



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:01 pm BST

PDB ID : 1WND  
Title : Escherichia coli YdcW gene product is a medium-chain aldehyde dehydrogenase as determined by kinetics and crystal structure  
Authors : Gruez, A.; Roig-Zamboni, V.; Tegoni, M.; Cambillau, C.  
Deposited on : 2004-07-29  
Resolution : 2.10 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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

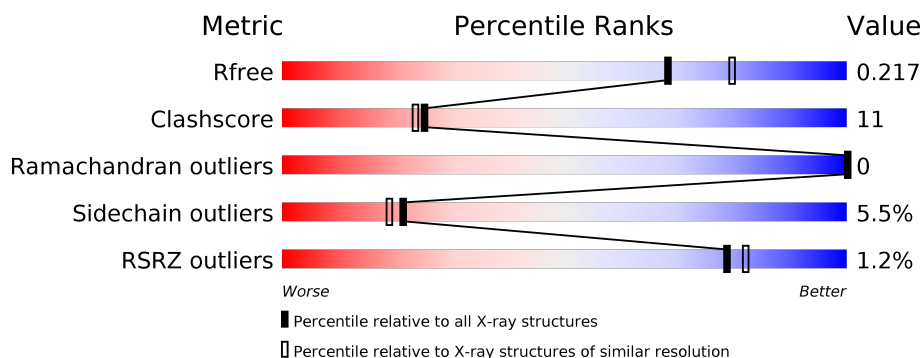
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	495	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	495	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• •</div> </div> </div>
1	C	495	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• •</div> </div> </div>
1	D	495	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14574 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 Putative betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	85	0	0
			3575	2263	616	679	17			
1	B	474	Total	C	N	O	S	54	0	0
			3575	2263	616	679	17			
1	C	474	Total	C	N	O	S	59	0	0
			3575	2263	616	679	17			
1	D	474	Total	C	N	O	S	52	0	0
			3575	2263	616	679	17			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	EXPRESSION TAG	UNP P77674
A	-19	TYR	-	EXPRESSION TAG	UNP P77674
A	-18	TYR	-	EXPRESSION TAG	UNP P77674
A	-17	HIS	-	EXPRESSION TAG	UNP P77674
A	-16	HIS	-	EXPRESSION TAG	UNP P77674
A	-15	HIS	-	EXPRESSION TAG	UNP P77674
A	-14	HIS	-	EXPRESSION TAG	UNP P77674
A	-13	HIS	-	EXPRESSION TAG	UNP P77674
A	-12	HIS	-	EXPRESSION TAG	UNP P77674
A	-11	LEU	-	EXPRESSION TAG	UNP P77674
A	-10	GLU	-	EXPRESSION TAG	UNP P77674
A	-9	SER	-	EXPRESSION TAG	UNP P77674
A	-8	THR	-	EXPRESSION TAG	UNP P77674
A	-7	SER	-	EXPRESSION TAG	UNP P77674
A	-6	LEU	-	EXPRESSION TAG	UNP P77674
A	-5	TYR	-	EXPRESSION TAG	UNP P77674
A	-4	LYS	-	EXPRESSION TAG	UNP P77674
A	-3	LYS	-	EXPRESSION TAG	UNP P77674
A	-2	ALA	-	EXPRESSION TAG	UNP P77674
A	-1	GLY	-	EXPRESSION TAG	UNP P77674
A	0	LEU	-	EXPRESSION TAG	UNP P77674

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	VAL	ILE	CONFLICT	UNP P77674
B	-20	SER	-	EXPRESSION TAG	UNP P77674
B	-19	TYR	-	EXPRESSION TAG	UNP P77674
B	-18	TYR	-	EXPRESSION TAG	UNP P77674
B	-17	HIS	-	EXPRESSION TAG	UNP P77674
B	-16	HIS	-	EXPRESSION TAG	UNP P77674
B	-15	HIS	-	EXPRESSION TAG	UNP P77674
B	-14	HIS	-	EXPRESSION TAG	UNP P77674
B	-13	HIS	-	EXPRESSION TAG	UNP P77674
B	-12	HIS	-	EXPRESSION TAG	UNP P77674
B	-11	LEU	-	EXPRESSION TAG	UNP P77674
B	-10	GLU	-	EXPRESSION TAG	UNP P77674
B	-9	SER	-	EXPRESSION TAG	UNP P77674
B	-8	THR	-	EXPRESSION TAG	UNP P77674
B	-7	SER	-	EXPRESSION TAG	UNP P77674
B	-6	LEU	-	EXPRESSION TAG	UNP P77674
B	-5	TYR	-	EXPRESSION TAG	UNP P77674
B	-4	LYS	-	EXPRESSION TAG	UNP P77674
B	-3	LYS	-	EXPRESSION TAG	UNP P77674
B	-2	ALA	-	EXPRESSION TAG	UNP P77674
B	-1	GLY	-	EXPRESSION TAG	UNP P77674
B	0	LEU	-	EXPRESSION TAG	UNP P77674
B	197	VAL	ILE	CONFLICT	UNP P77674
C	-20	SER	-	EXPRESSION TAG	UNP P77674
C	-19	TYR	-	EXPRESSION TAG	UNP P77674
C	-18	TYR	-	EXPRESSION TAG	UNP P77674
C	-17	HIS	-	EXPRESSION TAG	UNP P77674
C	-16	HIS	-	EXPRESSION TAG	UNP P77674
C	-15	HIS	-	EXPRESSION TAG	UNP P77674
C	-14	HIS	-	EXPRESSION TAG	UNP P77674
C	-13	HIS	-	EXPRESSION TAG	UNP P77674
C	-12	HIS	-	EXPRESSION TAG	UNP P77674
C	-11	LEU	-	EXPRESSION TAG	UNP P77674
C	-10	GLU	-	EXPRESSION TAG	UNP P77674
C	-9	SER	-	EXPRESSION TAG	UNP P77674
C	-8	THR	-	EXPRESSION TAG	UNP P77674
C	-7	SER	-	EXPRESSION TAG	UNP P77674
C	-6	LEU	-	EXPRESSION TAG	UNP P77674
C	-5	TYR	-	EXPRESSION TAG	UNP P77674
C	-4	LYS	-	EXPRESSION TAG	UNP P77674
C	-3	LYS	-	EXPRESSION TAG	UNP P77674
C	-2	ALA	-	EXPRESSION TAG	UNP P77674

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P77674
C	0	LEU	-	EXPRESSION TAG	UNP P77674
C	197	VAL	ILE	CONFLICT	UNP P77674
D	-20	SER	-	EXPRESSION TAG	UNP P77674
D	-19	TYR	-	EXPRESSION TAG	UNP P77674
D	-18	TYR	-	EXPRESSION TAG	UNP P77674
D	-17	HIS	-	EXPRESSION TAG	UNP P77674
D	-16	HIS	-	EXPRESSION TAG	UNP P77674
D	-15	HIS	-	EXPRESSION TAG	UNP P77674
D	-14	HIS	-	EXPRESSION TAG	UNP P77674
D	-13	HIS	-	EXPRESSION TAG	UNP P77674
D	-12	HIS	-	EXPRESSION TAG	UNP P77674
D	-11	LEU	-	EXPRESSION TAG	UNP P77674
D	-10	GLU	-	EXPRESSION TAG	UNP P77674
D	-9	SER	-	EXPRESSION TAG	UNP P77674
D	-8	THR	-	EXPRESSION TAG	UNP P77674
D	-7	SER	-	EXPRESSION TAG	UNP P77674
D	-6	LEU	-	EXPRESSION TAG	UNP P77674
D	-5	TYR	-	EXPRESSION TAG	UNP P77674
D	-4	LYS	-	EXPRESSION TAG	UNP P77674
D	-3	LYS	-	EXPRESSION TAG	UNP P77674
D	-2	ALA	-	EXPRESSION TAG	UNP P77674
D	-1	GLY	-	EXPRESSION TAG	UNP P77674
D	0	LEU	-	EXPRESSION TAG	UNP P77674
D	197	VAL	ILE	CONFLICT	UNP P77674

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

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

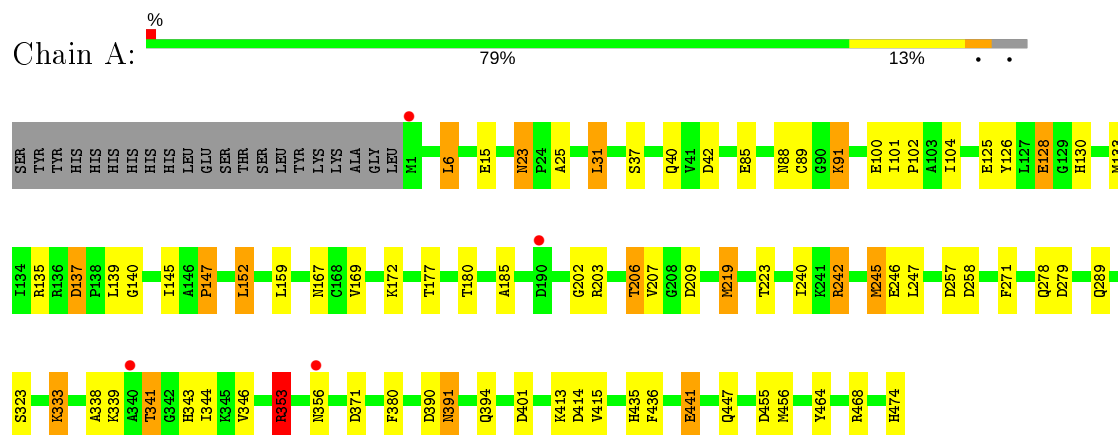
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total 67	O 67	0	0
3	B	65	Total 65	O 65	0	0
3	C	66	Total 66	O 66	0	0
3	D	72	Total 72	O 72	0	0

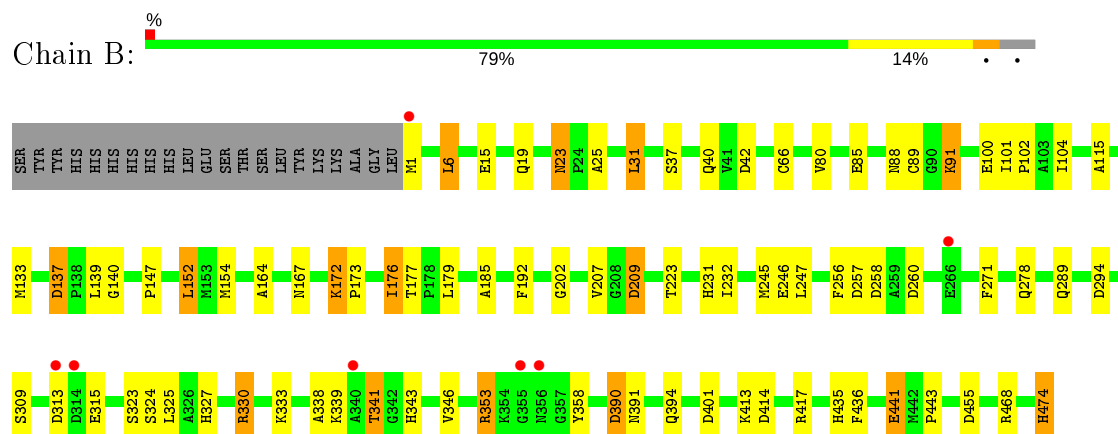
### 3 Residue-property plots [i](#)

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.

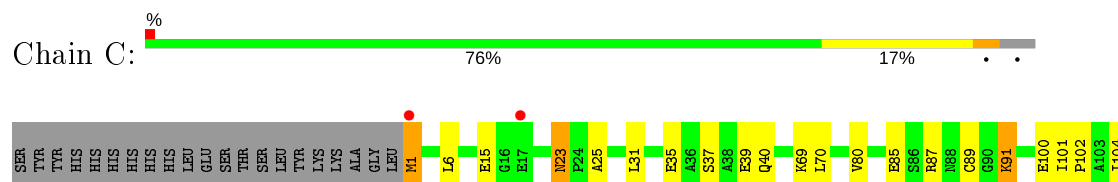
- Molecule 1: Putative betaine aldehyde dehydrogenase

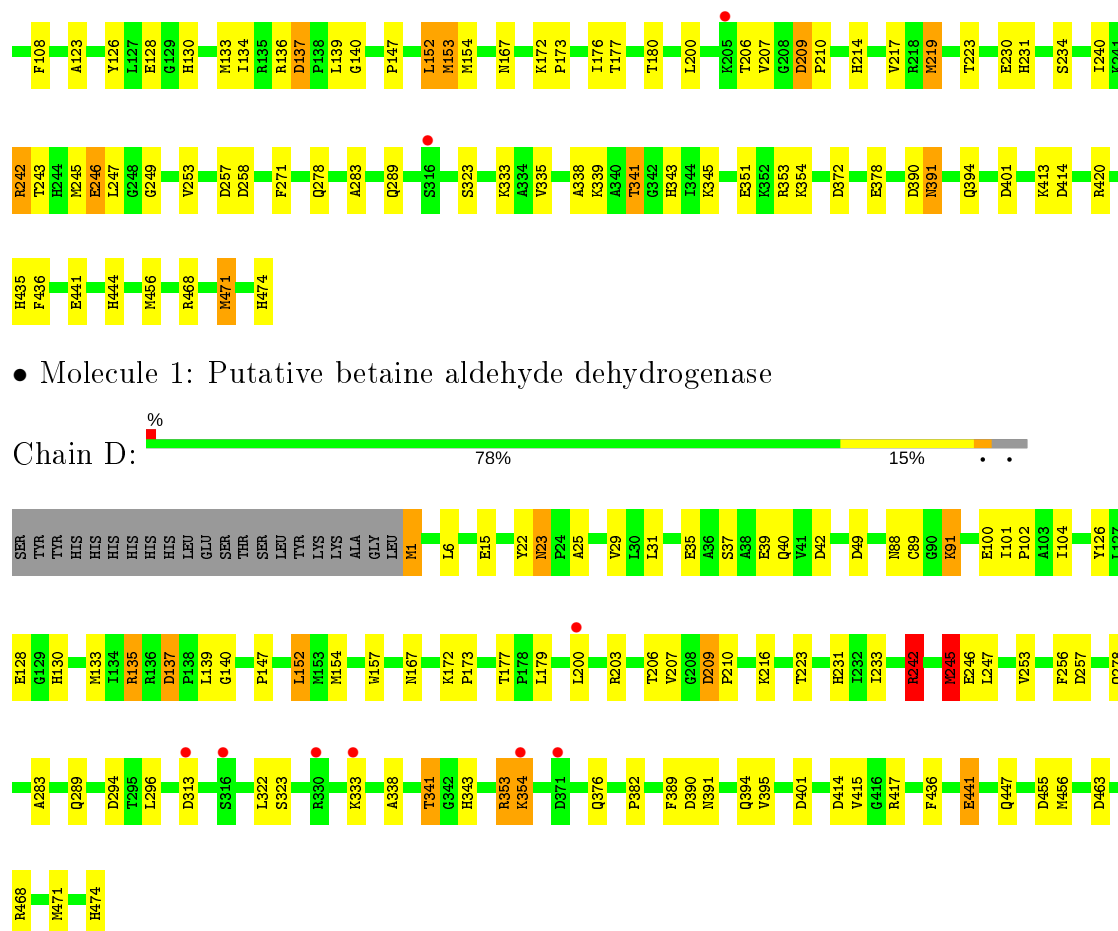


- Molecule 1: Putative betaine aldehyde dehydrogenase



- Molecule 1: Putative betaine aldehyde dehydrogenase





● Molecule 1: Putative betaine aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.04Å 79.68Å 158.67Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 98.8 (19.94-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.184 , 0.213 0.191 , 0.217	Depositor DCC
$R_{free}$ test set	6119 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.65	0/3649	0.86	12/4955 (0.2%)
1	B	0.62	0/3649	0.83	13/4955 (0.3%)
1	C	0.63	0/3649	0.85	11/4955 (0.2%)
1	D	0.65	1/3649 (0.0%)	0.85	14/4955 (0.3%)
All	All	0.64	1/14596 (0.0%)	0.85	50/19820 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	245	MET	C-N	6.01	1.47	1.34

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	MET	CA-C-N	-8.68	98.11	117.20
1	A	353	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	A	242	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	A	137	ASP	CB-CG-OD2	7.57	125.11	118.30
1	B	353	ARG	NE-CZ-NH2	7.32	123.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASP	CB-CG-OD2	7.30	124.88	118.30
1	D	137	ASP	CB-CG-OD2	7.27	124.84	118.30
1	C	353	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	414	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	137	ASP	CB-CG-OD2	6.60	124.24	118.30
1	D	313	ASP	CB-CG-OD2	6.54	124.18	118.30
1	D	209	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	242	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	C	414	ASP	CB-CG-OD2	6.23	123.91	118.30
1	D	414	ASP	CB-CG-OD2	6.15	123.84	118.30
1	D	245	MET	CG-SD-CE	6.15	110.04	100.20
1	B	313	ASP	CB-CG-OD2	6.14	123.82	118.30
1	D	471	MET	CG-SD-CE	6.10	109.96	100.20
1	C	471	MET	CG-SD-CE	-6.07	90.48	100.20
1	B	209	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	294	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	455	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	279	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	137	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	463	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	42	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	401	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	294	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	456	MET	CG-SD-CE	5.75	109.41	100.20
1	D	401	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	456	MET	CG-SD-CE	5.70	109.32	100.20
1	C	372	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	1	MET	N-CA-C	5.67	126.30	111.00
1	A	219	MET	CG-SD-CE	5.66	109.26	100.20
1	B	42	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	456	MET	CG-SD-CE	5.64	109.22	100.20
1	D	42	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	414	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	219	MET	CG-SD-CE	5.47	108.95	100.20
1	B	390	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	136	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	B	455	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	474	HIS	CA-C-O	-5.27	109.04	120.10
1	C	258	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	371	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	401	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	455	ASP	CB-CG-OD2	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	401	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	209	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Sidechain
1	B	353	ARG	Sidechain
1	D	245	MET	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3575	0	3558	78	0
1	B	3575	0	3558	75	0
1	C	3575	0	3558	90	0
1	D	3575	0	3558	79	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	67	0	0	0	0
3	B	65	0	0	5	0
3	C	66	0	0	4	0
3	D	72	0	0	2	0
All	All	14574	0	14232	300	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 11.

All (300) 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:242:ARG:NH1	1:C:243:THR:H	1.39	1.20
1:B:474:HIS:OXT	1:B:474:HIS:CD2	1.96	1.18
1:A:139:LEU:CD1	1:A:219:MET:CE	2.23	1.17
1:B:330:ARG:HH11	1:B:330:ARG:HG2	1.05	1.14
1:A:245:MET:HG2	1:A:247:LEU:HD21	1.19	1.12
1:C:474:HIS:CD2	1:C:474:HIS:OXT	2.05	1.09
1:C:139:LEU:CD1	1:C:219:MET:CE	2.36	1.03
1:D:474:HIS:CD2	1:D:474:HIS:OXT	2.14	1.01
1:A:139:LEU:CD1	1:A:219:MET:HE2	1.92	0.98
1:C:139:LEU:HD13	1:C:219:MET:HE2	1.41	0.98
1:D:390:ASP:H	1:D:394:GLN:HE22	1.08	0.97
1:B:474:HIS:OXT	1:B:474:HIS:HD2	1.44	0.96
1:C:390:ASP:H	1:C:394:GLN:HE22	1.09	0.96
1:A:203:ARG:HB2	1:A:206:THR:CG2	1.96	0.95
1:A:390:ASP:H	1:A:394:GLN:HE22	0.95	0.93
1:C:474:HIS:HD2	1:C:474:HIS:OXT	1.47	0.93
1:B:330:ARG:NH1	1:B:330:ARG:HG2	1.79	0.92
1:A:139:LEU:HD12	1:A:219:MET:CE	1.98	0.91
1:A:139:LEU:HD13	1:A:219:MET:HE2	1.51	0.91
1:B:390:ASP:H	1:B:394:GLN:HE22	1.19	0.89
1:C:242:ARG:HH11	1:C:243:THR:H	1.12	0.89
1:C:242:ARG:NH1	1:C:243:THR:N	2.21	0.89
1:A:474:HIS:OXT	1:A:474:HIS:CD2	2.25	0.89
1:C:37:SER:H	1:C:40:GLN:HE21	1.21	0.88
1:C:139:LEU:HD13	1:C:219:MET:CE	2.02	0.86
1:C:242:ARG:HH11	1:C:243:THR:N	1.72	0.85
1:B:80:VAL:HG23	3:B:487:HOH:O	1.75	0.85
1:D:390:ASP:H	1:D:394:GLN:NE2	1.74	0.84
1:A:133:MET:CE	1:B:133:MET:CE	2.56	0.83
1:A:139:LEU:HD12	1:A:219:MET:HE3	1.60	0.83
1:B:257:ASP:H	1:B:289:GLN:HE21	1.25	0.82
1:D:257:ASP:H	1:D:289:GLN:HE21	1.27	0.82
1:C:139:LEU:H	1:C:167:ASN:HD21	1.23	0.81
1:C:153:MET:CE	3:C:537:HOH:O	2.29	0.81
1:A:390:ASP:H	1:A:394:GLN:NE2	1.77	0.81
1:A:245:MET:HG2	1:A:247:LEU:CD2	2.07	0.80
1:C:130:HIS:ND1	1:C:471:MET:CE	2.44	0.80
1:D:341:THR:HG22	1:D:343:HIS:H	1.47	0.79
1:A:139:LEU:H	1:A:167:ASN:HD21	1.27	0.79
1:C:245:MET:HG2	1:C:247:LEU:HD21	1.62	0.79
1:A:133:MET:HE1	1:B:133:MET:CE	2.12	0.78
1:D:139:LEU:H	1:D:167:ASN:HD21	1.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLU:OE2	1:D:206:THR:HG21	1.84	0.78
1:B:139:LEU:H	1:B:167:ASN:HD21	1.31	0.77
1:B:37:SER:H	1:B:40:GLN:HE21	1.30	0.77
1:D:338:ALA:O	1:D:341:THR:HB	1.85	0.77
1:D:37:SER:H	1:D:40:GLN:HE21	1.31	0.77
1:C:91:LYS:HE2	1:C:100:GLU:OE2	1.86	0.76
1:A:133:MET:HE2	1:B:133:MET:SD	2.25	0.76
1:A:447:GLN:HA	1:D:242:ARG:NH2	2.01	0.75
1:A:447:GLN:HA	1:D:242:ARG:HH22	1.53	0.74
1:C:242:ARG:HH12	1:C:243:THR:H	1.35	0.74
1:B:278:GLN:HE22	1:B:323:SER:H	1.33	0.74
1:C:1:MET:HE1	1:C:87:ARG:HH22	1.53	0.74
1:A:139:LEU:CD1	1:A:219:MET:HE3	2.16	0.74
1:D:474:HIS:OXT	1:D:474:HIS:HD2	1.69	0.74
1:C:390:ASP:H	1:C:394:GLN:NE2	1.86	0.73
1:B:390:ASP:H	1:B:394:GLN:NE2	1.85	0.73
1:C:130:HIS:ND1	1:C:471:MET:HE2	2.04	0.73
1:A:133:MET:HE2	1:B:133:MET:CE	2.19	0.72
1:B:330:ARG:CG	1:B:330:ARG:HH11	1.94	0.72
1:A:37:SER:H	1:A:40:GLN:HE21	1.36	0.72
1:C:176:ILE:HG22	1:C:177:THR:HG23	1.70	0.72
1:A:278:GLN:HE22	1:A:323:SER:H	1.36	0.72
1:D:1:MET:HE2	1:D:179:LEU:HD22	1.72	0.72
1:C:140:GLY:H	1:C:167:ASN:HD22	1.38	0.71
1:D:257:ASP:H	1:D:289:GLN:NE2	1.87	0.71
1:A:390:ASP:N	1:A:394:GLN:HE22	1.79	0.71
1:D:278:GLN:HE22	1:D:323:SER:H	1.36	0.70
1:D:104:ILE:HD13	1:D:152:LEU:HD13	1.74	0.69
1:C:1:MET:CE	1:C:87:ARG:HH22	2.06	0.69
1:B:23:ASN:HD22	1:B:23:ASN:C	1.95	0.69
1:A:140:GLY:H	1:A:167:ASN:HD22	1.40	0.69
1:C:23:ASN:HD22	1:C:23:ASN:C	1.97	0.69
1:B:338:ALA:O	1:B:341:THR:HB	1.93	0.68
1:C:278:GLN:HE22	1:C:323:SER:H	1.38	0.68
1:A:133:MET:HE1	1:B:133:MET:HE2	1.76	0.67
1:C:153:MET:HE1	3:C:537:HOH:O	1.90	0.67
1:B:137:ASP:OD2	1:B:468:ARG:HD3	1.94	0.67
1:A:338:ALA:O	1:A:341:THR:HB	1.94	0.67
1:A:133:MET:CE	1:B:133:MET:HE2	2.23	0.67
1:D:245:MET:HG2	1:D:247:LEU:HD21	1.75	0.67
1:C:206:THR:HG23	1:C:207:VAL:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASP:CG	1:D:216:LYS:HE2	2.15	0.67
1:D:233:ILE:HD11	1:D:245:MET:HE1	1.77	0.67
1:B:257:ASP:H	1:B:289:GLN:NE2	1.92	0.67
1:A:139:LEU:HD11	1:A:219:MET:CE	2.25	0.66
1:B:104:ILE:HD13	1:B:152:LEU:HD13	1.76	0.66
1:C:338:ALA:O	1:C:341:THR:HB	1.96	0.66
1:D:474:HIS:CG	1:D:474:HIS:OXT	2.46	0.65
1:B:176:ILE:HG12	1:B:177:THR:HG23	1.77	0.65
1:A:333:LYS:HE2	1:A:333:LYS:HA	1.78	0.65
1:C:341:THR:HG22	1:C:343:HIS:H	1.61	0.65
1:D:140:GLY:H	1:D:167:ASN:HD22	1.42	0.65
1:B:341:THR:HG22	1:B:343:HIS:H	1.62	0.65
1:A:137:ASP:OD2	1:A:468:ARG:HD3	1.96	0.64
1:A:203:ARG:HB2	1:A:206:THR:HG22	1.76	0.64
1:B:15:GLU:H	1:B:40:GLN:HE22	1.46	0.64
1:D:1:MET:HE1	1:D:179:LEU:HD13	1.80	0.64
1:B:89:CYS:HB2	1:B:91:LYS:HD3	1.80	0.63
1:B:271:PHE:CD2	1:B:435:HIS:HB3	2.33	0.63
1:A:133:MET:HE1	1:B:133:MET:HE1	1.78	0.63
1:A:391:ASN:ND2	1:A:394:GLN:H	1.97	0.63
1:A:341:THR:HG22	1:A:343:HIS:H	1.63	0.62
1:C:101:ILE:HB	1:C:102:PRO:HD3	1.82	0.62
1:C:15:GLU:H	1:C:40:GLN:HE22	1.45	0.62
1:D:203:ARG:HB2	1:D:206:THR:HG22	1.81	0.62
1:D:233:ILE:HD11	1:D:245:MET:CE	2.30	0.62
1:D:447:GLN:HG2	3:D:490:HOH:O	2.00	0.62
1:B:339:LYS:HD3	1:B:346:VAL:HG21	1.82	0.61
1:C:91:LYS:CE	1:C:100:GLU:OE2	2.47	0.61
1:C:139:LEU:HD12	1:C:219:MET:CE	2.28	0.61
1:C:391:ASN:ND2	1:C:394:GLN:H	1.98	0.61
1:C:257:ASP:H	1:C:289:GLN:HE21	1.49	0.61
1:D:22:TYR:CE2	1:D:29:VAL:HG22	2.35	0.61
1:B:278:GLN:HE21	1:B:327:HIS:CD2	2.18	0.61
1:D:390:ASP:N	1:D:394:GLN:HE22	1.90	0.61
1:C:139:LEU:CD1	1:C:219:MET:HE2	2.08	0.61
1:A:133:MET:CE	1:B:133:MET:HE1	2.31	0.60
1:C:139:LEU:CD1	1:C:219:MET:HE3	2.30	0.60
1:B:278:GLN:HE21	1:B:327:HIS:HD2	1.48	0.60
1:B:140:GLY:H	1:B:167:ASN:HD22	1.47	0.60
1:D:15:GLU:H	1:D:40:GLN:HE22	1.49	0.60
1:A:441:GLU:HG3	1:D:126:TYR:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ASN:C	1:D:23:ASN:HD22	2.05	0.60
1:A:474:HIS:OXT	1:A:474:HIS:CG	2.53	0.60
1:C:37:SER:H	1:C:40:GLN:NE2	1.96	0.60
1:A:139:LEU:CD1	1:A:219:MET:HE1	2.27	0.59
3:B:513:HOH:O	1:C:130:HIS:HE1	1.83	0.59
1:D:354:LYS:O	1:D:354:LYS:HD3	2.02	0.59
1:B:325:LEU:HD13	1:B:358:TYR:CE1	2.37	0.59
1:A:23:ASN:C	1:A:23:ASN:HD22	2.04	0.59
1:D:49:ASP:OD2	1:D:216:LYS:HE2	2.03	0.59
1:C:341:THR:CG2	1:C:343:HIS:H	2.16	0.59
1:B:341:THR:HG23	1:B:343:HIS:CE1	2.38	0.59
1:C:139:LEU:CD1	1:C:219:MET:HE1	2.33	0.59
1:C:153:MET:HE2	3:C:537:HOH:O	1.97	0.58
1:B:474:HIS:CG	1:B:474:HIS:OXT	2.33	0.58
1:D:257:ASP:N	1:D:289:GLN:HE21	1.97	0.58
1:C:139:LEU:HD12	1:C:219:MET:HE3	1.86	0.58
1:A:139:LEU:HD13	1:A:219:MET:CE	2.12	0.57
1:A:257:ASP:H	1:A:289:GLN:HE21	1.49	0.57
1:A:245:MET:CG	1:A:247:LEU:HD21	2.13	0.57
1:A:31:LEU:HD12	1:A:31:LEU:N	2.19	0.57
1:C:390:ASP:N	1:C:394:GLN:HE22	1.92	0.57
1:B:23:ASN:HD22	1:B:25:ALA:H	1.52	0.57
1:D:1:MET:CE	1:D:179:LEU:HD22	2.34	0.56
1:D:89:CYS:HB2	1:D:91:LYS:HD3	1.85	0.56
1:D:341:THR:HG23	1:D:343:HIS:CE1	2.40	0.56
1:A:474:HIS:OXT	1:A:474:HIS:HD2	1.80	0.56
1:A:139:LEU:H	1:A:167:ASN:ND2	2.01	0.56
1:B:23:ASN:ND2	1:B:25:ALA:H	2.04	0.56
1:D:206:THR:HG23	1:D:207:VAL:HG23	1.87	0.56
1:C:23:ASN:ND2	1:C:25:ALA:H	2.03	0.56
1:C:137:ASP:OD2	1:C:468:ARG:HD3	2.06	0.56
1:D:278:GLN:HE22	1:D:323:SER:N	2.03	0.55
1:D:49:ASP:CG	1:D:216:LYS:CE	2.75	0.55
1:C:242:ARG:NH1	1:C:243:THR:O	2.40	0.55
1:D:154:MET:HE1	1:D:157:TRP:CZ3	2.41	0.55
1:A:278:GLN:HE22	1:A:323:SER:N	2.04	0.55
1:A:125:GLU:N	1:A:125:GLU:CD	2.59	0.55
1:C:139:LEU:H	1:C:167:ASN:ND2	1.98	0.55
1:A:126:TYR:CD2	1:D:441:GLU:HG3	2.42	0.55
1:A:258:ASP:O	1:A:413:LYS:HG3	2.06	0.54
1:B:91:LYS:HE3	1:B:100:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:CYS:CB	1:D:91:LYS:HD3	2.37	0.54
1:A:15:GLU:H	1:A:40:GLN:HE22	1.56	0.54
1:A:257:ASP:H	1:A:289:GLN:NE2	2.06	0.54
1:B:15:GLU:H	1:B:40:GLN:NE2	2.04	0.54
1:D:49:ASP:OD2	1:D:216:LYS:CE	2.55	0.54
1:C:35:GLU:OE2	1:C:206:THR:HG21	2.06	0.54
1:C:341:THR:HG23	1:C:343:HIS:ND1	2.23	0.54
1:C:147:PRO:HD3	1:C:223:THR:HB	1.90	0.53
1:C:23:ASN:HD22	1:C:25:ALA:H	1.57	0.53
1:C:278:GLN:HE22	1:C:323:SER:N	2.06	0.53
1:C:130:HIS:CG	1:C:471:MET:CE	2.92	0.53
1:C:80:VAL:HG23	3:C:520:HOH:O	2.08	0.53
1:B:245:MET:HG2	1:B:247:LEU:HD21	1.91	0.53
1:C:341:THR:HG23	1:C:343:HIS:CE1	2.44	0.53
1:D:128:GLU:O	1:D:130:HIS:HD2	1.92	0.53
1:A:341:THR:HG23	1:A:343:HIS:CE1	2.44	0.53
1:B:139:LEU:H	1:B:167:ASN:ND2	2.04	0.53
1:D:101:ILE:HB	1:D:102:PRO:HD3	1.90	0.53
1:C:257:ASP:H	1:C:289:GLN:NE2	2.05	0.52
1:D:173:PRO:HD2	1:D:200:LEU:O	2.09	0.52
1:B:257:ASP:N	1:B:289:GLN:HE21	2.02	0.52
1:A:104:ILE:HD13	1:A:152:LEU:HD13	1.91	0.52
1:C:271:PHE:CD2	1:C:435:HIS:HB3	2.45	0.52
1:D:322:LEU:HD21	1:D:382:PRO:HD3	1.90	0.52
1:C:130:HIS:CG	1:C:471:MET:HE3	2.45	0.51
1:C:474:HIS:OXT	1:C:474:HIS:CG	2.42	0.51
1:A:203:ARG:HB2	1:A:206:THR:HG21	1.89	0.51
1:A:88:ASN:HD21	1:A:177:THR:HA	1.76	0.50
1:B:202:GLY:HA3	1:B:207:VAL:HG21	1.94	0.50
1:B:441:GLU:CG	1:C:126:TYR:CD2	2.94	0.50
1:B:172:LYS:HD2	1:B:173:PRO:O	2.12	0.49
1:C:173:PRO:HD2	1:C:200:LEU:O	2.12	0.49
1:A:333:LYS:HE2	1:A:333:LYS:CA	2.42	0.49
1:B:147:PRO:HG2	1:B:154:MET:HG3	1.94	0.49
1:D:341:THR:CG2	1:D:343:HIS:H	2.22	0.49
1:C:140:GLY:H	1:C:167:ASN:ND2	2.09	0.49
1:B:91:LYS:CE	1:B:100:GLU:OE2	2.61	0.49
1:C:128:GLU:O	1:C:130:HIS:HD2	1.95	0.49
1:A:126:TYR:CD2	1:D:441:GLU:CG	2.95	0.49
1:A:271:PHE:CD2	1:A:435:HIS:HB3	2.48	0.49
1:A:219:MET:HE1	1:A:464:TYR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ILE:O	1:C:240:ILE:HG22	2.13	0.48
1:B:209:ASP:OD1	1:B:231:HIS:HE1	1.95	0.48
1:C:147:PRO:CG	1:C:154:MET:HG3	2.44	0.48
1:D:256:PHE:CD1	1:D:417:ARG:HD3	2.48	0.48
1:B:256:PHE:CD1	1:B:417:ARG:HD3	2.48	0.48
1:A:202:GLY:HA3	1:A:207:VAL:HG21	1.96	0.48
1:B:91:LYS:HG2	1:B:91:LYS:H	1.45	0.48
1:A:23:ASN:ND2	1:A:25:ALA:H	2.11	0.48
1:D:296:LEU:HD13	1:D:296:LEU:C	2.34	0.47
1:B:443:PRO:HD2	1:C:134:ILE:HD11	1.97	0.47
1:C:209:ASP:HB2	1:C:210:PRO:HD3	1.96	0.47
1:A:140:GLY:H	1:A:167:ASN:ND2	2.10	0.47
1:D:139:LEU:H	1:D:167:ASN:ND2	2.04	0.47
1:B:339:LYS:HD3	1:B:346:VAL:CG2	2.43	0.47
1:B:391:ASN:ND2	1:B:394:GLN:H	2.13	0.47
1:C:23:ASN:C	1:C:23:ASN:ND2	2.67	0.47
1:D:23:ASN:ND2	1:D:25:ALA:H	2.13	0.47
1:D:209:ASP:OD1	1:D:231:HIS:HE1	1.98	0.46
1:D:354:LYS:C	1:D:354:LYS:HD3	2.35	0.46
1:A:91:LYS:HE3	1:A:100:GLU:OE2	2.15	0.46
1:A:147:PRO:HD3	1:A:223:THR:HB	1.97	0.46
1:A:91:LYS:CE	1:A:100:GLU:OE2	2.64	0.46
1:A:474:HIS:CD2	1:C:420:ARG:HG2	2.50	0.46
1:C:15:GLU:H	1:C:40:GLN:NE2	2.13	0.46
1:D:23:ASN:HD22	1:D:25:ALA:H	1.63	0.46
1:D:137:ASP:OD2	1:D:468:ARG:HD3	2.14	0.46
1:C:335:VAL:O	1:C:339:LYS:HG3	2.16	0.46
1:D:91:LYS:HE3	1:D:100:GLU:OE2	2.16	0.46
1:D:376:GLN:NE2	3:D:503:HOH:O	2.50	0.45
1:B:101:ILE:HB	1:B:102:PRO:HD3	1.98	0.45
1:B:23:ASN:ND2	1:B:23:ASN:C	2.68	0.45
1:A:152:LEU:HG	1:A:180:THR:HB	1.98	0.45
1:A:89:CYS:HB2	1:A:91:LYS:HD3	1.98	0.45
1:C:209:ASP:OD1	1:C:231:HIS:HE1	1.99	0.45
1:C:253:VAL:HG21	1:C:283:ALA:HB1	1.97	0.45
1:D:390:ASP:N	1:D:394:GLN:NE2	2.55	0.45
1:D:147:PRO:HD3	1:D:223:THR:HB	1.99	0.45
1:C:104:ILE:HD13	1:C:152:LEU:HD13	1.99	0.45
1:B:441:GLU:HG3	1:C:126:TYR:CD2	2.52	0.44
1:B:6:LEU:HB2	1:B:185:ALA:HB1	1.99	0.44
1:A:128:GLU:O	1:A:130:HIS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:THR:HG21	1:A:344:ILE:HG13	2.00	0.44
1:B:441:GLU:HG2	1:C:126:TYR:CD2	2.53	0.44
1:D:154:MET:CE	1:D:157:TRP:CE3	3.01	0.44
1:A:101:ILE:HB	1:A:102:PRO:HD3	2.00	0.43
1:C:152:LEU:HG	1:C:180:THR:HB	2.00	0.43
1:D:1:MET:CE	1:D:179:LEU:HD13	2.47	0.43
1:D:35:GLU:CD	1:D:206:THR:HG21	2.36	0.43
3:B:513:HOH:O	1:C:130:HIS:CE1	2.65	0.43
1:D:209:ASP:HB2	1:D:210:PRO:HD3	2.00	0.43
1:D:389:PHE:CD1	1:D:395:VAL:HB	2.54	0.43
1:A:339:LYS:HD3	1:A:346:VAL:HG21	1.99	0.43
1:B:390:ASP:N	1:B:394:GLN:HE22	2.01	0.43
1:B:15:GLU:N	1:B:40:GLN:HE22	2.14	0.43
1:B:324:SER:HA	1:B:358:TYR:CE2	2.53	0.43
1:B:232:ILE:HD11	3:B:520:HOH:O	2.19	0.43
1:B:147:PRO:HG3	1:B:223:THR:HB	2.00	0.43
1:B:258:ASP:O	1:B:413:LYS:HG3	2.19	0.43
1:C:249:GLY:O	1:C:378:GLU:HG3	2.19	0.43
1:B:88:ASN:ND2	1:B:179:LEU:HG	2.34	0.42
1:C:413:LYS:O	1:D:415:VAL:HG23	2.19	0.42
1:D:88:ASN:HD21	1:D:177:THR:HA	1.84	0.42
1:A:341:THR:CG2	1:A:343:HIS:H	2.28	0.42
1:D:253:VAL:HG21	1:D:283:ALA:HB1	2.02	0.42
1:A:88:ASN:ND2	1:A:177:THR:HA	2.34	0.42
1:A:415:VAL:HG23	1:B:413:LYS:O	2.19	0.42
1:C:123:ALA:O	1:D:135:ARG:HB3	2.20	0.42
1:A:159:LEU:HD23	1:A:169:VAL:HG11	2.02	0.42
1:B:278:GLN:HE22	1:B:323:SER:N	2.09	0.42
1:D:37:SER:H	1:D:40:GLN:NE2	2.09	0.42
1:B:31:LEU:HD12	1:B:31:LEU:N	2.35	0.42
1:A:23:ASN:C	1:A:23:ASN:ND2	2.73	0.42
1:B:66:CYS:HB3	1:B:192:PHE:CE2	2.55	0.42
1:C:89:CYS:HB2	1:C:91:LYS:HD2	2.02	0.41
1:A:6:LEU:HB2	1:A:185:ALA:HB1	2.01	0.41
1:B:176:ILE:HD11	1:B:323:SER:HB2	2.01	0.41
1:D:91:LYS:HG2	1:D:91:LYS:H	1.50	0.41
1:D:140:GLY:H	1:D:167:ASN:ND2	2.13	0.41
1:D:1:MET:HE2	1:D:1:MET:HB3	1.78	0.41
1:C:139:LEU:HD11	1:C:219:MET:HE1	2.01	0.41
1:C:37:SER:N	1:C:40:GLN:HE21	2.03	0.41
1:B:232:ILE:CD1	3:B:520:HOH:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLU:OE2	1:C:444:HIS:HE1	2.04	0.41
1:A:240:ILE:O	1:A:240:ILE:HG22	2.20	0.41
1:B:115:ALA:HB2	1:B:164:ALA:HB1	2.01	0.41
1:C:133:MET:HE1	1:D:133:MET:SD	2.61	0.41
1:C:70:LEU:HD23	1:C:108:PHE:CE2	2.56	0.41
1:C:391:ASN:HD22	1:C:391:ASN:C	2.24	0.41
1:C:214:HIS:HB3	1:C:217:VAL:HG23	2.03	0.40
1:D:147:PRO:CG	1:D:154:MET:HG3	2.50	0.40
1:D:15:GLU:H	1:D:40:GLN:NE2	2.15	0.40
1:B:325:LEU:CD1	1:B:358:TYR:CE1	3.03	0.40
1:D:353:ARG:HE	1:D:353:ARG:HB3	1.61	0.40
1:D:391:ASN:ND2	1:D:394:GLN:H	2.20	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	472/495 (95%)	464 (98%)	8 (2%)	0	100	100
1	B	472/495 (95%)	462 (98%)	10 (2%)	0	100	100
1	C	472/495 (95%)	463 (98%)	9 (2%)	0	100	100
1	D	472/495 (95%)	461 (98%)	11 (2%)	0	100	100
All	All	1888/1980 (95%)	1850 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/390 (95%)	348 (94%)	23 (6%)	18	15
1	B	371/390 (95%)	354 (95%)	17 (5%)	27	26
1	C	371/390 (95%)	348 (94%)	23 (6%)	18	15
1	D	371/390 (95%)	353 (95%)	18 (5%)	25	23
All	All	1484/1560 (95%)	1403 (94%)	81 (6%)	21	19

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	23	ASN
1	A	31	LEU
1	A	85	GLU
1	A	91	LYS
1	A	128	GLU
1	A	135	ARG
1	A	145	ILE
1	A	147	PRO
1	A	152	LEU
1	A	172	LYS
1	A	206	THR
1	A	242	ARG
1	A	245	MET
1	A	246	GLU
1	A	333	LYS
1	A	341	THR
1	A	353	ARG
1	A	356	ASN
1	A	380	PHE
1	A	391	ASN
1	A	436	PHE
1	A	441	GLU
1	B	6	LEU
1	B	19	GLN
1	B	23	ASN
1	B	31	LEU
1	B	85	GLU

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Mol	Chain	Res	Type
1	B	91	LYS
1	B	152	LEU
1	B	172	LYS
1	B	176	ILE
1	B	246	GLU
1	B	309	SER
1	B	315	GLU
1	B	330	ARG
1	B	333	LYS
1	B	341	THR
1	B	436	PHE
1	B	441	GLU
1	C	1	MET
1	C	6	LEU
1	C	23	ASN
1	C	31	LEU
1	C	39	GLU
1	C	69	LYS
1	C	85	GLU
1	C	91	LYS
1	C	152	LEU
1	C	153	MET
1	C	172	LYS
1	C	230	GLU
1	C	234	SER
1	C	242	ARG
1	C	246	GLU
1	C	333	LYS
1	C	341	THR
1	C	345	LYS
1	C	351	GLU
1	C	354	LYS
1	C	391	ASN
1	C	436	PHE
1	C	441	GLU
1	D	1	MET
1	D	6	LEU
1	D	23	ASN
1	D	31	LEU
1	D	39	GLU
1	D	91	LYS
1	D	135	ARG

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Mol	Chain	Res	Type
1	D	152	LEU
1	D	172	LYS
1	D	242	ARG
1	D	245	MET
1	D	246	GLU
1	D	333	LYS
1	D	341	THR
1	D	353	ARG
1	D	354	LYS
1	D	436	PHE
1	D	441	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	23	ASN
1	A	40	GLN
1	A	77	ASN
1	A	88	ASN
1	A	119	ASN
1	A	130	HIS
1	A	167	ASN
1	A	231	HIS
1	A	278	GLN
1	A	289	GLN
1	A	391	ASN
1	A	394	GLN
1	A	403	GLN
1	A	474	HIS
1	B	23	ASN
1	B	40	GLN
1	B	77	ASN
1	B	88	ASN
1	B	130	HIS
1	B	167	ASN
1	B	231	HIS
1	B	278	GLN
1	B	289	GLN
1	B	391	ASN
1	B	394	GLN
1	B	403	GLN

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Mol	Chain	Res	Type
1	B	419	HIS
1	B	474	HIS
1	C	19	GLN
1	C	23	ASN
1	C	40	GLN
1	C	88	ASN
1	C	167	ASN
1	C	231	HIS
1	C	278	GLN
1	C	289	GLN
1	C	376	GLN
1	C	391	ASN
1	C	394	GLN
1	C	403	GLN
1	C	444	HIS
1	C	474	HIS
1	D	19	GLN
1	D	23	ASN
1	D	40	GLN
1	D	77	ASN
1	D	88	ASN
1	D	119	ASN
1	D	130	HIS
1	D	167	ASN
1	D	231	HIS
1	D	244	HIS
1	D	278	GLN
1	D	289	GLN
1	D	376	GLN
1	D	391	ASN
1	D	394	GLN
1	D	403	GLN
1	D	474	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

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	474/495 (95%)	-0.20	4 (0%) 86 88	13, 20, 27, 35	21 (4%)
1	B	474/495 (95%)	-0.20	7 (1%) 73 77	14, 20, 27, 35	13 (2%)
1	C	474/495 (95%)	-0.19	4 (0%) 86 88	14, 20, 27, 36	15 (3%)
1	D	474/495 (95%)	-0.19	7 (1%) 73 77	14, 20, 27, 39	13 (2%)
All	All	1896/1980 (95%)	-0.19	22 (1%) 79 82	13, 20, 27, 39	62 (3%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.7
1	D	313	ASP	3.1
1	D	354	LYS	3.1
1	B	266	GLU	2.9
1	B	314	ASP	2.8
1	A	340	ALA	2.8
1	B	1	MET	2.7
1	C	1	MET	2.6
1	B	313	ASP	2.6
1	D	330	ARG	2.5
1	B	356	ASN	2.4
1	A	190	ASP	2.4
1	D	333	LYS	2.4
1	D	371	ASP	2.3
1	C	17	GLU	2.3
1	D	200	LEU	2.3
1	C	205	LYS	2.3
1	A	356	ASN	2.3
1	B	355	GLY	2.2
1	C	316	SER	2.1
1	D	316	SER	2.0
1	B	340	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	475	1/1	0.99	0.03	25,25,25,25	0
2	CA	D	475	1/1	0.99	0.05	26,26,26,26	0
2	CA	B	475	1/1	0.99	0.05	27,27,27,27	0
2	CA	C	475	1/1	1.00	0.04	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.