



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:43 pm GMT

PDB ID : 2CG8  
Title : THE BIFUNCTIONAL DIHYDRONEOPTERIN ALDOLASE 6-HYDROXY  
METHYL-7,8-DIHYDROPTERIN SYNTHASE FROM STREPTOCOCCUS  
PNEUMONIAE  
Authors : Garcon, A.; Levy, C.; Derrick, J.P.  
Deposited on : 2006-02-28  
Resolution : 2.90 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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

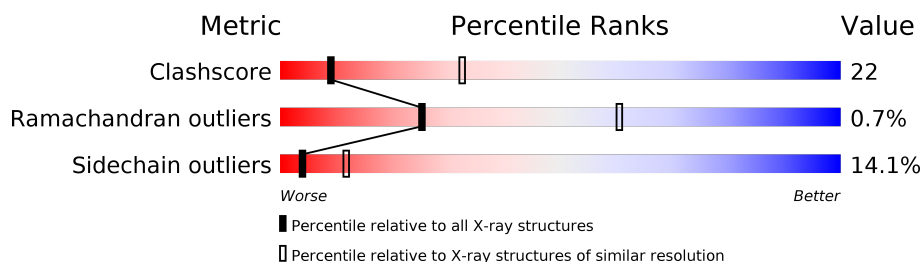
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.



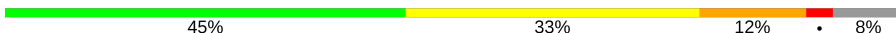

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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	270	
1	B	270	
1	C	270	
1	D	270	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7968 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 DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE.

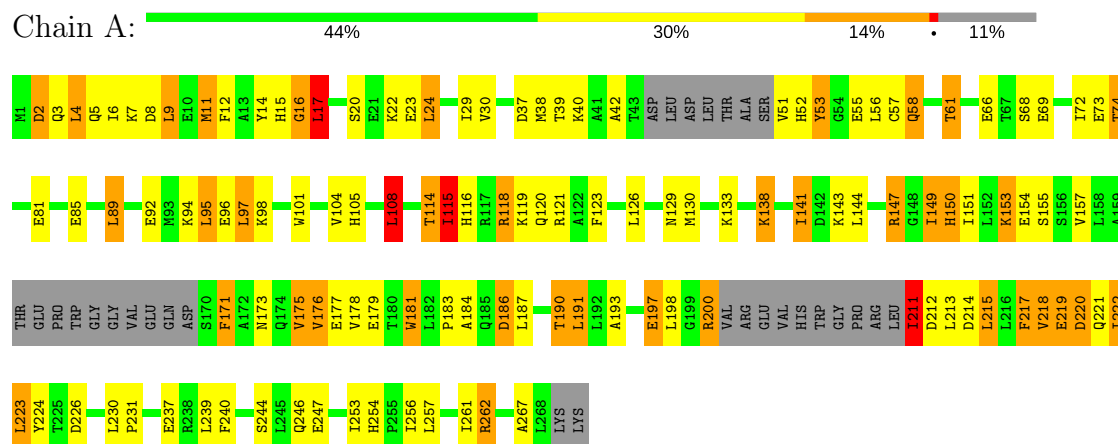
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	1
			1953	1263	321	362	7			
1	B	248	Total	C	N	O	S	0	0	1
			2006	1293	331	375	7			
1	C	249	Total	C	N	O	S	0	0	1
			2011	1299	329	376	7			
1	D	248	Total	C	N	O	S	0	0	2
			1998	1289	331	371	7			

### 3 Residue-property plots

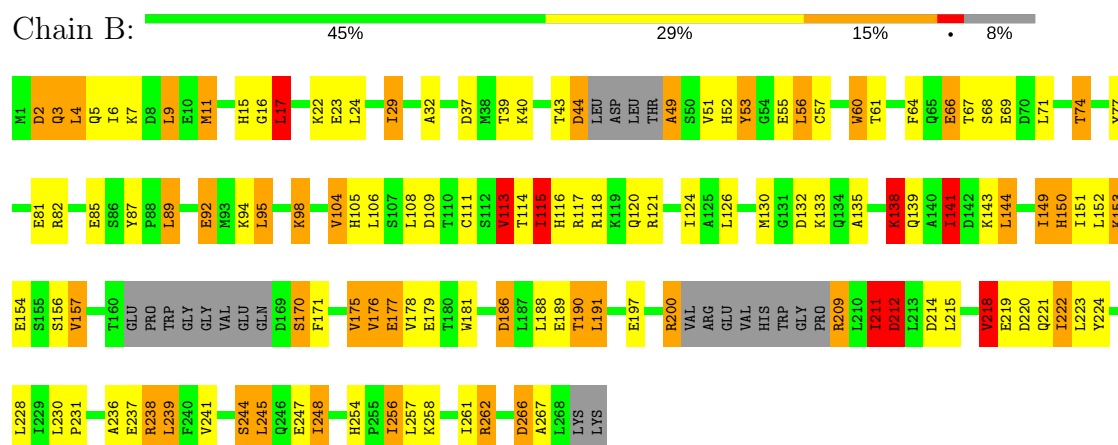
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE

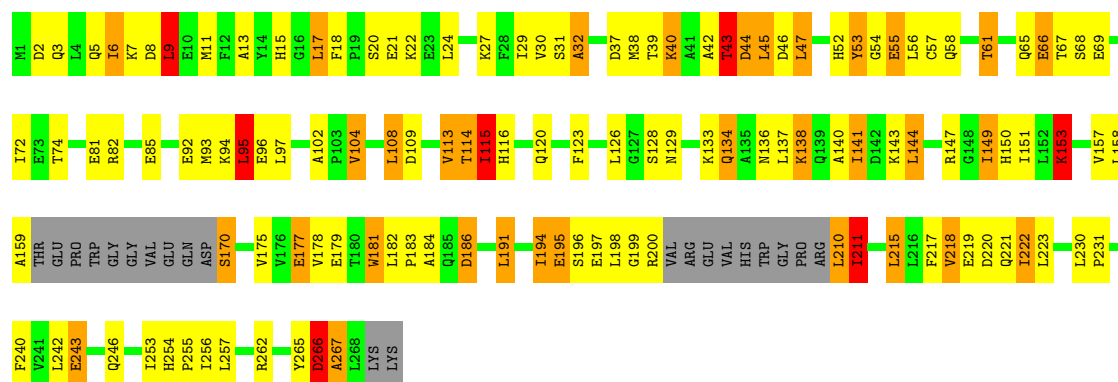


#### • Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE



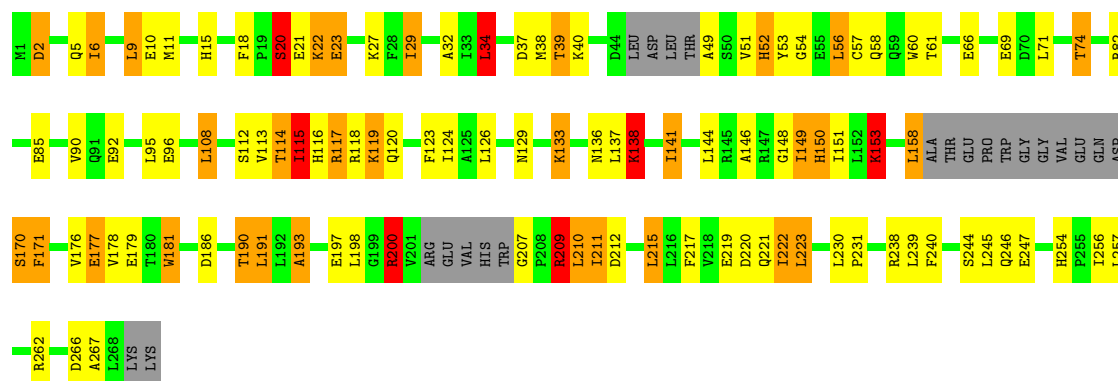
#### • Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE





• Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE

Chain D: 52% 26% 11% 8%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.44Å 149.44Å 238.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.8 (127.00-2.90)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.215 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.83	46/1993 (2.3%)	1.65	43/2700 (1.6%)
1	B	1.92	55/2046 (2.7%)	1.63	40/2772 (1.4%)
1	C	1.71	35/2052 (1.7%)	1.53	28/2783 (1.0%)
1	D	1.76	36/2039 (1.8%)	1.54	25/2763 (0.9%)
All	All	1.81	172/8130 (2.1%)	1.59	136/11018 (1.2%)

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	B	0	1
1	D	0	1
All	All	0	2

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	TRP	CG-CD1	11.50	1.52	1.36
1	A	181	TRP	CG-CD1	11.42	1.52	1.36
1	A	219	GLU	CD-OE2	11.05	1.37	1.25
1	D	153	LYS	CD-CE	10.99	1.78	1.51
1	C	55	GLU	CD-OE2	10.94	1.37	1.25
1	D	181	TRP	CD2-CE2	10.51	1.53	1.41
1	D	219	GLU	CD-OE1	10.50	1.37	1.25
1	B	181	TRP	CD2-CE2	10.36	1.53	1.41
1	C	153	LYS	CD-CE	10.31	1.77	1.51
1	D	219	GLU	CD-OE2	10.08	1.36	1.25
1	A	240	PHE	CD1-CE1	9.86	1.58	1.39
1	A	181	TRP	CD2-CE2	9.69	1.52	1.41
1	D	181	TRP	CG-CD1	9.54	1.50	1.36
1	B	66	GLU	CD-OE1	9.15	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	20	SER	CB-OG	8.86	1.53	1.42
1	A	153	LYS	CD-CE	8.74	1.73	1.51
1	A	153	LYS	CG-CD	8.65	1.81	1.52
1	B	138	LYS	CE-NZ	8.61	1.70	1.49
1	C	55	GLU	CD-OE1	8.33	1.34	1.25
1	B	179	GLU	CD-OE1	8.20	1.34	1.25
1	B	85	GLU	CG-CD	8.18	1.64	1.51
1	B	153	LYS	CG-CD	8.16	1.80	1.52
1	B	219	GLU	CD-OE2	8.13	1.34	1.25
1	D	22	LYS	CD-CE	8.12	1.71	1.51
1	A	218	VAL	CB-CG1	-8.10	1.35	1.52
1	B	55	GLU	CG-CD	8.10	1.64	1.51
1	B	181	TRP	CZ3-CH2	8.02	1.52	1.40
1	C	181	TRP	CD2-CE2	7.95	1.50	1.41
1	B	209	ARG	N-CA	7.86	1.62	1.46
1	D	153	LYS	CE-NZ	7.84	1.68	1.49
1	C	53	TYR	CD1-CE1	-7.78	1.27	1.39
1	D	85	GLU	CG-CD	7.78	1.63	1.51
1	A	85	GLU	CG-CD	7.62	1.63	1.51
1	B	181	TRP	CG-CD1	7.48	1.47	1.36
1	A	240	PHE	CD2-CE2	7.47	1.54	1.39
1	B	176	VAL	CB-CG1	-7.44	1.37	1.52
1	C	159	ALA	C-O	7.42	1.37	1.23
1	D	179	GLU	CB-CG	-7.34	1.38	1.52
1	D	181	TRP	CG-CD2	-7.33	1.31	1.43
1	A	17	LEU	CG-CD1	7.30	1.78	1.51
1	D	23	GLU	CD-OE2	7.29	1.33	1.25
1	D	85	GLU	CD-OE1	7.24	1.33	1.25
1	B	156	SER	CB-OG	-7.22	1.32	1.42
1	D	181	TRP	CZ3-CH2	7.19	1.51	1.40
1	D	49	ALA	CA-CB	7.17	1.67	1.52
1	B	179	GLU	CD-OE2	7.14	1.33	1.25
1	B	209	ARG	CZ-NH2	7.11	1.42	1.33
1	A	219	GLU	CD-OE1	7.05	1.33	1.25
1	A	171	PHE	CE2-CZ	7.04	1.50	1.37
1	C	219	GLU	CD-OE1	7.02	1.33	1.25
1	C	40	LYS	CE-NZ	6.98	1.66	1.49
1	B	153	LYS	CD-CE	6.97	1.68	1.51
1	C	179	GLU	CB-CG	-6.91	1.39	1.52
1	D	179	GLU	CD-OE2	6.91	1.33	1.25
1	D	113	VAL	CB-CG1	-6.90	1.38	1.52
1	C	66	GLU	CD-OE1	6.89	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	GLU	CD-OE2	6.86	1.33	1.25
1	A	181	TRP	CZ3-CH2	6.82	1.50	1.40
1	B	104	VAL	CB-CG1	-6.71	1.38	1.52
1	A	176	VAL	CB-CG1	-6.65	1.38	1.52
1	C	195	GLU	CG-CD	6.58	1.61	1.51
1	B	81	GLU	CB-CG	-6.56	1.39	1.52
1	B	197	GLU	CD-OE1	6.55	1.32	1.25
1	B	138	LYS	CD-CE	6.54	1.67	1.51
1	D	209	ARG	CB-CG	-6.50	1.35	1.52
1	B	247	GLU	CD-OE1	6.46	1.32	1.25
1	B	32	ALA	CA-CB	-6.43	1.39	1.52
1	B	237	GLU	CD-OE1	6.42	1.32	1.25
1	C	113	VAL	CB-CG1	-6.40	1.39	1.52
1	C	194	ILE	CA-CB	-6.38	1.40	1.54
1	D	247	GLU	CD-OE1	6.38	1.32	1.25
1	A	171	PHE	CG-CD1	6.38	1.48	1.38
1	C	55	GLU	CG-CD	6.37	1.61	1.51
1	C	153	LYS	CG-CD	6.36	1.74	1.52
1	B	219	GLU	CD-OE1	6.34	1.32	1.25
1	C	104	VAL	CB-CG1	-6.32	1.39	1.52
1	A	237	GLU	CD-OE2	6.32	1.32	1.25
1	C	32	ALA	CA-CB	-6.30	1.39	1.52
1	B	267	ALA	CA-C	6.29	1.69	1.52
1	A	53	TYR	CD2-CE2	-6.27	1.29	1.39
1	B	53	TYR	CD2-CE2	-6.26	1.29	1.39
1	A	58	GLN	CG-CD	6.26	1.65	1.51
1	A	247	GLU	CD-OE1	6.25	1.32	1.25
1	A	224	TYR	CE1-CZ	-6.24	1.30	1.38
1	C	218	VAL	CB-CG1	-6.18	1.39	1.52
1	A	81	GLU	CB-CG	-6.17	1.40	1.52
1	B	154	GLU	CB-CG	-6.13	1.40	1.52
1	B	153	LYS	CE-NZ	6.09	1.64	1.49
1	B	113	VAL	CB-CG1	-6.07	1.40	1.52
1	C	243	GLU	CB-CG	6.04	1.63	1.52
1	C	181	TRP	CG-CD2	-6.03	1.33	1.43
1	C	94	LYS	CD-CE	6.01	1.66	1.51
1	C	85	GLU	CD-OE2	6.00	1.32	1.25
1	B	237	GLU	CD-OE2	5.98	1.32	1.25
1	B	157	VAL	CB-CG1	-5.98	1.40	1.52
1	A	104	VAL	CB-CG1	-5.97	1.40	1.52
1	B	44	ASP	C-O	5.96	1.34	1.23
1	A	197	GLU	CB-CG	-5.94	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	60	TRP	CB-CG	-5.92	1.39	1.50
1	C	13	ALA	CA-CB	-5.88	1.40	1.52
1	A	94	LYS	CE-NZ	5.88	1.63	1.49
1	D	207	GLY	N-CA	5.87	1.54	1.46
1	A	154	GLU	C-O	-5.86	1.12	1.23
1	A	181	TRP	CG-CD2	-5.86	1.33	1.43
1	B	218	VAL	CB-CG1	-5.85	1.40	1.52
1	D	23	GLU	CD-OE1	5.85	1.32	1.25
1	C	81	GLU	CB-CG	-5.83	1.41	1.52
1	C	219	GLU	CD-OE2	5.81	1.32	1.25
1	B	60	TRP	CB-CG	-5.79	1.39	1.50
1	A	171	PHE	CD1-CE1	5.79	1.50	1.39
1	B	23	GLU	CD-OE2	5.77	1.31	1.25
1	A	16	GLY	C-O	5.74	1.32	1.23
1	C	53	TYR	CB-CG	-5.73	1.43	1.51
1	B	17	LEU	N-CA	5.72	1.57	1.46
1	B	171	PHE	CE2-CZ	5.71	1.48	1.37
1	B	94	LYS	CB-CG	-5.71	1.37	1.52
1	D	138	LYS	CD-CE	5.70	1.65	1.51
1	A	179	GLU	CB-CG	-5.68	1.41	1.52
1	A	55	GLU	CD-OE2	5.65	1.31	1.25
1	B	53	TYR	CD1-CE1	-5.64	1.30	1.39
1	B	87	TYR	CD2-CE2	5.64	1.47	1.39
1	A	133	LYS	CE-NZ	5.64	1.63	1.49
1	D	112	SER	CB-OG	5.60	1.49	1.42
1	B	224	TYR	CE1-CZ	-5.58	1.31	1.38
1	A	55	GLU	CD-OE1	5.57	1.31	1.25
1	A	217	PHE	CB-CG	-5.54	1.42	1.51
1	D	181	TRP	CE2-CZ2	-5.54	1.30	1.39
1	A	12	PHE	CD1-CE1	5.53	1.50	1.39
1	D	66	GLU	CB-CG	-5.52	1.41	1.52
1	B	77	TYR	CE1-CZ	-5.46	1.31	1.38
1	C	85	GLU	CG-CD	5.45	1.60	1.51
1	B	189	GLU	CD-OE2	5.45	1.31	1.25
1	A	53	TYR	CG-CD2	-5.45	1.32	1.39
1	C	153	LYS	CE-NZ	5.44	1.62	1.49
1	D	176	VAL	CB-CG1	-5.42	1.41	1.52
1	B	115	ILE	CB-CG1	-5.41	1.38	1.54
1	B	258	LYS	CD-CE	5.41	1.64	1.51
1	D	51	VAL	CB-CG2	5.40	1.64	1.52
1	B	223	LEU	CG-CD2	5.37	1.71	1.51
1	D	240	PHE	CE1-CZ	5.37	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	240	PHE	CG-CD2	5.36	1.46	1.38
1	D	58	GLN	CG-CD	5.36	1.63	1.51
1	B	17	LEU	CG-CD1	5.31	1.71	1.51
1	B	267	ALA	CA-CB	-5.29	1.41	1.52
1	A	108	LEU	C-O	-5.27	1.13	1.23
1	D	85	GLU	CD-OE2	5.26	1.31	1.25
1	A	30	VAL	CB-CG2	-5.26	1.41	1.52
1	B	92	GLU	CG-CD	5.26	1.59	1.51
1	A	223	LEU	CG-CD2	5.24	1.71	1.51
1	C	267	ALA	N-CA	5.20	1.56	1.46
1	A	53	TYR	CG-CD1	5.19	1.46	1.39
1	C	115	ILE	CA-CB	5.19	1.66	1.54
1	D	119	LYS	CD-CE	5.18	1.64	1.51
1	A	73	GLU	CD-OE1	5.18	1.31	1.25
1	B	89	LEU	CG-CD1	5.16	1.71	1.51
1	D	133	LYS	CD-CE	5.16	1.64	1.51
1	C	40	LYS	CD-CE	5.15	1.64	1.51
1	B	49	ALA	CA-CB	5.14	1.63	1.52
1	C	184	ALA	CA-CB	-5.14	1.41	1.52
1	A	23	GLU	CD-OE2	5.13	1.31	1.25
1	D	22	LYS	CE-NZ	5.12	1.61	1.49
1	A	141	ILE	CG1-CD1	5.12	1.85	1.50
1	A	89	LEU	CG-CD2	5.11	1.70	1.51
1	B	236	ALA	C-O	-5.11	1.13	1.23
1	B	197	GLU	CD-OE2	5.10	1.31	1.25
1	B	141	ILE	CG1-CD1	5.09	1.85	1.50
1	C	53	TYR	CD2-CE2	-5.05	1.31	1.39
1	C	219	GLU	CG-CD	5.04	1.59	1.51
1	A	85	GLU	CD-OE2	5.03	1.31	1.25
1	A	66	GLU	CD-OE1	5.03	1.31	1.25
1	D	193	ALA	CA-CB	-5.01	1.42	1.52
1	A	51	VAL	N-CA	5.00	1.56	1.46

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	NE-CZ-NH2	12.34	126.47	120.30
1	A	2	ASP	CB-CG-OD1	-10.10	109.21	118.30
1	A	220	ASP	CB-CG-OD2	9.90	127.21	118.30
1	D	71	LEU	CB-CG-CD2	-9.81	94.33	111.00
1	B	209	ARG	NE-CZ-NH1	-9.71	115.44	120.30
1	B	29	ILE	CG1-CB-CG2	-9.65	90.17	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ASP	CB-CG-OD2	9.41	126.77	118.30
1	A	11	MET	CA-CB-CG	-9.14	97.76	113.30
1	A	220	ASP	CB-CG-OD1	-9.09	110.12	118.30
1	A	147	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	D	29	ILE	CG1-CB-CG2	-8.54	92.62	111.40
1	B	267	ALA	O-C-N	-8.48	109.12	122.70
1	D	220	ASP	CB-CG-OD1	-8.47	110.67	118.30
1	A	4	LEU	CB-CG-CD2	-8.22	97.03	111.00
1	C	94	LYS	CD-CE-NZ	-8.17	92.91	111.70
1	D	266	ASP	CB-CG-OD2	8.08	125.57	118.30
1	B	6	ILE	CG1-CB-CG2	-8.07	93.64	111.40
1	A	211	ILE	CB-CA-C	-8.02	95.56	111.60
1	B	176	VAL	CG1-CB-CG2	-8.01	98.08	110.90
1	C	22	LYS	CD-CE-NZ	-7.98	93.35	111.70
1	B	238	ARG	NE-CZ-NH1	-7.97	116.32	120.30
1	D	220	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	226	ASP	CB-CG-OD1	-7.82	111.26	118.30
1	C	53	TYR	CB-CA-C	-7.81	94.77	110.40
1	B	220	ASP	N-CA-CB	-7.76	96.63	110.60
1	A	98	LYS	CD-CE-NZ	-7.59	94.23	111.70
1	A	176	VAL	CG1-CB-CG2	-7.55	98.83	110.90
1	D	2	ASP	CB-CG-OD1	-7.52	111.53	118.30
1	B	223	LEU	CB-CG-CD2	7.44	123.65	111.00
1	D	82	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	121	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	186	ASP	CB-CG-OD2	7.07	124.66	118.30
1	C	220	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	104	VAL	C-N-CA	-6.97	104.27	121.70
1	A	29	ILE	CG1-CB-CG2	-6.90	96.22	111.40
1	B	256	ILE	CA-CB-CG1	-6.90	97.89	111.00
1	A	6	ILE	CG1-CB-CG2	-6.86	96.32	111.40
1	A	118	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	D	133	LYS	CD-CE-NZ	-6.71	96.26	111.70
1	A	53	TYR	CD1-CE1-CZ	-6.71	113.77	119.80
1	C	182	LEU	CB-CG-CD1	-6.64	99.71	111.00
1	A	186	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	A	223	LEU	CB-CG-CD2	6.56	122.15	111.00
1	A	212	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	121	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	267	ALA	O-C-N	-6.52	112.27	122.70
1	C	61	THR	CA-CB-CG2	-6.39	103.46	112.40
1	C	115	ILE	CA-CB-CG2	6.38	123.65	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	C	177	GLU	OE1-CD-OE2	-6.33	115.71	123.30
1	C	266	ASP	CB-CG-OD2	6.32	123.99	118.30
1	D	181	TRP	CD1-NE1-CE2	-6.30	103.33	109.00
1	C	262	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	D	118	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	109	ASP	CB-CG-OD2	6.23	123.90	118.30
1	B	51	VAL	CG1-CB-CG2	6.22	120.85	110.90
1	C	210	LEU	CB-CG-CD2	-6.19	100.47	111.00
1	B	4	LEU	CB-CG-CD1	-6.18	100.49	111.00
1	A	24	LEU	CB-CA-C	-6.15	98.51	110.20
1	B	98	LYS	CD-CE-NZ	-6.15	97.56	111.70
1	C	47	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	B	245	LEU	CB-CG-CD1	6.09	121.35	111.00
1	A	95	LEU	CA-CB-CG	6.07	129.27	115.30
1	C	6	ILE	CG1-CB-CG2	-6.06	98.07	111.40
1	B	104	VAL	C-N-CA	-6.04	106.59	121.70
1	C	95	LEU	CA-CB-CG	6.04	129.20	115.30
1	B	186	ASP	CB-CG-OD2	6.04	123.73	118.30
1	D	6	ILE	CG1-CB-CG2	-6.01	98.18	111.40
1	B	2	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	A	8	ASP	CB-CG-OD1	5.94	123.64	118.30
1	B	220	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	104	VAL	C-N-CA	-5.93	106.88	121.70
1	D	219	GLU	OE1-CD-OE2	5.90	130.38	123.30
1	A	119	LYS	CD-CE-NZ	-5.90	98.13	111.70
1	B	209	ARG	N-CA-C	5.89	126.92	111.00
1	D	200	ARG	CA-C-N	5.86	130.10	117.20
1	B	212	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	219	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	B	11	MET	CA-CB-CG	-5.82	103.41	113.30
1	C	44	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	97	LEU	CB-CG-CD1	-5.79	101.15	111.00
1	C	211	ILE	CB-CA-C	-5.77	100.06	111.60
1	C	82	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	118	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	D	222	ILE	CG1-CB-CG2	-5.72	98.81	111.40
1	B	115	ILE	CA-CB-CG2	5.72	122.34	110.90
1	B	68	SER	CB-CA-C	-5.71	99.25	110.10
1	B	177	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	B	214	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	266	ASP	CB-CG-OD1	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	A	68	SER	CB-CA-C	-5.61	99.44	110.10
1	D	245	LEU	CB-CG-CD2	-5.57	101.54	111.00
1	A	53	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	D	262	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	141	ILE	CB-CG1-CD1	5.50	129.31	113.90
1	B	248	ILE	CG1-CB-CG2	-5.47	99.36	111.40
1	B	82	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	74	THR	CA-CB-CG2	5.46	120.05	112.40
1	A	226	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	115	ILE	CA-CB-CG2	5.38	121.66	110.90
1	B	170	SER	N-CA-C	5.34	125.43	111.00
1	A	214	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	210	LEU	CB-CA-C	-5.33	100.08	110.20
1	D	119	LYS	CG-CD-CE	-5.30	95.99	111.90
1	A	2	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	82	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	24	LEU	CB-CA-C	-5.29	100.14	110.20
1	B	115	ILE	CG1-CB-CG2	-5.27	99.80	111.40
1	B	211	ILE	CG1-CB-CG2	5.26	122.96	111.40
1	A	215	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	D	34	LEU	CB-CG-CD2	-5.22	102.13	111.00
1	B	154	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	C	43	THR	CA-CB-CG2	5.18	119.65	112.40
1	A	61	THR	OG1-CB-CG2	-5.17	98.10	110.00
1	C	9	LEU	CB-CG-CD2	5.16	119.77	111.00
1	C	223	LEU	CB-CA-C	-5.15	100.42	110.20
1	A	218	VAL	CA-CB-CG1	-5.14	103.18	110.90
1	D	141	ILE	CB-CG1-CD1	5.14	128.30	113.90
1	A	181	TRP	CD1-NE1-CE2	-5.14	104.38	109.00
1	B	267	ALA	N-CA-C	5.13	124.86	111.00
1	D	115	ILE	CA-CB-CG2	5.12	121.14	110.90
1	C	108	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	D	238	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	66	GLU	CB-CA-C	-5.10	100.19	110.40
1	A	211	ILE	N-CA-C	5.10	124.77	111.00
1	B	17	LEU	N-CA-CB	5.10	120.60	110.40
1	D	220	ASP	N-CA-CB	-5.10	101.42	110.60
1	C	66	GLU	CB-CA-C	-5.10	100.21	110.40
1	C	68	SER	CB-CA-C	-5.09	100.43	110.10
1	C	223	LEU	CB-CG-CD2	5.07	119.62	111.00
1	A	52	HIS	CB-CA-C	-5.07	100.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ILE	CG1-CB-CG2	5.07	122.55	111.40
1	B	138	LYS	CD-CE-NZ	5.03	123.28	111.70
1	C	181	TRP	CD1-NE1-CE2	-5.03	104.47	109.00
1	B	211	ILE	CB-CA-C	-5.02	101.55	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	266	ASP	Peptide
1	D	223	LEU	Peptide

## 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	1953	0	1967	94	0
1	B	2006	0	2016	87	0
1	C	2011	0	2026	107	0
1	D	1998	0	2010	88	0
All	All	7968	0	8019	357	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 22.

All (357) 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:C:153:LYS:CE	1:C:153:LYS:CD	1.77	1.62
1:A:153:LYS:CD	1:A:153:LYS:CG	1.81	1.58
1:A:17:LEU:CG	1:A:17:LEU:CD1	1.78	1.58
1:D:141:ILE:CD1	1:D:141:ILE:CG1	1.81	1.56
1:D:153:LYS:CD	1:D:153:LYS:CE	1.78	1.56
1:D:153:LYS:CE	1:D:153:LYS:NZ	1.68	1.55
1:B:153:LYS:CD	1:B:153:LYS:CG	1.80	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:CG1	1:B:141:ILE:CD1	1.85	1.52
1:B:138:LYS:NZ	1:B:138:LYS:CE	1.70	1.51
1:A:141:ILE:CG1	1:A:141:ILE:CD1	1.85	1.49
1:D:37:ASP:OD1	1:D:39:THR:HG22	1.38	1.21
1:D:149:ILE:HD12	1:D:149:ILE:C	1.56	1.20
1:D:211:ILE:HD12	1:D:211:ILE:H	1.12	1.11
1:A:37:ASP:OD1	1:A:39:THR:HG22	1.48	1.11
1:D:211:ILE:N	1:D:211:ILE:HD12	1.65	1.04
1:D:15:HIS:HD2	1:D:69:GLU:H	1.08	0.97
1:D:129:ASN:HA	1:D:133:LYS:HD3	1.46	0.97
1:C:123:PHE:CE1	1:C:177:GLU:HG3	1.99	0.96
1:B:149:ILE:C	1:B:149:ILE:HD12	1.87	0.95
1:B:108:LEU:HD11	1:B:111:CYS:SG	2.07	0.94
1:C:37:ASP:OD1	1:C:39:THR:HG22	1.68	0.94
1:D:115:ILE:C	1:D:115:ILE:HD12	1.88	0.93
1:B:4:LEU:HD11	1:B:53:TYR:HE2	1.34	0.92
1:D:120:GLN:HE21	1:D:221:GLN:HE22	1.10	0.91
1:A:120:GLN:HE21	1:A:221:GLN:HE22	1.10	0.91
1:D:149:ILE:HD12	1:D:150:HIS:N	1.87	0.90
1:B:15:HIS:HD2	1:B:69:GLU:H	1.19	0.90
1:D:37:ASP:OD1	1:D:39:THR:CG2	2.19	0.89
1:A:149:ILE:HD12	1:A:149:ILE:C	1.92	0.89
1:C:115:ILE:HD12	1:C:115:ILE:C	1.93	0.89
1:D:149:ILE:CD1	1:D:149:ILE:C	2.41	0.88
1:C:15:HIS:HD2	1:C:69:GLU:H	1.20	0.88
1:D:18:PHE:HB2	1:D:21:GLU:HG3	1.53	0.88
1:A:171:PHE:CD1	1:A:173:ASN:ND2	2.43	0.87
1:B:138:LYS:NZ	1:B:138:LYS:HB3	1.89	0.86
1:B:222:ILE:HD12	1:B:256:ILE:HD11	1.56	0.86
1:B:149:ILE:HD12	1:B:150:HIS:N	1.92	0.84
1:C:39:THR:HG21	1:D:186:ASP:OD2	1.78	0.84
1:D:15:HIS:CD2	1:D:69:GLU:H	1.96	0.83
1:A:37:ASP:OD1	1:A:39:THR:CG2	2.27	0.82
1:A:15:HIS:HD2	1:A:69:GLU:H	1.27	0.82
1:B:37:ASP:OD1	1:B:39:THR:HG22	1.79	0.82
1:C:253:ILE:HD13	1:D:256:ILE:HD13	1.60	0.81
1:A:42:ALA:O	1:B:74:THR:HB	1.80	0.81
1:C:42:ALA:O	1:D:74:THR:HB	1.80	0.81
1:C:120:GLN:HE21	1:C:221:GLN:HE22	1.28	0.81
1:C:9:LEU:HD13	1:C:11:MET:CE	2.10	0.81
1:A:9:LEU:HD13	1:A:11:MET:CE	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HD13	1:B:11:MET:CE	2.11	0.80
1:B:15:HIS:CD2	1:B:69:GLU:H	2.01	0.79
1:C:57:CYS:O	1:C:61:THR:HG22	1.83	0.79
1:C:9:LEU:HD13	1:C:11:MET:HE3	1.65	0.79
1:C:198:LEU:HD12	1:C:211:ILE:HG12	1.64	0.78
1:D:108:LEU:N	1:D:108:LEU:HD23	2.01	0.76
1:B:108:LEU:CD1	1:B:111:CYS:SG	2.72	0.76
1:A:171:PHE:CE1	1:A:173:ASN:ND2	2.53	0.76
1:A:254:HIS:HD2	1:A:256:ILE:H	1.32	0.76
1:D:223:LEU:HG	1:D:230:LEU:HD12	1.66	0.76
1:A:15:HIS:CD2	1:A:69:GLU:H	2.06	0.74
1:B:120:GLN:HE21	1:B:221:GLN:HE22	1.35	0.74
1:A:222:ILE:HD12	1:A:256:ILE:HD11	1.70	0.73
1:D:92:GLU:OE1	1:D:116:HIS:HE1	1.71	0.73
1:D:108:LEU:H	1:D:108:LEU:HD23	1.55	0.72
1:D:138:LYS:NZ	1:D:138:LYS:HB3	2.04	0.71
1:A:126:LEU:HD12	1:A:126:LEU:N	2.05	0.71
1:D:209:ARG:O	1:D:210:LEU:HB2	1.88	0.71
1:D:34:LEU:N	1:D:34:LEU:HD23	2.05	0.71
1:D:9:LEU:HD13	1:D:11:MET:CE	2.21	0.70
1:B:186:ASP:O	1:B:190:THR:HG23	1.91	0.70
1:C:18:PHE:HB2	1:C:21:GLU:HG3	1.74	0.70
1:D:198:LEU:O	1:D:210:LEU:HD13	1.92	0.69
1:B:9:LEU:HD13	1:B:11:MET:HE3	1.73	0.69
1:A:39:THR:HG21	1:B:186:ASP:OD2	1.92	0.69
1:C:15:HIS:CD2	1:C:69:GLU:H	2.08	0.69
1:A:17:LEU:CD1	1:A:17:LEU:CD2	2.69	0.68
1:B:4:LEU:HD11	1:B:53:TYR:CE2	2.24	0.68
1:A:120:GLN:NE2	1:A:221:GLN:HE22	1.88	0.68
1:C:198:LEU:CD1	1:C:211:ILE:HG12	2.24	0.68
1:D:211:ILE:N	1:D:211:ILE:CD1	2.47	0.68
1:D:120:GLN:NE2	1:D:221:GLN:HE22	1.90	0.67
1:C:254:HIS:HD2	1:C:257:LEU:H	1.43	0.67
1:C:149:ILE:CD1	1:C:178:VAL:HB	2.24	0.67
1:D:129:ASN:HB3	1:D:171:PHE:CD2	2.29	0.66
1:B:126:LEU:N	1:B:126:LEU:HD12	2.10	0.66
1:C:128:SER:HB2	1:C:210:LEU:O	1.95	0.66
1:A:15:HIS:HD2	1:A:69:GLU:N	1.94	0.66
1:C:92:GLU:OE1	1:C:116:HIS:HE1	1.79	0.65
1:C:15:HIS:HD2	1:C:69:GLU:N	1.94	0.65
1:B:16:GLY:O	1:B:22:LYS:HE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG21	1:D:186:ASP:CG	2.18	0.65
1:C:108:LEU:N	1:C:108:LEU:HD23	2.12	0.64
1:C:231:PRO:HD2	1:C:256:ILE:HD12	1.80	0.64
1:C:39:THR:HB	1:D:117:ARG:NH2	2.13	0.64
1:B:15:HIS:HD2	1:B:69:GLU:N	1.94	0.64
1:D:129:ASN:HB2	1:D:170:SER:O	1.97	0.64
1:C:253:ILE:HD13	1:D:256:ILE:CD1	2.28	0.63
1:C:196:SER:C	1:C:198:LEU:H	2.02	0.63
1:C:37:ASP:OD1	1:C:39:THR:CG2	2.46	0.63
1:A:9:LEU:HD13	1:A:11:MET:HE3	1.79	0.62
1:C:57:CYS:O	1:C:61:THR:CG2	2.48	0.62
1:D:209:ARG:O	1:D:210:LEU:CB	2.47	0.62
1:B:9:LEU:HD13	1:B:11:MET:HE2	1.82	0.61
1:D:115:ILE:HD12	1:D:116:HIS:N	2.14	0.61
1:C:128:SER:CB	1:C:210:LEU:O	2.48	0.61
1:D:15:HIS:HD2	1:D:69:GLU:N	1.90	0.61
1:A:129:ASN:O	1:A:130:MET:HG2	2.00	0.61
1:C:115:ILE:HD12	1:C:116:HIS:N	2.14	0.61
1:D:9:LEU:HD13	1:D:11:MET:HE2	1.82	0.61
1:C:254:HIS:CD2	1:C:257:LEU:H	2.19	0.61
1:B:138:LYS:HB3	1:B:138:LYS:HZ2	1.64	0.61
1:A:222:ILE:O	1:A:222:ILE:HG12	2.00	0.60
1:B:17:LEU:HD12	1:B:17:LEU:N	2.16	0.60
1:D:108:LEU:N	1:D:108:LEU:CD2	2.65	0.60
1:A:218:VAL:HG13	1:A:218:VAL:O	2.01	0.60
1:A:200:ARG:HB2	1:A:200:ARG:HH11	1.66	0.60
1:B:149:ILE:CD1	1:B:178:VAL:HB	2.31	0.60
1:A:254:HIS:CD2	1:A:256:ILE:H	2.17	0.60
1:A:149:ILE:CD1	1:A:178:VAL:HB	2.32	0.59
1:A:4:LEU:HD11	1:A:53:TYR:CE2	2.37	0.59
1:C:217:PHE:CD2	1:C:231:PRO:HB3	2.38	0.59
1:A:9:LEU:HD13	1:A:11:MET:HE2	1.83	0.59
1:C:120:GLN:NE2	1:C:221:GLN:HE22	2.01	0.59
1:B:37:ASP:OD1	1:B:39:THR:CG2	2.50	0.59
1:C:151:ILE:HD12	1:C:151:ILE:N	2.17	0.59
1:C:39:THR:HB	1:D:117:ARG:HH21	1.68	0.58
1:A:24:LEU:HG	1:D:20:SER:HB2	1.84	0.58
1:D:217:PHE:CD2	1:D:231:PRO:HB3	2.38	0.58
1:B:149:ILE:HD11	1:B:178:VAL:HB	1.85	0.58
1:A:171:PHE:HD1	1:A:173:ASN:ND2	2.01	0.57
1:A:175:VAL:HG23	1:A:176:VAL:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:HB3	1:B:138:LYS:HZ3	1.68	0.57
1:C:240:PHE:HD2	1:C:240:PHE:H	1.50	0.57
1:C:195:GLU:HA	1:C:211:ILE:HD13	1.87	0.57
1:A:175:VAL:CG2	1:A:176:VAL:N	2.68	0.57
1:B:209:ARG:HD3	1:B:212:ASP:OD1	2.05	0.57
1:D:52:HIS:O	1:D:56:LEU:HB2	2.05	0.56
1:C:129:ASN:HA	1:C:133:LYS:HG2	1.85	0.56
1:C:45:LEU:HD23	1:C:45:LEU:N	2.20	0.56
1:D:9:LEU:HD13	1:D:11:MET:HE3	1.87	0.56
1:A:149:ILE:HD12	1:A:150:HIS:N	2.20	0.56
1:A:186:ASP:O	1:A:190:THR:HG23	2.05	0.56
1:C:5:GLN:HG3	1:C:7:LYS:HE3	1.88	0.56
1:C:2:ASP:HB2	1:C:38:MET:HG3	1.87	0.56
1:B:254:HIS:HD2	1:B:256:ILE:H	1.53	0.56
1:A:200:ARG:NH1	1:A:200:ARG:HB2	2.20	0.56
1:A:138:LYS:HB3	1:A:138:LYS:HZ2	1.71	0.56
1:B:115:ILE:HD12	1:B:115:ILE:C	2.27	0.55
1:A:5:GLN:HG3	1:A:7:LYS:HE3	1.88	0.55
1:A:253:ILE:HD12	1:B:256:ILE:HD13	1.89	0.55
1:A:37:ASP:CG	1:A:39:THR:HG22	2.26	0.55
1:A:96:GLU:HA	1:A:114:THR:HB	1.87	0.55
1:B:57:CYS:O	1:B:61:THR:HG22	2.05	0.55
1:D:57:CYS:O	1:D:61:THR:HG22	2.05	0.55
1:A:218:VAL:O	1:A:221:GLN:HB2	2.06	0.55
1:D:200:ARG:NH1	1:D:212:ASP:OD1	2.39	0.55
1:A:149:ILE:HD13	1:A:178:VAL:HB	1.89	0.54
1:A:17:LEU:HD12	1:A:17:LEU:N	2.23	0.54
1:C:199:GLY:O	1:C:210:LEU:HD13	2.07	0.54
1:C:9:LEU:HD13	1:C:11:MET:HE2	1.89	0.54
1:A:123:PHE:CE1	1:A:177:GLU:HG3	2.42	0.54
1:B:151:ILE:N	1:B:151:ILE:HD12	2.22	0.54
1:D:193:ALA:O	1:D:197:GLU:HG2	2.08	0.54
1:A:231:PRO:HD2	1:A:256:ILE:HD12	1.91	0.53
1:B:254:HIS:CD2	1:B:256:ILE:H	2.27	0.53
1:A:149:ILE:C	1:A:149:ILE:CD1	2.71	0.53
1:C:126:LEU:HD12	1:C:126:LEU:N	2.24	0.53
1:C:138:LYS:NZ	1:C:138:LYS:HB3	2.24	0.53
1:A:193:ALA:O	1:A:197:GLU:HG2	2.10	0.52
1:A:16:GLY:O	1:A:22:LYS:HE2	2.10	0.52
1:C:53:TYR:CD2	1:C:53:TYR:N	2.72	0.52
1:D:53:TYR:O	1:D:54:GLY:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:O	1:A:222:ILE:CG1	2.58	0.51
1:C:134:GLN:OE1	1:C:134:GLN:HA	2.10	0.51
1:C:265:TYR:O	1:C:266:ASP:C	2.44	0.51
1:C:133:LYS:HE2	1:C:170:SER:O	2.09	0.51
1:D:186:ASP:O	1:D:190:THR:HG23	2.11	0.51
1:C:158:LEU:N	1:C:158:LEU:HD12	2.25	0.51
1:A:57:CYS:O	1:A:61:THR:HG22	2.11	0.51
1:B:92:GLU:OE1	1:B:116:HIS:HE1	1.94	0.51
1:B:29:ILE:HB	1:B:98:LYS:HB2	1.92	0.50
1:C:211:ILE:HD12	1:C:211:ILE:H	1.76	0.50
1:C:240:PHE:HA	1:C:243:GLU:HB2	1.92	0.50
1:D:96:GLU:HG3	1:D:114:THR:HB	1.93	0.50
1:B:254:HIS:CD2	1:B:257:LEU:H	2.30	0.50
1:A:2:ASP:OD1	1:B:115:ILE:HA	2.11	0.50
1:C:95:LEU:HD13	1:C:95:LEU:C	2.31	0.50
1:D:2:ASP:HB2	1:D:38:MET:HG3	1.93	0.50
1:A:39:THR:HB	1:B:117:ARG:HH21	1.75	0.50
1:B:175:VAL:CG1	1:B:244:SER:HB2	2.42	0.50
1:C:27:LYS:HD3	1:C:29:ILE:HD11	1.93	0.50
1:A:120:GLN:HE21	1:A:221:GLN:NE2	1.93	0.50
1:A:115:ILE:HD12	1:A:115:ILE:C	2.31	0.49
1:A:151:ILE:HD12	1:A:151:ILE:N	2.27	0.49
1:A:175:VAL:HG23	1:A:176:VAL:H	1.77	0.49
1:D:126:LEU:N	1:D:126:LEU:HD12	2.26	0.49
1:D:200:ARG:HD2	1:D:211:ILE:O	2.13	0.49
1:B:188:LEU:HD22	1:B:228:LEU:HB2	1.95	0.49
1:A:58:GLN:HA	1:A:61:THR:HG22	1.95	0.49
1:C:30:VAL:HG12	1:C:31:SER:N	2.27	0.49
1:C:240:PHE:N	1:C:240:PHE:CD2	2.79	0.49
1:A:92:GLU:HB2	1:A:118:ARG:HG3	1.93	0.48
1:B:149:ILE:C	1:B:149:ILE:CD1	2.62	0.48
1:B:211:ILE:O	1:B:211:ILE:HD12	2.13	0.48
1:B:66:GLU:HB3	1:B:67:THR:HG23	1.95	0.48
1:A:218:VAL:HG12	1:A:230:LEU:HD13	1.95	0.48
1:B:124:ILE:HD13	1:B:191:LEU:HD11	1.93	0.48
1:A:72:ILE:HB	1:A:97:LEU:HD22	1.94	0.48
1:C:72:ILE:HB	1:C:97:LEU:HD13	1.95	0.48
1:D:23:GLU:HA	1:D:23:GLU:OE1	2.13	0.48
1:A:186:ASP:O	1:A:190:THR:CG2	2.62	0.48
1:A:155:SER:OG	1:A:244:SER:HB2	2.14	0.48
1:C:158:LEU:CD1	1:C:158:LEU:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLU:CB	1:C:67:THR:HG23	2.44	0.48
1:D:115:ILE:C	1:D:115:ILE:CD1	2.68	0.48
1:C:194:ILE:O	1:C:195:GLU:C	2.51	0.48
1:C:8:ASP:O	1:D:108:LEU:HA	2.14	0.47
1:B:218:VAL:O	1:B:221:GLN:HB2	2.14	0.47
1:C:196:SER:C	1:C:198:LEU:N	2.67	0.47
1:C:66:GLU:HB3	1:C:67:THR:HG23	1.94	0.47
1:A:92:GLU:OE1	1:A:116:HIS:HE1	1.97	0.47
1:C:96:GLU:HB2	1:C:114:THR:HB	1.95	0.47
1:B:17:LEU:HD12	1:B:17:LEU:H	1.80	0.47
1:C:2:ASP:C	1:C:3:GLN:HG2	2.34	0.47
1:A:17:LEU:N	1:A:17:LEU:CD1	2.78	0.47
1:C:2:ASP:OD1	1:D:117:ARG:NH1	2.47	0.47
1:B:135:ALA:O	1:B:139:GLN:HG3	2.15	0.47
1:B:71:LEU:HB2	1:B:74:THR:HG23	1.97	0.47
1:C:17:LEU:HD12	1:C:17:LEU:N	2.29	0.47
1:C:183:PRO:HG2	1:C:186:ASP:OD2	2.15	0.47
1:C:265:TYR:O	1:C:267:ALA:N	2.48	0.47
1:D:230:LEU:HA	1:D:231:PRO:C	2.36	0.47
1:C:108:LEU:H	1:C:108:LEU:HD23	1.78	0.46
1:D:90:VAL:O	1:D:119:LYS:HE3	2.15	0.46
1:D:254:HIS:CD2	1:D:257:LEU:H	2.33	0.46
1:B:108:LEU:HD11	1:B:111:CYS:HG	1.76	0.46
1:A:108:LEU:N	1:A:108:LEU:HD23	2.31	0.46
1:A:39:THR:HG21	1:B:186:ASP:CG	2.36	0.46
1:B:175:VAL:HG12	1:B:244:SER:HB2	1.98	0.46
1:B:200:ARG:CZ	1:B:200:ARG:HB2	2.45	0.46
1:A:253:ILE:CD1	1:B:256:ILE:HD13	2.46	0.46
1:A:129:ASN:C	1:A:130:MET:CG	2.84	0.46
1:B:222:ILE:O	1:B:222:ILE:HG12	2.15	0.46
1:B:254:HIS:HD2	1:B:257:LEU:H	1.62	0.46
1:A:138:LYS:HB3	1:A:138:LYS:NZ	2.31	0.45
1:B:5:GLN:OE1	1:B:7:LYS:HE2	2.16	0.45
1:C:217:PHE:CE2	1:C:231:PRO:HB3	2.52	0.45
1:D:138:LYS:HZ3	1:D:138:LYS:HB3	1.79	0.45
1:C:92:GLU:OE1	1:C:116:HIS:CE1	2.67	0.45
1:D:149:ILE:O	1:D:149:ILE:HD12	2.06	0.45
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.57	0.45
1:D:92:GLU:OE1	1:D:116:HIS:CE1	2.61	0.45
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.68	0.45
1:C:5:GLN:HB2	1:C:32:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ILE:HG21	1:C:222:ILE:HD13	1.50	0.45
1:D:200:ARG:NH1	1:D:209:ARG:HG2	2.32	0.45
1:A:254:HIS:CD2	1:A:257:LEU:H	2.35	0.45
1:D:53:TYR:N	1:D:53:TYR:CD2	2.84	0.45
1:C:123:PHE:CE1	1:C:177:GLU:CG	2.86	0.45
1:A:38:MET:CE	1:B:113:VAL:HG22	2.47	0.45
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.62	0.45
1:D:124:ILE:HD13	1:D:191:LEU:HD11	1.98	0.45
1:D:198:LEU:O	1:D:210:LEU:CD1	2.64	0.45
1:D:6:ILE:HD12	1:D:6:ILE:N	2.32	0.45
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.50	0.44
1:B:17:LEU:CD1	1:B:17:LEU:N	2.80	0.44
1:C:140:ALA:O	1:C:141:ILE:C	2.54	0.44
1:C:46:ASP:OD1	1:C:46:ASP:C	2.56	0.44
1:B:261:ILE:O	1:B:262:ARG:C	2.55	0.44
1:C:243:GLU:HA	1:C:265:TYR:CE1	2.52	0.44
1:C:52:HIS:HD2	1:C:55:GLU:HG3	1.82	0.44
1:A:200:ARG:HH11	1:A:200:ARG:CB	2.30	0.44
1:B:153:LYS:CB	1:B:153:LYS:CD	2.82	0.44
1:B:49:ALA:C	1:B:89:LEU:HD11	2.37	0.44
1:C:231:PRO:HG3	1:C:255:PRO:HG2	2.00	0.44
1:A:115:ILE:HD12	1:A:116:HIS:N	2.33	0.44
1:D:5:GLN:HB2	1:D:32:ALA:O	2.17	0.44
1:B:222:ILE:HG21	1:B:222:ILE:HD13	1.62	0.44
1:A:4:LEU:HD11	1:A:53:TYR:HE2	1.83	0.43
1:B:4:LEU:CD1	1:B:53:TYR:HE2	2.19	0.43
1:C:102:ALA:O	1:C:104:VAL:N	2.51	0.43
1:A:14:TYR:N	1:A:14:TYR:CD1	2.86	0.43
1:A:217:PHE:CD2	1:A:231:PRO:HB3	2.53	0.43
1:A:58:GLN:CA	1:A:61:THR:HG22	2.49	0.43
1:B:2:ASP:C	1:B:3:GLN:HG2	2.39	0.43
1:C:53:TYR:HB2	1:C:54:GLY:H	1.56	0.43
1:D:210:LEU:HD23	1:D:210:LEU:HA	1.86	0.43
1:B:209:ARG:HH11	1:B:209:ARG:HD3	1.58	0.43
1:C:149:ILE:HD11	1:C:178:VAL:HB	1.99	0.43
1:C:97:LEU:C	1:C:97:LEU:HD23	2.39	0.43
1:D:133:LYS:O	1:D:136:ASN:HB2	2.18	0.43
1:D:149:ILE:CD1	1:D:178:VAL:HB	2.49	0.43
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.83	0.43
1:B:144:LEU:HD12	1:B:144:LEU:HA	1.72	0.43
1:B:248:ILE:HG21	1:B:248:ILE:HD13	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:O	1:C:65:GLN:HG3	2.18	0.43
1:B:230:LEU:HA	1:B:231:PRO:C	2.38	0.43
1:C:58:GLN:O	1:C:61:THR:CG2	2.67	0.43
1:D:256:ILE:HD13	1:D:256:ILE:HG21	1.87	0.43
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.85	0.42
1:D:123:PHE:CE1	1:D:177:GLU:HG3	2.54	0.42
1:C:123:PHE:CZ	1:C:177:GLU:HG3	2.51	0.42
1:D:146:ALA:C	1:D:148:GLY:H	2.22	0.42
1:C:149:ILE:HD12	1:C:150:HIS:N	2.35	0.42
1:A:181:TRP:C	1:A:181:TRP:CD1	2.93	0.42
1:B:238:ARG:O	1:B:239:LEU:C	2.57	0.42
1:A:222:ILE:HG21	1:A:222:ILE:HD13	1.49	0.42
1:C:136:ASN:H	1:C:136:ASN:ND2	2.18	0.42
1:C:242:LEU:O	1:C:243:GLU:C	2.58	0.42
1:A:183:PRO:O	1:A:184:ALA:C	2.58	0.42
1:A:219:GLU:HB3	1:A:220:ASP:H	1.17	0.42
1:B:241:VAL:O	1:B:245:LEU:HB2	2.20	0.42
1:C:215:LEU:HA	1:C:215:LEU:HD23	1.73	0.42
1:B:176:VAL:HG12	1:B:177:GLU:N	2.33	0.42
1:B:60:TRP:O	1:B:64:PHE:HB2	2.19	0.42
1:C:218:VAL:HG12	1:C:230:LEU:HD11	2.01	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.81	0.42
1:C:43:THR:HG22	1:C:44:ASP:OD1	2.20	0.42
1:C:53:TYR:O	1:C:54:GLY:C	2.56	0.42
1:D:254:HIS:HD2	1:D:257:LEU:H	1.67	0.42
1:B:175:VAL:CG2	1:B:176:VAL:N	2.83	0.41
1:D:158:LEU:HD12	1:D:158:LEU:HA	1.82	0.41
1:D:27:LYS:HD3	1:D:29:ILE:HD11	2.02	0.41
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.83	0.41
1:B:95:LEU:HD13	1:B:95:LEU:C	2.41	0.41
1:C:195:GLU:HA	1:C:211:ILE:CD1	2.49	0.41
1:C:24:LEU:HD23	1:C:24:LEU:HA	1.79	0.41
1:C:6:ILE:O	1:C:31:SER:HA	2.19	0.41
1:D:37:ASP:CG	1:D:39:THR:HG22	2.29	0.41
1:D:10:GLU:O	1:D:11:MET:HG3	2.20	0.41
1:D:151:ILE:HD12	1:D:151:ILE:N	2.35	0.41
1:A:101:TRP:CD1	1:A:101:TRP:N	2.88	0.41
1:A:191:LEU:HG	1:A:213:LEU:HB3	2.03	0.41
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.92	0.41
1:C:47:LEU:HA	1:C:47:LEU:HD23	1.62	0.41
1:A:223:LEU:H	1:A:230:LEU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:H	1:B:17:LEU:CD1	2.32	0.41
1:A:129:ASN:OD1	1:A:130:MET:HG3	2.21	0.41
1:B:104:VAL:HG12	1:B:105:HIS:N	2.35	0.41
1:B:132:ASP:O	1:B:133:LYS:C	2.59	0.41
1:B:153:LYS:HD2	1:B:153:LYS:HA	2.03	0.41
1:C:191:LEU:HD12	1:C:191:LEU:HA	1.79	0.41
1:C:3:GLN:O	1:D:114:THR:HG23	2.21	0.41
1:D:153:LYS:HD2	1:D:153:LYS:HA	1.20	0.41
1:D:200:ARG:HB3	1:D:200:ARG:HE	1.81	0.41
1:A:254:HIS:HD2	1:A:256:ILE:N	2.09	0.41
1:C:95:LEU:CD1	1:C:95:LEU:C	2.89	0.41
1:B:37:ASP:CG	1:B:39:THR:HG22	2.41	0.41
1:C:136:ASN:ND2	1:C:136:ASN:N	2.69	0.41
1:C:196:SER:O	1:C:198:LEU:N	2.54	0.41
1:A:261:ILE:O	1:A:262:ARG:C	2.59	0.40
1:B:175:VAL:HG12	1:B:244:SER:CB	2.51	0.40
1:D:254:HIS:HD2	1:D:256:ILE:H	1.69	0.40
1:C:153:LYS:HD2	1:C:153:LYS:HA	1.21	0.40
1:A:198:LEU:HB2	1:A:211:ILE:HD11	2.04	0.40
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.86	0.40
1:C:218:VAL:HG12	1:C:230:LEU:CD1	2.52	0.40
1:D:254:HIS:CD2	1:D:256:ILE:H	2.40	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	233/270 (86%)	223 (96%)	10 (4%)	0	100	100
1	B	240/270 (89%)	229 (95%)	10 (4%)	1 (0%)	38	72
1	C	243/270 (90%)	223 (92%)	16 (7%)	4 (2%)	11	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	240/270 (89%)	220 (92%)	18 (8%)	2 (1%)	22	57
All	All	956/1080 (88%)	895 (94%)	54 (6%)	7 (1%)	25	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	SER
1	C	266	ASP
1	D	210	LEU
1	D	267	ALA
1	C	134	GLN
1	C	147	ARG
1	C	197	GLU

### 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	215/241 (89%)	188 (87%)	27 (13%)	5	15
1	B	221/241 (92%)	188 (85%)	33 (15%)	3	10
1	C	222/241 (92%)	191 (86%)	31 (14%)	4	12
1	D	220/241 (91%)	187 (85%)	33 (15%)	3	10
All	All	878/964 (91%)	754 (86%)	124 (14%)	4	12

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	LEU
1	A	17	LEU
1	A	20	SER
1	A	40	LYS
1	A	56	LEU
1	A	74	THR

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Mol	Chain	Res	Type
1	A	95	LEU
1	A	105	HIS
1	A	108	LEU
1	A	114	THR
1	A	115	ILE
1	A	138	LYS
1	A	143	LYS
1	A	149	ILE
1	A	150	HIS
1	A	157	VAL
1	A	175	VAL
1	A	190	THR
1	A	191	LEU
1	A	200	ARG
1	A	211	ILE
1	A	215	LEU
1	A	222	ILE
1	A	239	LEU
1	A	246	GLN
1	A	262	ARG
1	B	3	GLN
1	B	9	LEU
1	B	17	LEU
1	B	40	LYS
1	B	43	THR
1	B	44	ASP
1	B	52	HIS
1	B	56	LEU
1	B	74	THR
1	B	95	LEU
1	B	113	VAL
1	B	114	THR
1	B	115	ILE
1	B	130	MET
1	B	138	LYS
1	B	141	ILE
1	B	143	LYS
1	B	144	LEU
1	B	149	ILE
1	B	150	HIS
1	B	157	VAL
1	B	175	VAL

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Mol	Chain	Res	Type
1	B	190	THR
1	B	191	LEU
1	B	200	ARG
1	B	211	ILE
1	B	212	ASP
1	B	215	LEU
1	B	218	VAL
1	B	222	ILE
1	B	239	LEU
1	B	244	SER
1	B	262	ARG
1	C	9	LEU
1	C	17	LEU
1	C	20	SER
1	C	40	LYS
1	C	43	THR
1	C	45	LEU
1	C	56	LEU
1	C	74	THR
1	C	93	MET
1	C	95	LEU
1	C	109	ASP
1	C	113	VAL
1	C	114	THR
1	C	115	ILE
1	C	137	LEU
1	C	138	LYS
1	C	141	ILE
1	C	143	LYS
1	C	144	LEU
1	C	149	ILE
1	C	153	LYS
1	C	157	VAL
1	C	170	SER
1	C	175	VAL
1	C	181	TRP
1	C	191	LEU
1	C	200	ARG
1	C	211	ILE
1	C	215	LEU
1	C	222	ILE
1	C	246	GLN

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Mol	Chain	Res	Type
1	D	9	LEU
1	D	20	SER
1	D	22	LYS
1	D	34	LEU
1	D	39	THR
1	D	40	LYS
1	D	52	HIS
1	D	56	LEU
1	D	74	THR
1	D	95	LEU
1	D	108	LEU
1	D	114	THR
1	D	115	ILE
1	D	137	LEU
1	D	138	LYS
1	D	144	LEU
1	D	149	ILE
1	D	150	HIS
1	D	153	LYS
1	D	158	LEU
1	D	170	SER
1	D	171	PHE
1	D	181	TRP
1	D	190	THR
1	D	191	LEU
1	D	200	ARG
1	D	209	ARG
1	D	211	ILE
1	D	215	LEU
1	D	222	ILE
1	D	239	LEU
1	D	244	SER
1	D	246	GLN

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	15	HIS
1	A	116	HIS
1	A	120	GLN
1	A	174	GLN
1	A	254	HIS

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Mol	Chain	Res	Type
1	B	15	HIS
1	B	105	HIS
1	B	116	HIS
1	B	120	GLN
1	B	134	GLN
1	B	136	ASN
1	B	139	GLN
1	B	173	ASN
1	B	174	GLN
1	B	254	HIS
1	C	15	HIS
1	C	52	HIS
1	C	105	HIS
1	C	116	HIS
1	C	120	GLN
1	C	136	ASN
1	C	139	GLN
1	C	174	GLN
1	C	254	HIS
1	D	15	HIS
1	D	116	HIS
1	D	120	GLN
1	D	136	ASN
1	D	139	GLN
1	D	174	GLN
1	D	254	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

There are no ligands in this entry.

## 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.