



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:54 AM GMT

PDB ID : 2V8Z
Title : CRYSTAL STRUCTURE OF YAGE, A PROPHAGE PROTEIN BELONGING TO THE DIHYDRODIPICOLINIC ACID SYNTHASE FAMILY FROM E. COLI K12
Authors : Manicka, S.; Peleg, Y.; Unger, T.; Albeck, S.; Dym, O.; Greenblatt, H.M.; Bourenkov, G.; Lamzin, V.; Krishnaswamy, S.; Sussman, J.L.
Deposited on : 2007-08-16
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

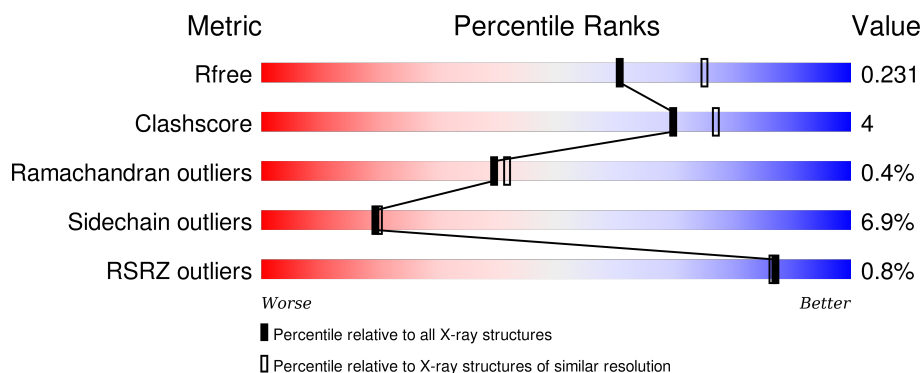
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	343	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>••</div> <div>13%</div> </div> </div>
1	B	343	<div> <div>77%</div> <div>8%</div> <div>•</div> <div>13%</div> </div>
1	C	343	<div> <div>72%</div> <div>11%</div> <div>••</div> <div>13%</div> </div>
1	D	343	<div> <div>%</div> <div>73%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9478 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 YAGE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2250	1443	381	420	6			
1	B	298	Total	C	N	O	S	0	0	0
			2257	1446	385	420	6			
1	C	298	Total	C	N	O	S	0	0	0
			2252	1444	383	419	6			
1	D	298	Total	C	N	O	S	0	0	0
			2255	1445	385	419	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP P75682
A	-16	GLY	-	EXPRESSION TAG	UNP P75682
A	-15	SER	-	EXPRESSION TAG	UNP P75682
A	-14	SER	-	EXPRESSION TAG	UNP P75682
A	-13	HIS	-	EXPRESSION TAG	UNP P75682
A	-12	HIS	-	EXPRESSION TAG	UNP P75682
A	-11	HIS	-	EXPRESSION TAG	UNP P75682
A	-10	HIS	-	EXPRESSION TAG	UNP P75682
A	-9	HIS	-	EXPRESSION TAG	UNP P75682
A	-8	HIS	-	EXPRESSION TAG	UNP P75682
A	-7	SER	-	EXPRESSION TAG	UNP P75682
A	-6	ALA	-	EXPRESSION TAG	UNP P75682
A	-5	GLY	-	EXPRESSION TAG	UNP P75682
A	-4	GLU	-	EXPRESSION TAG	UNP P75682
A	-3	ASN	-	EXPRESSION TAG	UNP P75682
A	-2	LEU	-	EXPRESSION TAG	UNP P75682
A	-1	TYR	-	EXPRESSION TAG	UNP P75682
A	0	PHE	-	EXPRESSION TAG	UNP P75682
A	1	GLN	-	EXPRESSION TAG	UNP P75682
A	2	GLY	-	EXPRESSION TAG	UNP P75682
A	310	CYS	-	EXPRESSION TAG	UNP P75682

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	GLY	-	EXPRESSION TAG	UNP P75682
A	312	ARG	-	EXPRESSION TAG	UNP P75682
A	313	THR	-	EXPRESSION TAG	UNP P75682
A	314	ARG	-	EXPRESSION TAG	UNP P75682
A	315	ALA	-	EXPRESSION TAG	UNP P75682
A	316	PRO	-	EXPRESSION TAG	UNP P75682
A	317	PRO	-	EXPRESSION TAG	UNP P75682
A	318	PRO	-	EXPRESSION TAG	UNP P75682
A	319	PRO	-	EXPRESSION TAG	UNP P75682
A	320	PRO	-	EXPRESSION TAG	UNP P75682
A	321	LEU	-	EXPRESSION TAG	UNP P75682
A	322	ARG	-	EXPRESSION TAG	UNP P75682
A	323	SER	-	EXPRESSION TAG	UNP P75682
A	324	GLY	-	EXPRESSION TAG	UNP P75682
A	325	CYS	-	EXPRESSION TAG	UNP P75682
B	-17	MET	-	EXPRESSION TAG	UNP P75682
B	-16	GLY	-	EXPRESSION TAG	UNP P75682
B	-15	SER	-	EXPRESSION TAG	UNP P75682
B	-14	SER	-	EXPRESSION TAG	UNP P75682
B	-13	HIS	-	EXPRESSION TAG	UNP P75682
B	-12	HIS	-	EXPRESSION TAG	UNP P75682
B	-11	HIS	-	EXPRESSION TAG	UNP P75682
B	-10	HIS	-	EXPRESSION TAG	UNP P75682
B	-9	HIS	-	EXPRESSION TAG	UNP P75682
B	-8	HIS	-	EXPRESSION TAG	UNP P75682
B	-7	SER	-	EXPRESSION TAG	UNP P75682
B	-6	ALA	-	EXPRESSION TAG	UNP P75682
B	-5	GLY	-	EXPRESSION TAG	UNP P75682
B	-4	GLU	-	EXPRESSION TAG	UNP P75682
B	-3	ASN	-	EXPRESSION TAG	UNP P75682
B	-2	LEU	-	EXPRESSION TAG	UNP P75682
B	-1	TYR	-	EXPRESSION TAG	UNP P75682
B	0	PHE	-	EXPRESSION TAG	UNP P75682
B	1	GLN	-	EXPRESSION TAG	UNP P75682
B	2	GLY	-	EXPRESSION TAG	UNP P75682
B	310	CYS	-	EXPRESSION TAG	UNP P75682
B	311	GLY	-	EXPRESSION TAG	UNP P75682
B	312	ARG	-	EXPRESSION TAG	UNP P75682
B	313	THR	-	EXPRESSION TAG	UNP P75682
B	314	ARG	-	EXPRESSION TAG	UNP P75682
B	315	ALA	-	EXPRESSION TAG	UNP P75682
B	316	PRO	-	EXPRESSION TAG	UNP P75682

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	PRO	-	EXPRESSION TAG	UNP P75682
B	318	PRO	-	EXPRESSION TAG	UNP P75682
B	319	PRO	-	EXPRESSION TAG	UNP P75682
B	320	PRO	-	EXPRESSION TAG	UNP P75682
B	321	LEU	-	EXPRESSION TAG	UNP P75682
B	322	ARG	-	EXPRESSION TAG	UNP P75682
B	323	SER	-	EXPRESSION TAG	UNP P75682
B	324	GLY	-	EXPRESSION TAG	UNP P75682
B	325	CYS	-	EXPRESSION TAG	UNP P75682
C	-17	MET	-	EXPRESSION TAG	UNP P75682
C	-16	GLY	-	EXPRESSION TAG	UNP P75682
C	-15	SER	-	EXPRESSION TAG	UNP P75682
C	-14	SER	-	EXPRESSION TAG	UNP P75682
C	-13	HIS	-	EXPRESSION TAG	UNP P75682
C	-12	HIS	-	EXPRESSION TAG	UNP P75682
C	-11	HIS	-	EXPRESSION TAG	UNP P75682
C	-10	HIS	-	EXPRESSION TAG	UNP P75682
C	-9	HIS	-	EXPRESSION TAG	UNP P75682
C	-8	HIS	-	EXPRESSION TAG	UNP P75682
C	-7	SER	-	EXPRESSION TAG	UNP P75682
C	-6	ALA	-	EXPRESSION TAG	UNP P75682
C	-5	GLY	-	EXPRESSION TAG	UNP P75682
C	-4	GLU	-	EXPRESSION TAG	UNP P75682
C	-3	ASN	-	EXPRESSION TAG	UNP P75682
C	-2	LEU	-	EXPRESSION TAG	UNP P75682
C	-1	TYR	-	EXPRESSION TAG	UNP P75682
C	0	PHE	-	EXPRESSION TAG	UNP P75682
C	1	GLN	-	EXPRESSION TAG	UNP P75682
C	2	GLY	-	EXPRESSION TAG	UNP P75682
C	310	CYS	-	EXPRESSION TAG	UNP P75682
C	311	GLY	-	EXPRESSION TAG	UNP P75682
C	312	ARG	-	EXPRESSION TAG	UNP P75682
C	313	THR	-	EXPRESSION TAG	UNP P75682
C	314	ARG	-	EXPRESSION TAG	UNP P75682
C	315	ALA	-	EXPRESSION TAG	UNP P75682
C	316	PRO	-	EXPRESSION TAG	UNP P75682
C	317	PRO	-	EXPRESSION TAG	UNP P75682
C	318	PRO	-	EXPRESSION TAG	UNP P75682
C	319	PRO	-	EXPRESSION TAG	UNP P75682
C	320	PRO	-	EXPRESSION TAG	UNP P75682
C	321	LEU	-	EXPRESSION TAG	UNP P75682
C	322	ARG	-	EXPRESSION TAG	UNP P75682

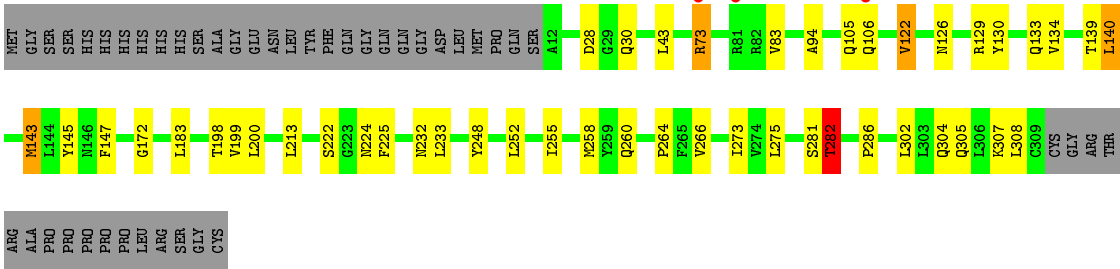
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	323	SER	-	EXPRESSION TAG	UNP P75682
C	324	GLY	-	EXPRESSION TAG	UNP P75682
C	325	CYS	-	EXPRESSION TAG	UNP P75682
D	-17	MET	-	EXPRESSION TAG	UNP P75682
D	-16	GLY	-	EXPRESSION TAG	UNP P75682
D	-15	SER	-	EXPRESSION TAG	UNP P75682
D	-14	SER	-	EXPRESSION TAG	UNP P75682
D	-13	HIS	-	EXPRESSION TAG	UNP P75682
D	-12	HIS	-	EXPRESSION TAG	UNP P75682
D	-11	HIS	-	EXPRESSION TAG	UNP P75682
D	-10	HIS	-	EXPRESSION TAG	UNP P75682
D	-9	HIS	-	EXPRESSION TAG	UNP P75682
D	-8	HIS	-	EXPRESSION TAG	UNP P75682
D	-7	SER	-	EXPRESSION TAG	UNP P75682
D	-6	ALA	-	EXPRESSION TAG	UNP P75682
D	-5	GLY	-	EXPRESSION TAG	UNP P75682
D	-4	GLU	-	EXPRESSION TAG	UNP P75682
D	-3	ASN	-	EXPRESSION TAG	UNP P75682
D	-2	LEU	-	EXPRESSION TAG	UNP P75682
D	-1	TYR	-	EXPRESSION TAG	UNP P75682
D	0	PHE	-	EXPRESSION TAG	UNP P75682
D	1	GLN	-	EXPRESSION TAG	UNP P75682
D	2	GLY	-	EXPRESSION TAG	UNP P75682
D	310	CYS	-	EXPRESSION TAG	UNP P75682
D	311	GLY	-	EXPRESSION TAG	UNP P75682
D	312	ARG	-	EXPRESSION TAG	UNP P75682
D	313	THR	-	EXPRESSION TAG	UNP P75682
D	314	ARG	-	EXPRESSION TAG	UNP P75682
D	315	ALA	-	EXPRESSION TAG	UNP P75682
D	316	PRO	-	EXPRESSION TAG	UNP P75682
D	317	PRO	-	EXPRESSION TAG	UNP P75682
D	318	PRO	-	EXPRESSION TAG	UNP P75682
D	319	PRO	-	EXPRESSION TAG	UNP P75682
D	320	PRO	-	EXPRESSION TAG	UNP P75682
D	321	LEU	-	EXPRESSION TAG	UNP P75682
D	322	ARG	-	EXPRESSION TAG	UNP P75682
D	323	SER	-	EXPRESSION TAG	UNP P75682
D	324	GLY	-	EXPRESSION TAG	UNP P75682
D	325	CYS	-	EXPRESSION TAG	UNP P75682

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	104	Total 104	O 104	0	0
2	B	144	Total 144	O 144	0	0
2	C	119	Total 119	O 119	0	0
2	D	97	Total 97	O 97	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.69 Å 156.49 Å 55.88 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.20 19.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.92-2.20) 99.8 (19.92-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 2.19 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.232 0.190 , 0.231	Depositor DCC
R_{free} test set	3252 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63805 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9478	wwPDB-VP
Average B, all atoms (Å ²)	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.0417e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

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	0.76	3/2298 (0.1%)	0.85	8/3133 (0.3%)
1	B	0.81	2/2305 (0.1%)	0.92	11/3141 (0.4%)
1	C	0.74	2/2300 (0.1%)	0.86	7/3135 (0.2%)
1	D	0.74	3/2303 (0.1%)	0.92	6/3139 (0.2%)
All	All	0.76	10/9206 (0.1%)	0.89	32/12548 (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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	ARG	CZ-NH2	7.80	1.43	1.33
1	A	83	VAL	CB-CG1	-7.08	1.38	1.52
1	D	83	VAL	CB-CG2	-6.74	1.38	1.52
1	B	198	THR	CB-CG2	-6.61	1.30	1.52
1	A	83	VAL	CB-CG2	-6.48	1.39	1.52
1	B	83	VAL	CB-CG1	-6.24	1.39	1.52
1	C	83	VAL	CB-CG1	-6.10	1.40	1.52
1	D	83	VAL	CB-CG1	-6.09	1.40	1.52
1	C	83	VAL	CB-CG2	-5.73	1.40	1.52
1	A	242	VAL	CB-CG1	-5.67	1.41	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	ARG	NE-CZ-NH2	-21.42	109.59	120.30
1	B	73	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	B	73	ARG	NE-CZ-NH1	11.83	126.22	120.30
1	A	282	THR	N-CA-C	8.74	134.61	111.00
1	D	282	THR	N-CA-C	8.50	133.94	111.00
1	D	83	VAL	CG1-CB-CG2	-8.44	97.39	110.90
1	C	282	THR	N-CA-C	8.30	133.41	111.00
1	A	83	VAL	CG1-CB-CG2	-8.03	98.05	110.90
1	D	305	GLN	N-CA-C	-7.62	90.43	111.00
1	B	305	GLN	N-CA-C	-7.55	90.61	111.00
1	C	83	VAL	CG1-CB-CG2	-7.43	99.02	110.90
1	B	83	VAL	CG1-CB-CG2	-7.11	99.53	110.90
1	D	73	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	28	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	28	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	73	ARG	NH1-CZ-NH2	6.38	126.42	119.40
1	C	140	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	122	VAL	CG1-CB-CG2	5.64	119.92	110.90
1	B	282	THR	N-CA-CB	5.57	120.88	110.30
1	C	73	ARG	CA-CB-CG	-5.53	101.23	113.40
1	A	275	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	275	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	242	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	B	198	THR	OG1-CB-CG2	-5.30	97.81	110.00
1	C	304	GLN	N-CA-C	5.23	125.11	111.00
1	A	28	ASP	CB-CG-OD1	-5.18	113.63	118.30
1	B	200	LEU	CB-CG-CD1	5.18	119.81	111.00
1	C	183	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	213	LEU	CB-CG-CD1	5.16	119.77	111.00
1	B	28	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	B	183	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	213	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	SER	Peptide
1	A	304	GLN	Peptide
1	B	281	SER	Peptide
1	B	304	GLN	Peptide
1	C	281	SER	Peptide
1	C	304	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	281	SER	Peptide
1	D	304	GLN	Peptide

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	2250	0	2268	26	0
1	B	2257	0	2281	15	0
1	C	2252	0	2274	29	0
1	D	2255	0	2279	24	0
2	A	104	0	0	5	0
2	B	144	0	0	0	0
2	C	119	0	0	3	0
2	D	97	0	0	6	0
All	All	9478	0	9102	81	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 4.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLN:HE22	1:B:139:THR:H	1.04	0.99
1:C:122:VAL:HG22	1:D:264:PRO:HD3	1.60	0.84
1:D:106:GLN:HG3	2:D:2031:HOH:O	1.75	0.84
1:A:122:VAL:HG22	1:B:264:PRO:HD3	1.61	0.83
1:A:188:HIS:CD2	2:A:2069:HOH:O	2.34	0.80
1:A:73:ARG:HG3	2:A:2019:HOH:O	1.82	0.78
1:A:188:HIS:HE1	1:C:257:GLN:NE2	1.82	0.78
1:D:106:GLN:CG	2:D:2031:HOH:O	2.29	0.78
1:A:257:GLN:CG	2:A:2030:HOH:O	2.31	0.77
1:B:105:GLN:NE2	1:B:139:THR:H	1.85	0.73
1:A:28:ASP:OD1	1:A:28:ASP:N	2.20	0.72
1:C:286:PRO:HB2	1:D:94:ALA:HB3	1.71	0.72
1:D:106:GLN:HB2	2:D:2027:HOH:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:O	1:B:198:THR:HG21	1.91	0.70
1:A:264:PRO:HD3	1:B:122:VAL:HG22	1.72	0.69
1:C:264:PRO:HD3	1:D:122:VAL:HG22	1.74	0.69
1:A:24:ILE:HB	1:A:36:THR:HG22	1.82	0.62
1:C:73:ARG:HG3	1:C:73:ARG:O	2.01	0.60
1:D:28:ASP:CB	2:D:2004:HOH:O	2.50	0.60
1:C:129:ARG:O	1:C:133:GLN:HG3	2.02	0.59
1:C:94:ALA:HB3	1:D:286:PRO:HB2	1.84	0.59
1:C:105:GLN:HB2	1:C:140:LEU:HD22	1.85	0.59
1:C:297:ALA:HA	2:C:2118:HOH:O	2.02	0.59
1:C:297:ALA:O	1:C:301:THR:HG23	2.03	0.59
1:A:188:HIS:HE1	1:C:257:GLN:HE22	1.51	0.56
1:A:105:GLN:NE2	1:A:139:THR:OG1	2.37	0.55
1:D:122:VAL:HG13	1:D:126:ASN:HB2	1.89	0.54
1:D:129:ARG:O	1:D:133:GLN:HG2	2.08	0.53
1:D:105:GLN:HB2	1:D:140:LEU:HD22	1.91	0.53
1:A:94:ALA:HB3	1:B:286:PRO:HB2	1.91	0.52
1:B:255:ILE:O	1:B:258:MET:HG2	2.10	0.52
1:D:105:GLN:NE2	1:D:139:THR:OG1	2.38	0.52
1:B:229:VAL:HG11	1:B:252:LEU:HD13	1.93	0.51
1:C:130:TYR:O	1:C:134:VAL:HG13	2.11	0.50
1:A:188:HIS:CE1	1:C:257:GLN:NE2	2.70	0.49
1:B:292:ASP:H	1:B:295:ARG:HH21	1.58	0.49
1:A:255:ILE:O	1:A:258:MET:HG2	2.12	0.48
1:D:255:ILE:O	1:D:258:MET:HG2	2.13	0.48
1:C:254:GLN:O	1:C:257:GLN:HG2	2.14	0.48
1:A:267:ASN:O	1:A:271:GLU:HG2	2.14	0.47
1:B:229:VAL:CG1	1:B:252:LEU:HD13	2.44	0.47
1:D:233:LEU:HD23	1:D:233:LEU:C	2.35	0.47
1:B:105:GLN:HB2	1:B:140:LEU:HD22	1.97	0.47
1:D:130:TYR:O	1:D:134:VAL:HG13	2.15	0.47
1:C:62:GLN:NE2	2:C:2014:HOH:O	2.48	0.46
1:C:17:ILE:HD12	1:C:230:SER:HB3	1.97	0.46
1:A:122:VAL:HG13	1:A:126:ASN:HB2	1.98	0.46
1:A:115:ILE:HA	1:A:145:TYR:HB3	1.96	0.46
1:D:143:MET:HB2	1:D:143:MET:HE3	1.76	0.46
1:D:302:LEU:HD22	2:D:2097:HOH:O	2.16	0.46
1:A:184:ARG:HD3	1:C:253:LEU:O	2.16	0.46
1:C:172:GLY:HA3	1:C:198:THR:HG23	1.97	0.45
1:C:143:MET:HE3	1:C:143:MET:HB2	1.81	0.45
1:D:122:VAL:HG13	1:D:126:ASN:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:VAL:HG13	1:C:126:ASN:HB2	1.98	0.45
1:A:213:LEU:HD13	1:C:253:LEU:HB3	1.98	0.45
1:B:130:TYR:O	1:B:134:VAL:HG13	2.17	0.45
1:C:260:GLN:NE2	2:C:2108:HOH:O	2.47	0.45
1:B:115:ILE:HA	1:B:145:TYR:HB3	1.98	0.44
1:A:77:ASP:HB3	2:A:2021:HOH:O	2.18	0.43
1:D:232:ASN:HB3	1:D:248:TYR:CZ	2.54	0.43
1:A:297:ALA:O	1:A:301:THR:HG23	2.19	0.43
1:A:229:VAL:CG1	1:A:252:LEU:HD13	2.50	0.42
1:C:289:SER:HB2	1:C:290:PRO:HD2	2.01	0.42
1:A:229:VAL:HG11	1:A:252:LEU:HD13	2.02	0.42
1:A:242:VAL:CG1	1:C:243:ALA:HA	2.50	0.41
1:D:260:GLN:NE2	2:D:2081:HOH:O	2.36	0.41
1:D:224:ASN:HB3	1:D:273:ILE:HD11	2.02	0.41
1:D:282:THR:H	1:D:282:THR:HG23	1.63	0.41
1:A:83:VAL:HB	1:A:84:PRO:CD	2.51	0.41
1:D:172:GLY:HA3	1:D:198:THR:HG23	2.03	0.41
1:B:270:LYS:HA	1:B:273:ILE:HD12	2.03	0.41
1:A:188:HIS:HD2	2:A:2069:HOH:O	1.90	0.41
1:C:13:LEU:O	1:C:198:THR:HG21	2.21	0.41
1:D:222:SER:HA	1:D:225:PHE:CE1	2.56	0.41
1:A:61:SER:OG	1:A:62:GLN:NE2	2.54	0.41
1:C:278:ARG:HA	1:C:279:PRO:HD2	1.96	0.40
1:C:292:ASP:OD1	1:C:295:ARG:HB2	2.21	0.40
1:C:115:ILE:HA	1:C:145:TYR:HB3	2.02	0.40
1:C:233:LEU:C	1:C:233:LEU:HD23	2.42	0.40
1:B:122:VAL:HG13	1:B:126:ASN:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/343 (86%)	289 (98%)	5 (2%)	2 (1%)	26	25
1	B	296/343 (86%)	292 (99%)	4 (1%)	0	100	100
1	C	296/343 (86%)	288 (97%)	6 (2%)	2 (1%)	26	25
1	D	296/343 (86%)	291 (98%)	4 (1%)	1 (0%)	46	50
All	All	1184/1372 (86%)	1160 (98%)	19 (2%)	5 (0%)	39	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	THR
1	A	305	GLN
1	C	282	THR
1	C	305	GLN
1	D	282	THR

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	240/280 (86%)	220 (92%)	20 (8%)	14	13
1	B	241/280 (86%)	229 (95%)	12 (5%)	30	35
1	C	240/280 (86%)	223 (93%)	17 (7%)	18	19
1	D	241/280 (86%)	224 (93%)	17 (7%)	18	19
All	All	962/1120 (86%)	896 (93%)	66 (7%)	19	20

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	36	THR
1	A	43	LEU
1	A	106	GLN
1	A	122	VAL
1	A	134	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	MET
1	A	145	TYR
1	A	147	PHE
1	A	183	LEU
1	A	199	VAL
1	A	200	LEU
1	A	213	LEU
1	A	242	VAL
1	A	252	LEU
1	A	275	LEU
1	A	282	THR
1	A	296	LYS
1	A	301	THR
1	A	308	LEU
1	B	43	LEU
1	B	122	VAL
1	B	140	LEU
1	B	143	MET
1	B	145	TYR
1	B	147	PHE
1	B	183	LEU
1	B	198	THR
1	B	200	LEU
1	B	252	LEU
1	B	275	LEU
1	B	308	LEU
1	C	43	LEU
1	C	73	ARG
1	C	122	VAL
1	C	134	VAL
1	C	143	MET
1	C	145	TYR
1	C	147	PHE
1	C	183	LEU
1	C	199	VAL
1	C	200	LEU
1	C	213	LEU
1	C	252	LEU
1	C	275	LEU
1	C	301	THR
1	C	305	GLN
1	C	307	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	308	LEU
1	D	30	GLN
1	D	43	LEU
1	D	73	ARG
1	D	122	VAL
1	D	140	LEU
1	D	143	MET
1	D	145	TYR
1	D	147	PHE
1	D	183	LEU
1	D	199	VAL
1	D	200	LEU
1	D	213	LEU
1	D	252	LEU
1	D	266	VAL
1	D	275	LEU
1	D	307	LYS
1	D	308	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	102	GLN
1	A	105	GLN
1	A	106	GLN
1	A	188	HIS
1	A	196	HIS
1	B	62	GLN
1	B	102	GLN
1	B	105	GLN
1	B	188	HIS
1	C	62	GLN
1	C	106	GLN
1	C	257	GLN
1	C	260	GLN
1	D	62	GLN
1	D	126	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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, 95th 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 ²)	Q<0.9
1	A	298/343 (86%)	-0.23	4 (1%) 79 78	2, 4, 11, 14	0
1	B	298/343 (86%)	-0.50	1 (0%) 94 94	2, 4, 11, 14	0
1	C	298/343 (86%)	-0.35	1 (0%) 94 94	2, 5, 11, 16	0
1	D	298/343 (86%)	-0.20	3 (1%) 84 83	2, 5, 12, 16	0
All	All	1192/1372 (86%)	-0.32	9 (0%) 87 87	2, 4, 11, 16	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	GLN	3.8
1	A	73	ARG	3.2
1	A	28	ASP	3.1
1	D	73	ARG	2.6
1	C	292	ASP	2.5
1	B	73	ARG	2.3
1	D	81	ARG	2.1
1	A	45	LYS	2.1
1	A	80	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.