



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 09:58 AM BST

PDB ID : 1EZR  
Title : CRYSTAL STRUCTURE OF NUCLEOSIDE HYDROLASE FROM LEISH-MANIA MAJOR  
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Deposited on : 2000-05-11  
Resolution : 2.50 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.

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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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

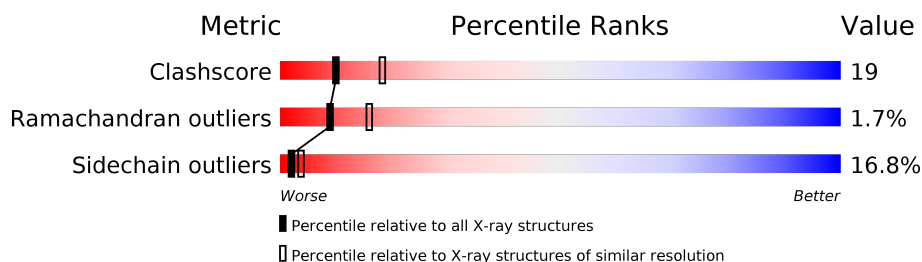
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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	314	
1	B	314	
1	C	314	
1	D	314	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9444 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 NUCLEOSIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2335	1491	401	430	13			
1	B	312	Total	C	N	O	S	0	0	0
			2335	1491	401	430	13			
1	C	312	Total	C	N	O	S	0	0	0
			2335	1491	401	430	13			
1	D	312	Total	C	N	O	S	0	0	0
			2335	1491	401	430	13			

- 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.

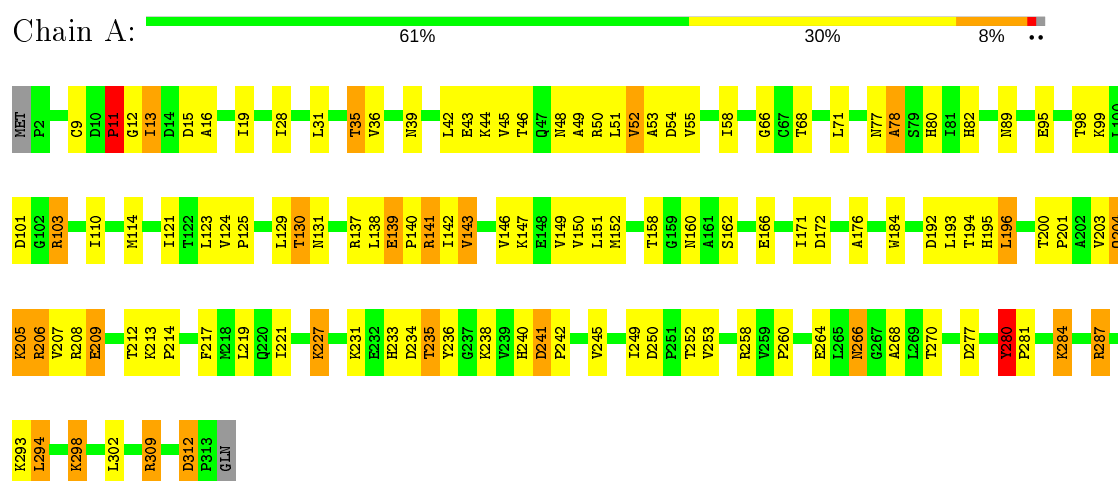
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	22	Total	O	0	0
			22	22		
3	C	29	Total	O	0	0
			29	29		
3	D	22	Total	O	0	0
			22	22		

### 3 Residue-property plots

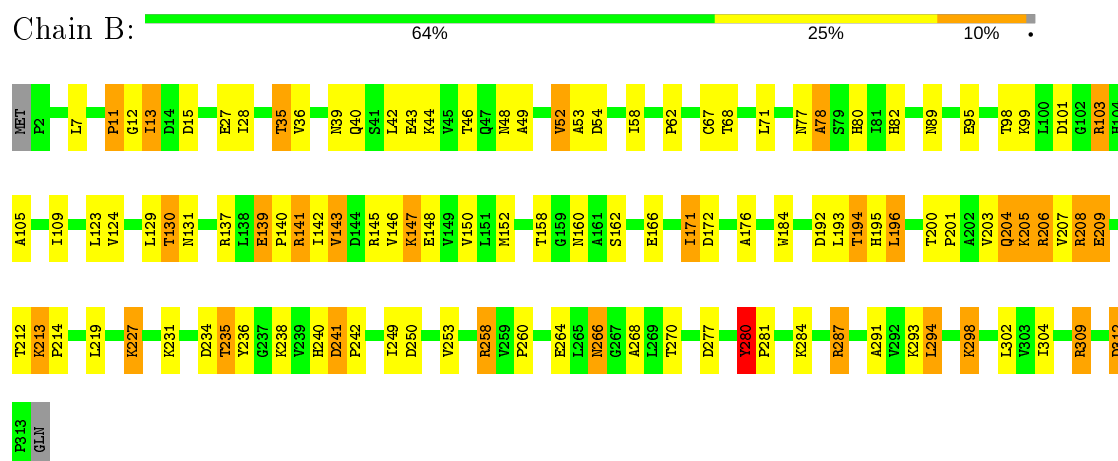
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

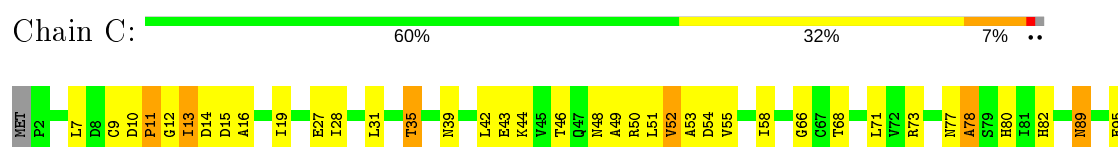
#### • Molecule 1: NUCLEOSIDE HYDROLASE

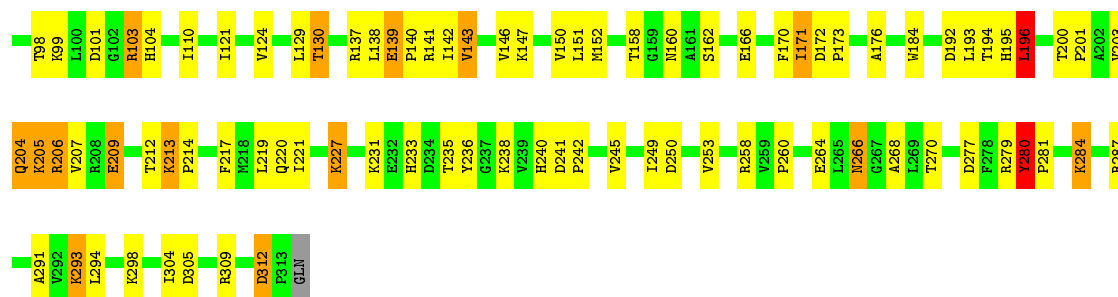


#### • Molecule 1: NUCLEOSIDE HYDROLASE



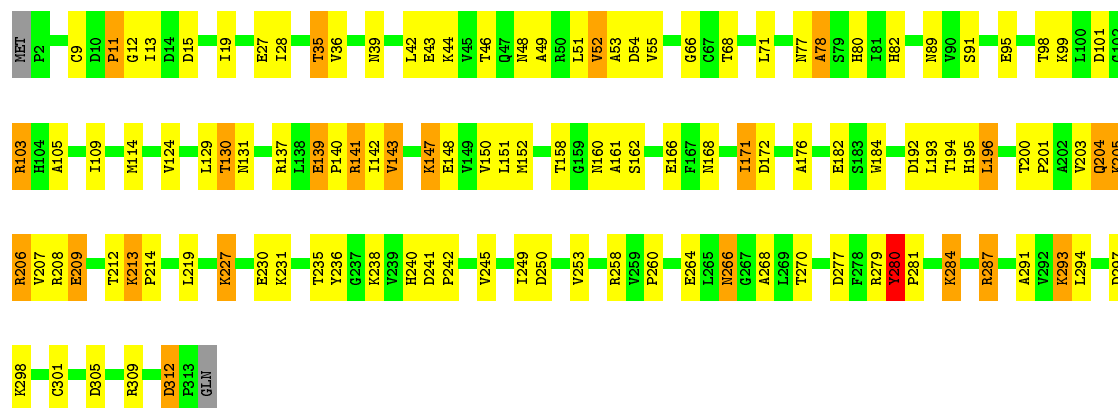
#### • Molecule 1: NUCLEOSIDE HYDROLASE





• Molecule 1: NUCLEOSIDE HYDROLASE

Chain D: 62% 30% 7%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.80 Å 79.20 Å 109.80 Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.5 (20.00-2.50)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.203 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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	0.38	0/2381	0.63	1/3252 (0.0%)
1	B	0.39	0/2381	0.63	1/3252 (0.0%)
1	C	0.39	0/2381	0.63	2/3252 (0.1%)
1	D	0.39	0/2381	0.63	1/3252 (0.0%)
All	All	0.39	0/9524	0.63	5/13008 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	GLY	N-CA-C	-7.53	94.26	113.10
1	C	12	GLY	N-CA-C	-7.50	94.36	113.10
1	B	12	GLY	N-CA-C	-7.47	94.42	113.10
1	A	12	GLY	N-CA-C	-7.36	94.69	113.10
1	C	196	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2335	0	2353	96	0
1	B	2335	0	2353	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2335	0	2353	98	0
1	D	2335	0	2353	93	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	27	0	0	3	0
3	B	22	0	0	6	0
3	C	29	0	0	2	0
3	D	22	0	0	0	0
All	All	9444	0	9412	358	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 19.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TYR:HB3	1:A:281:PRO:HD3	1.32	1.08
1:B:280:TYR:HB3	1:B:281:PRO:HD3	1.35	1.06
1:D:280:TYR:HB3	1:D:281:PRO:HD3	1.35	1.03
1:C:266:ASN:HD22	1:C:266:ASN:H	1.03	1.03
1:B:250:ASP:O	1:B:253:VAL:HG23	1.61	1.01
1:C:280:TYR:HB3	1:C:281:PRO:HD3	1.39	1.00
1:C:250:ASP:O	1:C:253:VAL:HG23	1.64	0.97
1:D:250:ASP:O	1:D:253:VAL:HG23	1.64	0.97
1:A:250:ASP:O	1:A:253:VAL:HG23	1.65	0.95
1:D:201:PRO:HA	1:D:204:GLN:HG3	1.48	0.95
1:B:201:PRO:HA	1:B:204:GLN:HG3	1.52	0.91
1:A:266:ASN:H	1:A:266:ASN:HD22	1.22	0.88
1:C:266:ASN:HD22	1:C:266:ASN:N	1.71	0.86
1:B:266:ASN:H	1:B:266:ASN:HD22	1.24	0.86
1:A:201:PRO:HA	1:A:204:GLN:HG3	1.56	0.85
1:C:201:PRO:HA	1:C:204:GLN:HG3	1.57	0.85
1:B:28:ILE:HD13	1:B:249:ILE:HG12	1.58	0.85
1:A:280:TYR:HB3	1:A:281:PRO:CD	2.06	0.85
1:D:266:ASN:HD22	1:D:266:ASN:H	1.21	0.84
1:D:280:TYR:HB3	1:D:281:PRO:CD	2.08	0.82
1:B:280:TYR:HB3	1:B:281:PRO:CD	2.08	0.82
1:B:287:ARG:HG2	3:B:585:HOH:O	1.81	0.81
1:B:54:ASP:OD1	1:B:98:THR:HG23	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:HD22	1:A:266:ASN:N	1.79	0.80
1:C:280:TYR:HB3	1:C:281:PRO:CD	2.12	0.80
1:D:28:ILE:HD13	1:D:249:ILE:HG12	1.64	0.79
1:D:54:ASP:OD1	1:D:98:THR:HG23	1.83	0.79
1:B:266:ASN:N	1:B:266:ASN:HD22	1.81	0.78
1:D:266:ASN:N	1:D:266:ASN:HD22	1.80	0.76
1:C:266:ASN:HD21	1:D:268:ALA:CB	2.00	0.74
1:C:28:ILE:HD13	1:C:249:ILE:HG12	1.66	0.74
1:C:227:LYS:HA	1:C:231:LYS:CB	2.18	0.73
1:A:11:PRO:HA	1:A:15:ASP:HB2	1.71	0.72
1:B:11:PRO:HA	1:B:15:ASP:HB2	1.72	0.72
1:C:35:THR:HG21	1:C:46:THR:OG1	1.89	0.72
1:B:28:ILE:CD1	1:B:249:ILE:HG12	2.19	0.72
1:C:42:LEU:HD22	1:C:68:THR:HG22	1.73	0.71
1:A:266:ASN:HB2	1:D:266:ASN:HB2	1.71	0.71
1:A:227:LYS:HA	1:A:231:LYS:CB	2.21	0.71
1:C:160:ASN:OD1	1:C:166:GLU:HA	1.91	0.71
1:B:227:LYS:HA	1:B:231:LYS:CB	2.21	0.70
1:A:28:ILE:HD13	1:A:249:ILE:HG12	1.72	0.70
1:D:35:THR:HG22	1:D:42:LEU:HD11	1.74	0.70
1:D:227:LYS:HA	1:D:231:LYS:CB	2.22	0.69
1:C:28:ILE:CD1	1:C:249:ILE:HG12	2.22	0.69
1:C:11:PRO:HA	1:C:15:ASP:HB2	1.74	0.69
1:C:54:ASP:OD1	1:C:98:THR:HG23	1.93	0.69
1:D:11:PRO:HA	1:D:15:ASP:HB2	1.76	0.68
1:B:35:THR:HG21	1:B:46:THR:OG1	1.94	0.68
1:A:54:ASP:OD1	1:A:98:THR:HG23	1.94	0.68
1:D:28:ILE:CD1	1:D:249:ILE:HG12	2.25	0.67
1:B:48:ASN:O	1:B:52:VAL:HG13	1.96	0.66
1:C:141:ARG:HG3	1:C:141:ARG:HH11	1.61	0.66
1:C:205:LYS:HB2	1:C:205:LYS:NZ	2.10	0.66
1:B:129:LEU:HD12	1:B:176:ALA:HA	1.77	0.65
1:C:35:THR:HG22	1:C:42:LEU:HD11	1.77	0.65
1:A:206:ARG:HH21	1:A:209:GLU:HB3	1.61	0.65
1:A:28:ILE:CD1	1:A:249:ILE:HG12	2.25	0.65
1:A:98:THR:HG22	3:A:565:HOH:O	1.96	0.65
1:C:48:ASN:O	1:C:52:VAL:HG13	1.96	0.65
1:B:35:THR:HG22	1:B:42:LEU:HD11	1.79	0.65
1:A:280:TYR:CB	1:A:281:PRO:HD3	2.18	0.65
1:B:205:LYS:NZ	1:B:205:LYS:HB2	2.11	0.64
1:A:205:LYS:HB2	1:A:205:LYS:NZ	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LYS:NZ	1:D:205:LYS:HB2	2.11	0.64
1:B:212:THR:HB	1:B:214:PRO:HD2	1.79	0.64
1:A:266:ASN:HD21	1:B:268:ALA:CB	2.11	0.64
1:C:141:ARG:NH1	1:C:141:ARG:HG3	2.12	0.64
1:C:280:TYR:CB	1:C:281:PRO:HD3	2.24	0.64
1:D:206:ARG:HH21	1:D:209:GLU:HB3	1.62	0.64
1:D:48:ASN:O	1:D:52:VAL:HG13	1.98	0.64
1:A:42:LEU:HD22	1:A:68:THR:HG22	1.79	0.63
1:B:67:CYS:HA	3:B:516:HOH:O	1.97	0.63
1:C:206:ARG:HH21	1:C:209:GLU:HB3	1.63	0.63
1:B:206:ARG:HH21	1:B:209:GLU:HB3	1.63	0.63
1:A:266:ASN:HD21	1:B:268:ALA:HB2	1.64	0.63
1:A:137:ARG:NH1	1:D:71:LEU:O	2.32	0.63
1:A:35:THR:HG21	1:A:46:THR:OG1	1.99	0.62
1:A:260:PRO:HG2	1:A:277:ASP:HB3	1.81	0.62
1:B:309:ARG:HH11	1:B:309:ARG:HG2	1.64	0.62
1:A:48:ASN:O	1:A:52:VAL:HG13	1.98	0.62
1:D:35:THR:HG21	1:D:46:THR:OG1	1.99	0.62
1:C:266:ASN:ND2	1:C:266:ASN:N	2.43	0.61
1:C:268:ALA:HB2	1:D:266:ASN:HD21	1.65	0.61
1:D:9:CYS:SG	1:D:11:PRO:HD3	2.41	0.61
1:B:160:ASN:OD1	1:B:166:GLU:HA	2.01	0.61
1:A:35:THR:HG22	1:A:42:LEU:HD11	1.83	0.60
1:A:140:PRO:HD2	3:A:572:HOH:O	2.02	0.60
1:C:11:PRO:HG2	1:C:49:ALA:HB2	1.84	0.60
1:C:14:ASP:HB2	3:C:593:HOH:O	2.00	0.60
1:A:212:THR:HB	1:A:214:PRO:HD2	1.83	0.60
1:C:266:ASN:HD21	1:D:268:ALA:HB2	1.67	0.60
1:A:206:ARG:HE	1:A:206:ARG:HA	1.68	0.59
1:D:141:ARG:HH11	1:D:141:ARG:HG3	1.66	0.59
1:D:206:ARG:HE	1:D:206:ARG:HA	1.67	0.59
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.17	0.59
1:C:206:ARG:HE	1:C:206:ARG:HA	1.67	0.59
1:A:196:LEU:HD12	1:A:294:LEU:H	1.68	0.59
1:D:141:ARG:NH1	1:D:141:ARG:HG3	2.15	0.58
1:B:213:LYS:HD2	1:B:312:ASP:OD2	2.04	0.58
1:C:129:LEU:HD12	1:C:176:ALA:HA	1.86	0.58
1:D:309:ARG:HG2	1:D:309:ARG:HH11	1.68	0.57
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.67	0.57
1:D:196:LEU:HD23	1:D:196:LEU:N	2.19	0.57
1:D:280:TYR:CB	1:D:281:PRO:HD3	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HD22	1:B:68:THR:HG22	1.85	0.57
1:B:280:TYR:CB	1:B:281:PRO:HD3	2.23	0.57
1:D:42:LEU:HD22	1:D:68:THR:HG22	1.87	0.57
1:C:212:THR:HB	1:C:214:PRO:HD2	1.87	0.56
1:A:142:ILE:HG13	1:A:143:VAL:N	2.19	0.56
1:B:140:PRO:O	1:B:143:VAL:HG13	2.06	0.56
1:D:213:LYS:HD2	1:D:312:ASP:OD2	2.06	0.56
1:A:129:LEU:HD12	1:A:176:ALA:HA	1.87	0.56
1:C:43:GLU:CD	1:C:43:GLU:H	2.08	0.56
1:A:110:ILE:CD1	1:A:138:LEU:HD23	2.37	0.55
1:B:206:ARG:HA	1:B:206:ARG:HE	1.71	0.55
1:A:43:GLU:CD	1:A:43:GLU:H	2.09	0.55
1:B:124:VAL:HA	1:B:150:VAL:O	2.07	0.55
1:A:11:PRO:HG2	1:A:49:ALA:HB2	1.88	0.55
1:B:266:ASN:ND2	1:B:266:ASN:N	2.53	0.55
1:C:151:LEU:O	1:C:151:LEU:HD12	2.07	0.54
1:A:200:THR:OG1	1:A:203:VAL:HG23	2.07	0.54
1:C:142:ILE:HG13	1:C:143:VAL:N	2.23	0.54
1:C:201:PRO:HD3	1:C:236:TYR:CE2	2.42	0.54
1:C:130:THR:HB	1:C:172:ASP:OD1	2.07	0.54
1:B:141:ARG:NH1	1:B:141:ARG:HG3	2.23	0.54
1:C:124:VAL:HA	1:C:150:VAL:O	2.08	0.54
1:C:151:LEU:HD12	1:C:151:LEU:C	2.28	0.54
1:B:43:GLU:CD	1:B:43:GLU:H	2.10	0.54
1:B:141:ARG:HH11	1:B:141:ARG:HG3	1.72	0.53
1:C:309:ARG:HG2	1:C:309:ARG:HH11	1.73	0.53
1:C:35:THR:HG22	1:C:42:LEU:CD1	2.38	0.53
1:D:212:THR:HB	1:D:214:PRO:HD2	1.90	0.53
1:D:139:GLU:OE1	1:D:141:ARG:HG3	2.08	0.53
1:B:71:LEU:O	1:C:137:ARG:NH1	2.40	0.53
1:B:196:LEU:HD12	1:B:294:LEU:H	1.74	0.53
1:C:213:LYS:HD2	1:C:312:ASP:OD2	2.09	0.53
1:C:51:LEU:O	1:C:55:VAL:HG23	2.08	0.53
1:D:266:ASN:ND2	1:D:266:ASN:N	2.52	0.53
1:A:207:VAL:HG21	1:A:219:LEU:HD21	1.91	0.53
1:C:241:ASP:N	1:C:242:PRO:HD2	2.24	0.53
1:B:200:THR:OG1	1:B:203:VAL:HG23	2.09	0.52
1:B:137:ARG:NH1	1:C:71:LEU:O	2.42	0.52
1:D:43:GLU:CD	1:D:43:GLU:H	2.11	0.52
1:B:234:ASP:O	1:B:235:THR:HG23	2.10	0.52
1:B:131:ASN:HB2	3:B:518:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:PRO:HG2	1:D:49:ALA:HB2	1.91	0.52
1:D:168:ASN:O	1:D:171:ILE:HG22	2.09	0.52
1:A:140:PRO:O	1:A:143:VAL:HG13	2.10	0.52
1:B:204:GLN:O	1:B:207:VAL:HG22	2.10	0.52
1:B:62:PRO:HA	3:B:577:HOH:O	2.09	0.52
1:D:142:ILE:HG13	1:D:143:VAL:N	2.23	0.52
1:D:193:LEU:HG	1:D:291:ALA:HB1	1.91	0.51
1:B:196:LEU:N	1:B:196:LEU:HD23	2.25	0.51
1:D:101:ASP:OD2	1:D:103:ARG:HD3	2.10	0.51
1:D:124:VAL:HA	1:D:150:VAL:O	2.11	0.51
1:D:201:PRO:HD3	1:D:236:TYR:CE2	2.46	0.51
1:A:266:ASN:ND2	1:A:266:ASN:N	2.51	0.51
1:B:105:ALA:O	1:B:109:ILE:HG13	2.10	0.51
1:C:170:PHE:O	1:C:173:PRO:HD3	2.11	0.51
1:A:19:ILE:HD13	1:A:52:VAL:HG21	1.92	0.51
1:A:71:LEU:O	1:D:137:ARG:NH1	2.43	0.50
1:C:140:PRO:O	1:C:143:VAL:HG13	2.11	0.50
1:A:266:ASN:CB	1:D:266:ASN:HB2	2.41	0.50
1:A:31:LEU:HD12	1:A:121:ILE:HG12	1.94	0.50
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.76	0.50
1:C:260:PRO:HG2	1:C:277:ASP:HB3	1.93	0.50
1:D:196:LEU:HD12	1:D:294:LEU:H	1.77	0.50
1:A:245:VAL:O	1:A:249:ILE:HG13	2.12	0.50
1:D:129:LEU:HD12	1:D:176:ALA:HA	1.93	0.50
1:A:130:THR:HB	1:A:172:ASP:OD1	2.12	0.50
1:B:11:PRO:HG2	1:B:49:ALA:HB2	1.94	0.50
1:B:260:PRO:HG2	1:B:277:ASP:HB3	1.94	0.50
1:A:204:GLN:O	1:A:207:VAL:HG22	2.12	0.49
1:C:279:ARG:NH1	1:D:160:ASN:O	2.42	0.49
1:B:101:ASP:OD2	1:B:103:ARG:HD3	2.12	0.49
1:C:42:LEU:CD2	1:C:68:THR:HG22	2.39	0.49
1:A:241:ASP:N	1:A:242:PRO:HD2	2.27	0.49
1:C:19:ILE:HD13	1:C:52:VAL:HG21	1.94	0.49
1:A:124:VAL:HA	1:A:150:VAL:O	2.12	0.49
1:A:160:ASN:OD1	1:A:166:GLU:HA	2.13	0.49
1:A:196:LEU:N	1:A:196:LEU:HD23	2.28	0.49
1:C:196:LEU:HD23	1:C:196:LEU:N	2.27	0.49
1:B:266:ASN:HB2	1:C:266:ASN:HB2	1.94	0.49
1:B:53:ALA:HA	1:B:58:ILE:HD12	1.95	0.48
1:C:264:GLU:HG2	1:C:270:THR:OG1	2.13	0.48
1:D:160:ASN:OD1	1:D:166:GLU:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:VAL:HG21	1:B:219:LEU:HD21	1.95	0.48
1:C:240:HIS:C	1:C:242:PRO:HD2	2.32	0.48
1:D:171:ILE:O	1:D:171:ILE:HD13	2.13	0.48
1:B:101:ASP:OD2	1:B:103:ARG:HG2	2.13	0.48
1:C:266:ASN:HD21	1:D:268:ALA:HB3	1.76	0.48
1:C:141:ARG:HH11	1:C:141:ARG:CG	2.27	0.48
1:C:193:LEU:HG	1:C:291:ALA:HB1	1.96	0.48
1:A:264:GLU:HG2	1:A:270:THR:OG1	2.14	0.48
1:B:147:LYS:HG3	1:B:148:GLU:HG2	1.95	0.48
1:A:266:ASN:ND2	1:A:266:ASN:H	2.03	0.48
1:D:130:THR:HB	1:D:172:ASP:OD1	2.14	0.48
1:B:142:ILE:HG13	1:B:143:VAL:N	2.27	0.48
1:D:114:MET:HE2	1:D:141:ARG:HB2	1.96	0.48
1:A:207:VAL:HG23	1:A:219:LEU:HD11	1.95	0.47
1:D:206:ARG:HE	1:D:206:ARG:CA	2.26	0.47
1:D:260:PRO:HG2	1:D:277:ASP:HB3	1.94	0.47
1:D:297:ASP:O	1:D:301:CYS:SG	2.71	0.47
1:A:201:PRO:HD3	1:A:236:TYR:CE2	2.48	0.47
1:B:42:LEU:CD2	1:B:68:THR:HG22	2.43	0.47
1:C:7:LEU:HD12	1:C:124:VAL:O	2.15	0.47
1:C:207:VAL:HG21	1:C:219:LEU:HD21	1.95	0.47
1:D:204:GLN:O	1:D:207:VAL:HG22	2.14	0.47
1:A:101:ASP:OD2	1:A:103:ARG:HD3	2.14	0.47
1:D:147:LYS:HG3	1:D:148:GLU:HG2	1.96	0.47
1:A:42:LEU:CD2	1:A:68:THR:HG22	2.44	0.47
1:D:207:VAL:HG21	1:D:219:LEU:HD21	1.96	0.47
1:D:105:ALA:O	1:D:109:ILE:HG13	2.14	0.47
1:A:194:THR:OG1	1:A:240:HIS:HD2	1.98	0.47
1:D:160:ASN:OD1	1:D:161:ALA:N	2.46	0.47
1:A:284:LYS:H	1:A:284:LYS:HG2	1.52	0.46
1:B:36:VAL:HG13	1:B:131:ASN:ND2	2.29	0.46
1:D:200:THR:OG1	1:D:203:VAL:HG23	2.15	0.46
1:A:213:LYS:N	1:A:214:PRO:CD	2.78	0.46
1:B:309:ARG:NH1	1:B:309:ARG:HG2	2.28	0.46
1:D:280:TYR:CB	1:D:281:PRO:CD	2.86	0.46
1:D:277:ASP:OD1	1:D:279:ARG:HB2	2.15	0.46
1:A:206:ARG:HE	1:A:206:ARG:CA	2.27	0.46
1:D:193:LEU:O	1:D:196:LEU:HG	2.16	0.46
1:A:213:LYS:HD2	1:A:312:ASP:OD2	2.16	0.46
1:A:268:ALA:HB2	1:B:266:ASN:HD21	1.80	0.46
1:C:110:ILE:CD1	1:C:138:LEU:HD23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HE	1:C:206:ARG:CA	2.29	0.46
1:D:141:ARG:HH11	1:D:141:ARG:CG	2.29	0.46
1:C:101:ASP:OD2	1:C:103:ARG:HD3	2.16	0.46
1:D:139:GLU:O	1:D:142:ILE:HG12	2.16	0.46
1:D:241:ASP:N	1:D:242:PRO:HD2	2.30	0.46
1:C:268:ALA:CB	1:D:266:ASN:HD21	2.29	0.46
1:A:142:ILE:O	1:A:146:VAL:HG23	2.16	0.46
1:A:151:LEU:C	1:A:151:LEU:HD12	2.36	0.46
1:C:19:ILE:CD1	1:C:52:VAL:HG21	2.46	0.46
1:C:9:CYS:SG	1:C:11:PRO:HD3	2.56	0.46
1:B:201:PRO:HD3	1:B:236:TYR:CE2	2.50	0.45
1:C:53:ALA:HA	1:C:58:ILE:HD12	1.97	0.45
1:C:73:ARG:HG2	3:C:540:HOH:O	2.16	0.45
1:B:287:ARG:HB2	1:B:287:ARG:HE	1.61	0.45
1:C:204:GLN:O	1:C:207:VAL:HG22	2.17	0.45
1:A:193:LEU:HD13	1:A:193:LEU:C	2.36	0.45
1:B:287:ARG:HG3	1:B:287:ARG:H	1.61	0.45
1:D:114:MET:CE	1:D:141:ARG:HB2	2.46	0.45
1:A:51:LEU:O	1:A:55:VAL:HG23	2.17	0.45
1:A:53:ALA:HB1	1:A:98:THR:HG21	1.99	0.45
1:B:141:ARG:O	1:B:145:ARG:HG3	2.17	0.45
1:B:193:LEU:O	1:B:196:LEU:HG	2.16	0.45
1:C:194:THR:OG1	1:C:240:HIS:HD2	2.00	0.45
1:A:141:ARG:CG	1:A:141:ARG:HH11	2.30	0.45
1:D:207:VAL:HG23	1:D:219:LEU:HD11	1.98	0.45
1:B:258:ARG:NH1	3:B:522:HOH:O	2.50	0.45
1:B:207:VAL:HG23	1:B:208:ARG:N	2.32	0.44
1:B:241:ASP:N	1:B:242:PRO:HD2	2.32	0.44
1:B:77:ASN:O	1:B:78:ALA:C	2.55	0.44
1:D:35:THR:HG22	1:D:42:LEU:CD1	2.43	0.44
1:A:16:ALA:HA	1:A:19:ILE:HD12	1.98	0.44
1:C:196:LEU:HD12	1:C:294:LEU:H	1.83	0.44
1:B:213:LYS:N	1:B:214:PRO:CD	2.80	0.44
1:D:19:ILE:HD12	1:D:52:VAL:HG21	1.99	0.44
1:D:309:ARG:HG2	1:D:309:ARG:NH1	2.31	0.44
1:C:280:TYR:HE1	1:D:230:GLU:HA	1.83	0.44
1:D:245:VAL:O	1:D:249:ILE:HG13	2.17	0.44
1:B:35:THR:HG22	1:B:42:LEU:CD1	2.47	0.44
1:D:203:VAL:O	1:D:207:VAL:HG13	2.17	0.44
1:B:139:GLU:OE1	1:B:141:ARG:HG3	2.18	0.44
1:C:16:ALA:HA	1:C:19:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LYS:HG2	1:D:284:LYS:H	1.49	0.44
1:C:89:ASN:OD1	1:C:220:GLN:NE2	2.50	0.44
1:D:194:THR:OG1	1:D:240:HIS:HD2	2.01	0.44
1:D:51:LEU:O	1:D:55:VAL:HG23	2.18	0.44
1:A:217:PHE:O	1:A:221:ILE:HG12	2.18	0.44
1:B:266:ASN:ND2	1:B:266:ASN:H	2.04	0.43
1:C:142:ILE:O	1:C:146:VAL:HG23	2.16	0.43
1:D:264:GLU:HG2	1:D:270:THR:OG1	2.18	0.43
1:B:142:ILE:O	1:B:146:VAL:HG23	2.19	0.43
1:C:13:ILE:HG13	1:C:13:ILE:H	1.51	0.43
1:B:194:THR:OG1	1:B:240:HIS:HD2	2.01	0.43
1:A:233:HIS:CB	1:B:280:TYR:OH	2.66	0.43
1:A:250:ASP:OD2	1:A:252:THR:HG23	2.19	0.43
1:A:77:ASN:O	1:A:78:ALA:C	2.56	0.43
1:B:13:ILE:H	1:B:13:ILE:HG13	1.50	0.43
1:B:298:LYS:O	1:B:302:LEU:HG	2.19	0.43
1:C:266:ASN:ND2	1:D:268:ALA:H	2.17	0.43
1:C:207:VAL:HG12	1:C:304:ILE:HD13	2.01	0.43
1:C:46:THR:O	1:C:50:ARG:HG3	2.19	0.43
1:A:36:VAL:HG13	1:A:131:ASN:ND2	2.34	0.43
1:C:200:THR:OG1	1:C:203:VAL:HG23	2.18	0.43
1:A:234:ASP:O	1:A:235:THR:HG23	2.19	0.43
1:B:193:LEU:HG	1:B:291:ALA:HB1	2.00	0.43
1:B:171:ILE:HD13	1:B:171:ILE:O	2.18	0.43
1:D:66:GLY:CA	1:D:105:ALA:HB3	2.49	0.43
1:A:46:THR:O	1:A:50:ARG:HG3	2.19	0.42
1:C:305:ASP:CG	1:C:309:ARG:HE	2.22	0.42
1:A:298:LYS:O	1:A:302:LEU:HG	2.19	0.42
1:B:193:LEU:HD13	1:B:193:LEU:C	2.40	0.42
1:C:217:PHE:O	1:C:221:ILE:HG12	2.19	0.42
1:D:77:ASN:O	1:D:78:ALA:C	2.56	0.42
1:D:36:VAL:HG12	1:D:131:ASN:CG	2.40	0.42
1:A:193:LEU:O	1:A:196:LEU:HG	2.20	0.42
1:B:130:THR:HB	1:B:172:ASP:OD1	2.19	0.42
1:B:206:ARG:HE	1:B:206:ARG:CA	2.31	0.42
1:C:213:LYS:N	1:C:214:PRO:CD	2.82	0.42
1:C:77:ASN:O	1:C:78:ALA:C	2.57	0.42
1:A:123:LEU:HB2	1:A:149:VAL:HG22	2.01	0.42
1:D:53:ALA:HB1	1:D:98:THR:HG21	2.02	0.42
1:A:19:ILE:CD1	1:A:52:VAL:HG21	2.50	0.41
1:B:207:VAL:HG23	1:B:219:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:CB	1:C:214:PRO:HD2	2.49	0.41
1:C:207:VAL:HG12	1:C:304:ILE:CD1	2.50	0.41
1:D:293:LYS:HG3	1:D:294:LEU:N	2.35	0.41
1:A:114:MET:CE	1:A:141:ARG:HB2	2.50	0.41
1:A:13:ILE:H	1:A:13:ILE:HG13	1.54	0.41
1:A:35:THR:HG22	1:A:42:LEU:CD1	2.49	0.41
1:B:205:LYS:HB2	1:B:205:LYS:HZ3	1.85	0.41
1:C:233:HIS:CB	1:D:280:TYR:OH	2.68	0.41
1:C:284:LYS:HG2	1:C:284:LYS:H	1.51	0.41
1:A:101:ASP:OD2	1:A:103:ARG:HG2	2.21	0.41
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.93	0.41
1:B:264:GLU:HG2	1:B:270:THR:OG1	2.21	0.41
1:C:245:VAL:O	1:C:249:ILE:HG13	2.19	0.41
1:D:140:PRO:O	1:D:143:VAL:HG13	2.21	0.41
1:A:240:HIS:C	1:A:242:PRO:HD2	2.41	0.41
1:D:213:LYS:N	1:D:214:PRO:CD	2.84	0.41
1:C:293:LYS:HG3	1:C:294:LEU:N	2.35	0.41
1:A:139:GLU:OE1	1:A:141:ARG:HG3	2.21	0.41
1:B:131:ASN:N	3:B:518:HOH:O	2.46	0.41
1:B:212:THR:CB	1:B:214:PRO:HD2	2.48	0.41
1:A:287:ARG:H	1:A:287:ARG:HG3	1.66	0.41
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.93	0.41
1:A:53:ALA:HA	1:A:58:ILE:HD12	2.02	0.41
1:C:171:ILE:O	1:C:171:ILE:HD13	2.20	0.41
1:C:31:LEU:HD12	1:C:121:ILE:HG12	2.02	0.41
1:C:139:GLU:O	1:C:142:ILE:HG12	2.21	0.41
1:A:287:ARG:HE	1:A:287:ARG:HB2	1.68	0.41
1:B:240:HIS:O	1:B:241:ASP:C	2.59	0.41
1:A:139:GLU:O	1:A:142:ILE:HG12	2.22	0.40
1:A:268:ALA:CB	1:B:266:ASN:HD21	2.33	0.40
1:C:207:VAL:HG23	1:C:219:LEU:HD11	2.01	0.40
1:C:66:GLY:HA2	1:C:104:HIS:CE1	2.55	0.40
1:D:151:LEU:HD12	1:D:151:LEU:C	2.42	0.40
1:D:287:ARG:HG3	1:D:287:ARG:H	1.59	0.40
1:A:131:ASN:HB2	3:A:573:HOH:O	2.22	0.40
1:B:207:VAL:HG12	1:B:304:ILE:CD1	2.51	0.40
1:C:284:LYS:HB3	1:C:284:LYS:HE2	1.83	0.40
1:A:66:GLY:HA3	1:A:131:ASN:HD21	1.85	0.40
1:B:141:ARG:CG	1:B:141:ARG:HH11	2.34	0.40
1:C:73:ARG:HG3	1:C:173:PRO:HD2	2.03	0.40
1:C:207:VAL:CG2	1:C:219:LEU:HD21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ARG:NH2	1:D:182:GLU:OE2	2.53	0.40
1:D:305:ASP:CG	1:D:309:ARG:HE	2.25	0.40
1:B:7:LEU:HD12	1:B:124:VAL:O	2.21	0.40
1:D:66:GLY:HA2	1:D:105:ALA:HB3	2.03	0.40
1:A:114:MET:HE2	1:A:141:ARG:HB2	2.04	0.40
1:A:9:CYS:SG	1:A:11:PRO:HD3	2.62	0.40
1:C:10:ASP:OD1	1:C:10:ASP:N	2.54	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	310/314 (99%)	281 (91%)	24 (8%)	5 (2%)	9	17
1	B	310/314 (99%)	282 (91%)	22 (7%)	6 (2%)	8	13
1	C	310/314 (99%)	282 (91%)	23 (7%)	5 (2%)	9	17
1	D	310/314 (99%)	284 (92%)	21 (7%)	5 (2%)	9	17
All	All	1240/1256 (99%)	1129 (91%)	90 (7%)	21 (2%)	9	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	TYR
1	B	280	TYR
1	C	280	TYR
1	D	280	TYR
1	A	11	PRO
1	B	80	HIS
1	C	80	HIS
1	D	80	HIS

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Mol	Chain	Res	Type
1	A	78	ALA
1	A	80	HIS
1	B	11	PRO
1	B	82	HIS
1	C	11	PRO
1	D	11	PRO
1	D	82	HIS
1	B	78	ALA
1	B	194	THR
1	C	82	HIS
1	D	78	ALA
1	A	82	HIS
1	C	78	ALA

### 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	248/263 (94%)	204 (82%)	44 (18%)	2	3
1	B	248/263 (94%)	204 (82%)	44 (18%)	2	3
1	C	248/263 (94%)	210 (85%)	38 (15%)	2	5
1	D	248/263 (94%)	207 (84%)	41 (16%)	2	4
All	All	992/1052 (94%)	825 (83%)	167 (17%)	2	4

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	13	ILE
1	A	35	THR
1	A	39	ASN
1	A	44	LYS
1	A	45	VAL
1	A	52	VAL
1	A	89	ASN

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Mol	Chain	Res	Type
1	A	95	GLU
1	A	99	LYS
1	A	103	ARG
1	A	125	PRO
1	A	130	THR
1	A	139	GLU
1	A	141	ARG
1	A	143	VAL
1	A	147	LYS
1	A	152	MET
1	A	158	THR
1	A	162	SER
1	A	171	ILE
1	A	184	TRP
1	A	192	ASP
1	A	195	HIS
1	A	196	LEU
1	A	204	GLN
1	A	205	LYS
1	A	206	ARG
1	A	208	ARG
1	A	209	GLU
1	A	227	LYS
1	A	235	THR
1	A	238	LYS
1	A	241	ASP
1	A	258	ARG
1	A	266	ASN
1	A	280	TYR
1	A	284	LYS
1	A	287	ARG
1	A	293	LYS
1	A	294	LEU
1	A	298	LYS
1	A	309	ARG
1	A	312	ASP
1	B	13	ILE
1	B	27	GLU
1	B	35	THR
1	B	39	ASN
1	B	40	GLN
1	B	44	LYS

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Mol	Chain	Res	Type
1	B	52	VAL
1	B	89	ASN
1	B	95	GLU
1	B	99	LYS
1	B	103	ARG
1	B	130	THR
1	B	139	GLU
1	B	141	ARG
1	B	143	VAL
1	B	147	LYS
1	B	152	MET
1	B	158	THR
1	B	162	SER
1	B	171	ILE
1	B	184	TRP
1	B	192	ASP
1	B	195	HIS
1	B	196	LEU
1	B	204	GLN
1	B	205	LYS
1	B	206	ARG
1	B	208	ARG
1	B	209	GLU
1	B	213	LYS
1	B	227	LYS
1	B	235	THR
1	B	238	LYS
1	B	241	ASP
1	B	258	ARG
1	B	266	ASN
1	B	280	TYR
1	B	284	LYS
1	B	287	ARG
1	B	293	LYS
1	B	294	LEU
1	B	298	LYS
1	B	309	ARG
1	B	312	ASP
1	C	13	ILE
1	C	27	GLU
1	C	35	THR
1	C	39	ASN

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Mol	Chain	Res	Type
1	C	44	LYS
1	C	52	VAL
1	C	89	ASN
1	C	95	GLU
1	C	99	LYS
1	C	103	ARG
1	C	130	THR
1	C	139	GLU
1	C	143	VAL
1	C	147	LYS
1	C	152	MET
1	C	158	THR
1	C	162	SER
1	C	171	ILE
1	C	184	TRP
1	C	192	ASP
1	C	195	HIS
1	C	196	LEU
1	C	204	GLN
1	C	205	LYS
1	C	206	ARG
1	C	209	GLU
1	C	213	LYS
1	C	227	LYS
1	C	235	THR
1	C	238	LYS
1	C	258	ARG
1	C	266	ASN
1	C	280	TYR
1	C	284	LYS
1	C	287	ARG
1	C	293	LYS
1	C	298	LYS
1	C	312	ASP
1	D	13	ILE
1	D	27	GLU
1	D	35	THR
1	D	39	ASN
1	D	44	LYS
1	D	52	VAL
1	D	89	ASN
1	D	91	SER

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Mol	Chain	Res	Type
1	D	95	GLU
1	D	99	LYS
1	D	103	ARG
1	D	130	THR
1	D	139	GLU
1	D	141	ARG
1	D	143	VAL
1	D	147	LYS
1	D	152	MET
1	D	158	THR
1	D	162	SER
1	D	171	ILE
1	D	184	TRP
1	D	192	ASP
1	D	195	HIS
1	D	196	LEU
1	D	204	GLN
1	D	205	LYS
1	D	206	ARG
1	D	208	ARG
1	D	209	GLU
1	D	213	LYS
1	D	227	LYS
1	D	235	THR
1	D	238	LYS
1	D	258	ARG
1	D	266	ASN
1	D	280	TYR
1	D	284	LYS
1	D	287	ARG
1	D	293	LYS
1	D	298	LYS
1	D	312	ASP

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

Mol	Chain	Res	Type
1	A	40	GLN
1	A	157	HIS
1	A	177	HIS
1	A	181	ASN
1	A	240	HIS

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Mol	Chain	Res	Type
1	A	266	ASN
1	B	116	HIS
1	B	157	HIS
1	B	220	GLN
1	B	240	HIS
1	B	266	ASN
1	C	157	HIS
1	C	220	GLN
1	C	240	HIS
1	C	266	ASN
1	D	157	HIS
1	D	220	GLN
1	D	240	HIS
1	D	266	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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.