1.47	0.73
3:A:601:HOH:O	3:B:754:HOH:O[3_656]	1.53	0.67
1:A:64:ARG:NH2	3:D:1422:HOH:O[3_656]	1.56	0.64
1:A:173:THR:O	3:B:754:HOH:O[3_656]	1.59	0.61
1:A:64:ARG:NH1	3:D:1422:HOH:O[3_656]	1.62	0.58
3:A:525:HOH:O	3:D:1450:HOH:O[3_656]	1.68	0.52
3:A:583:HOH:O	3:D:1318:HOH:O[2_675]	1.68	0.52
3:A:591:HOH:O	3:D:1281:HOH:O[3_656]	1.72	0.48
1:D:173:THR:CB	3:C:1151:HOH:O[4_466]	1.73	0.47
1:A:64:ARG:CZ	3:D:1422:HOH:O[3_656]	1.74	0.46
1:D:173:THR:CG2	3:C:1151:HOH:O[4_466]	1.84	0.36
1:A:175:GLU:CG	1:B:143:ASN:OD1[3_656]	1.99	0.21
1:A:239:THR:CG2	1:B:195:ASN:ND2[3_656]	1.99	0.21
1:D:173:THR:CA	3:C:1151:HOH:O[4_466]	2.04	0.16
1:C:143:ASN:ND2	1:D:208:ASP:OD1[4_566]	2.06	0.14
3:A:523:HOH:O	3:D:1454:HOH:O[3_656]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/347 (99%)	331 (96%)	11 (3%)	1 (0%)	50	31
1	B	343/347 (99%)	332 (97%)	11 (3%)	0	100	100
1	C	343/347 (99%)	332 (97%)	11 (3%)	0	100	100
1	D	343/347 (99%)	330 (96%)	13 (4%)	0	100	100
All	All	1372/1388 (99%)	1325 (97%)	46 (3%)	1 (0%)	59	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/284 (100%)	271 (96%)	12 (4%)	40	20
1	B	283/284 (100%)	269 (95%)	14 (5%)	35	15
1	C	283/284 (100%)	273 (96%)	10 (4%)	48	28
1	D	283/284 (100%)	271 (96%)	12 (4%)	40	20
All	All	1132/1136 (100%)	1084 (96%)	48 (4%)	40	20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	88	GLN

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Mol	Chain	Res	Type
1	A	132	SER
1	A	161	ASP
1	A	162	GLU
1	A	166	ARG
1	A	168	ARG
1	A	223	ILE
1	A	227	ARG
1	A	322	ASP
1	A	331	LEU
1	A	345	SER
1	B	25	THR
1	B	67	SER
1	B	88	GLN
1	B	132	SER
1	B	143	ASN
1	B	146	ARG
1	B	158	GLU
1	B	161	ASP
1	B	162	GLU
1	B	166	ARG
1	B	168	ARG
1	B	198	GLN
1	B	223	ILE
1	B	331	LEU
1	C	25	THR
1	C	53	SER
1	C	88	GLN
1	C	162	GLU
1	C	166	ARG
1	C	168	ARG
1	C	223	ILE
1	C	227	ARG
1	C	329	ASP
1	C	331	LEU
1	D	88	GLN
1	D	132	SER
1	D	146	ARG
1	D	161	ASP
1	D	162	GLU
1	D	166	ARG
1	D	168	ARG
1	D	223	ILE

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Mol	Chain	Res	Type
1	D	227	ARG
1	D	266	ARG
1	D	329	ASP
1	D	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	88	GLN
1	A	107	HIS
1	A	114	HIS
1	A	147	GLN
1	A	153	GLN
1	A	203	ASN
1	A	317	HIS
1	A	318	GLN
1	B	61	ASN
1	B	88	GLN
1	B	107	HIS
1	B	114	HIS
1	B	153	GLN
1	B	195	ASN
1	B	203	ASN
1	B	317	HIS
1	B	319	ASN
1	B	332	GLN
1	C	61	ASN
1	C	88	GLN
1	C	107	HIS
1	C	114	HIS
1	C	195	ASN
1	C	203	ASN
1	C	317	HIS
1	D	88	GLN
1	D	107	HIS
1	D	114	HIS
1	D	195	ASN
1	D	203	ASN
1	D	317	HIS
1	D	318	GLN
1	D	319	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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