



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:51 PM GMT

PDB ID : 1YNY  
Title : Molecular Structure of D-Hydantoinase from a Bacillus sp. AR9: Evidence for mercury inhibition  
Authors : Radha Kishan, K.V.; Vohra, R.M.; Ganeshan, K.; Agrawal, V.; Sharma, V.M.; Sharma, R.  
Deposited on : 2005-01-26  
Resolution : 2.30 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  
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

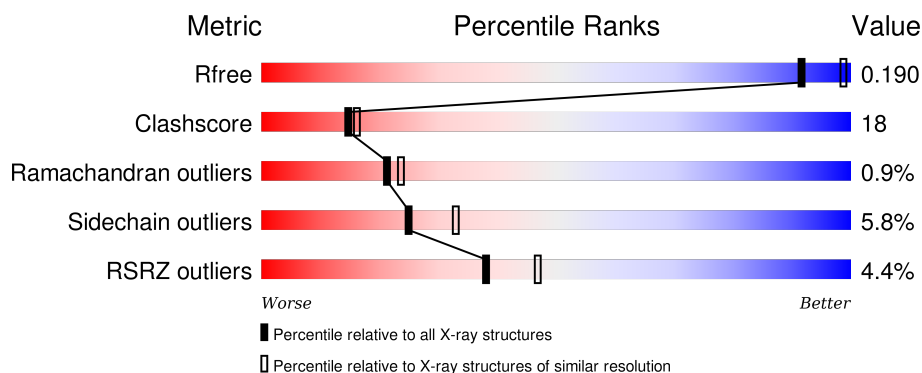
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	461	<div> <div>3%</div> <div>70%</div> <div>24%</div> <div>5%</div> </div>
1	B	461	<div> <div>5%</div> <div>66%</div> <div>31%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7333 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 D-Hydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3509	2226	598	673	12			
1	B	459	Total	C	N	O	S	0	0	0
			3538	2244	603	679	12			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	137	Total	O	0	0
			137	137		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.54Å 129.54Å 102.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.00-2.30) 98.5 (49.24-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.243 0.203 , 0.190	Depositor DCC
$R_{free}$ test set	2165 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.4	EDS
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 42938 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.33	0/3583	0.64	2/4855 (0.0%)
1	B	0.35	0/3613	0.63	1/4898 (0.0%)
All	All	0.34	0/7196	0.64	3/9753 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	HIS	N-CA-C	-5.43	96.35	111.00
1	A	98	GLY	N-CA-C	-5.29	99.87	113.10
1	B	183	HIS	N-CA-C	-5.20	96.96	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3509	0	3444	112	0
1	B	3538	0	3476	136	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	145	0	0	5	0
3	B	137	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7333	0	6920	248	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 18.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG11	1:A:361:LEU:HD12	1.29	1.14
1:B:57:PRO:HA	1:B:90:VAL:HG12	1.33	1.10
1:A:97:LYS:HZ2	1:A:98:GLY:H	1.13	0.91
1:B:35:LEU:H	1:B:35:LEU:HD13	1.39	0.88
1:A:376:PHE:O	1:A:455:ARG:HG2	1.74	0.88
1:B:286:VAL:HB	3:B:5098:HOH:O	1.74	0.86
1:B:347:THR:HG22	1:B:423:VAL:HG21	1.57	0.86
1:B:160:GLN:HE22	1:B:187:GLY:HA3	1.40	0.86
1:A:96:LYS:O	1:A:99:GLU:HB3	1.77	0.85
1:B:97:LYS:HE3	1:B:128:GLU:HB3	1.58	0.83
1:B:148:SER:HB2	1:B:455:ARG:HH22	1.42	0.83
1:A:92:PHE:CE1	1:A:150:LYS:HD2	2.14	0.83
1:A:190:LEU:HD13	1:A:212:ARG:HB3	1.60	0.81
1:A:11:VAL:HG11	1:A:361:LEU:CD1	2.13	0.77
1:A:9:THR:HG22	1:A:18:GLN:HG2	1.66	0.76
1:A:347:THR:HG21	1:A:402:ARG:NH2	2.01	0.76
1:B:92:PHE:CE1	1:B:150:LYS:HD2	2.20	0.75
1:B:57:PRO:HA	1:B:90:VAL:CG1	2.16	0.75
1:B:130:ASN:O	1:B:134:LEU:HD13	1.86	0.75
1:B:11:VAL:HG13	1:B:51:ILE:HG22	1.69	0.73
1:B:103:SER:O	1:B:107:THR:HG23	1.87	0.73
1:A:99:GLU:OE1	1:A:127:ALA:HB3	1.89	0.73
1:B:243:ALA:H	1:B:296:ASN:ND2	1.87	0.73
1:B:243:ALA:H	1:B:296:ASN:HD22	1.35	0.72
1:A:97:LYS:NZ	1:A:98:GLY:H	1.87	0.70
1:B:360:SER:H	1:B:363:GLN:HE21	1.38	0.70
1:B:2:LYS:HG2	1:B:40:ALA:HB2	1.73	0.70
1:B:160:GLN:NE2	1:B:187:GLY:HA3	2.07	0.70
1:A:97:LYS:HE2	1:A:128:GLU:OE1	1.92	0.69
1:B:102:LYS:HA	3:B:5096:HOH:O	1.92	0.69
1:A:310:GLN:O	1:A:367:ILE:HD12	1.93	0.69
1:B:344:ASP:O	1:B:348:ILE:HG23	1.94	0.68
1:A:243:ALA:H	1:A:296:ASN:HD22	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:HD23	1:B:101:LEU:H	1.59	0.66
1:B:33:HIS:O	1:B:35:LEU:N	2.29	0.66
1:A:189:VAL:HG23	1:A:190:LEU:HD23	1.77	0.66
1:B:2:LYS:HA	1:B:23:ILE:O	1.96	0.65
1:A:141:ILE:HD12	1:A:176:LEU:HD13	1.78	0.65
1:B:367:ILE:HD11	3:B:5018:HOH:O	1.97	0.65
1:B:137:LEU:O	1:B:140:VAL:HG22	1.97	0.65
1:A:304:LEU:HD22	1:A:367:ILE:CD1	2.27	0.65
1:A:243:ALA:H	1:A:296:ASN:ND2	1.95	0.64
1:A:206:ILE:HD13	1:A:206:ILE:O	1.97	0.64
1:B:96:LYS:HD2	3:B:5061:HOH:O	1.96	0.64
1:A:43:ILE:HD11	1:A:395:ILE:HD13	1.80	0.64
1:A:126:ILE:HD11	1:A:149:LEU:HD13	1.80	0.64
1:B:351:SER:CB	1:B:423:VAL:HG23	2.27	0.64
1:A:326:GLU:O	1:A:329:ARG:HG2	1.98	0.64
1:A:296:ASN:O	1:A:300:LEU:HD22	1.97	0.64
1:A:351:SER:HB2	1:A:423:VAL:HG13	1.80	0.63
1:B:79:ARG:NH1	1:B:79:ARG:HB3	2.13	0.63
1:B:320:ASN:HD22	1:B:414:ASP:H	1.47	0.63
1:A:304:LEU:HD22	1:A:367:ILE:HD11	1.81	0.62
1:A:347:THR:HG21	1:A:402:ARG:HH21	1.63	0.62
1:A:322:ARG:HH11	1:A:322:ARG:HG3	1.64	0.62
1:A:344:ASP:O	1:A:348:ILE:HG23	2.00	0.61
1:A:318:PRO:HB2	1:A:413:VAL:HG21	1.81	0.61
1:B:361:LEU:O	1:B:364:PHE:HB3	2.00	0.61
1:A:115:LYS:HG2	3:A:1137:HOH:O	2.00	0.61
1:B:350:TYR:OH	1:B:355:ARG:NH1	2.34	0.60
1:B:43:ILE:HD11	1:B:395:ILE:HD13	1.81	0.60
1:B:35:LEU:CD1	1:B:35:LEU:H	2.12	0.60
1:B:328:GLY:HA3	1:B:335:ILE:HG12	1.81	0.60
1:B:40:ALA:HA	3:B:5118:HOH:O	2.00	0.60
1:B:239:HIS:CE1	1:B:289:PRO:HD3	2.37	0.60
1:A:351:SER:CB	1:A:423:VAL:HG13	2.32	0.60
1:A:190:LEU:HD22	1:A:212:ARG:HA	1.84	0.60
1:A:310:GLN:HB2	1:A:371:LYS:HG2	1.84	0.60
1:A:97:LYS:HD3	1:A:98:GLY:N	2.17	0.59
1:B:43:ILE:HD13	1:B:43:ILE:C	2.22	0.59
1:A:78:THR:HB	1:A:118:ILE:HG12	1.84	0.59
1:A:239:HIS:CE1	1:A:289:PRO:HD3	2.38	0.59
1:B:240:VAL:O	1:B:263:THR:HG23	2.02	0.59
1:B:397:ASP:O	1:B:425:GLY:HA2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PRO:HB2	1:B:413:VAL:HG21	1.86	0.58
1:B:347:THR:CG2	1:B:423:VAL:HG21	2.32	0.58
1:A:97:LYS:HZ2	1:A:98:GLY:N	1.93	0.58
1:B:320:ASN:H	1:B:324:GLN:HE21	1.51	0.58
1:A:6:ARG:HH11	1:A:6:ARG:HG3	1.68	0.58
1:A:206:ILE:HD12	1:A:210:TYR:CZ	2.40	0.57
1:A:361:LEU:O	1:A:364:PHE:HB3	2.04	0.56
1:B:37:VAL:HG13	1:B:37:VAL:O	2.05	0.56
1:A:272:VAL:HG13	1:A:291:LEU:O	2.05	0.56
1:B:79:ARG:HH11	1:B:79:ARG:HB3	1.69	0.56
1:A:114:GLY:C	1:A:115:LYS:HD2	2.26	0.56
1:B:286:VAL:HG21	1:B:335:ILE:HG21	1.88	0.55
1:A:64:PRO:HA	1:A:69:VAL:HG12	1.89	0.55
1:B:283:ALA:O	1:B:286:VAL:HG22	2.07	0.55
1:A:160:GLN:OE1	1:A:187:GLY:HA3	2.06	0.55
1:B:263:THR:HG21	1:B:300:LEU:HD13	1.87	0.55
1:A:288:SER:HA	1:A:289:PRO:C	2.27	0.55
1:B:113:ARG:HB3	1:B:113:ARG:NH1	2.21	0.55
1:B:126:ILE:HD13	1:B:149:LEU:HB3	1.88	0.55
1:A:340:PRO:HG2	1:A:417:PRO:HD3	1.88	0.54
1:B:288:SER:HA	1:B:289:PRO:C	2.28	0.54
1:A:378:MET:HE2	1:A:453:ILE:HD12	1.90	0.54
1:B:190:LEU:HD22	1:B:212:ARG:HA	1.89	0.54
1:A:337:ASN:N	1:A:337:ASN:HD22	2.05	0.54
1:A:137:LEU:O	1:A:140:VAL:HG12	2.09	0.53
1:A:43:ILE:O	1:A:43:ILE:HG13	2.07	0.53
1:B:348:ILE:C	1:B:348:ILE:HD12	2.29	0.53
1:A:137:LEU:HA	1:A:140:VAL:HG12	1.91	0.52
1:A:316:HIS:CG	1:A:342:ILE:HB	2.43	0.52
1:A:97:LYS:HZ3	1:A:97:LYS:HA	1.73	0.52
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.74	0.52
1:A:39:GLY:O	1:A:40:ALA:HB2	2.09	0.52
1:A:348:ILE:HD12	1:A:348:ILE:C	2.30	0.52
1:B:141:ILE:C	1:B:141:ILE:HD12	2.29	0.52
1:B:35:LEU:HB2	1:B:37:VAL:HG12	1.90	0.52
1:B:459:GLU:OE2	1:B:460:GLN:NE2	2.43	0.52
1:B:43:ILE:HD13	1:B:43:ILE:O	2.10	0.52
1:A:240:VAL:O	1:A:263:THR:HG23	2.10	0.52
1:B:78:THR:HB	1:B:118:ILE:HG12	1.91	0.51
1:B:35:LEU:N	1:B:35:LEU:HD13	2.18	0.51
1:B:328:GLY:HA3	1:B:335:ILE:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HD12	1:A:210:TYR:CE2	2.45	0.51
1:B:126:ILE:HD11	1:B:149:LEU:HD22	1.91	0.51
1:A:455:ARG:HH11	1:A:455:ARG:HG2	1.76	0.51
1:B:337:ASN:HD22	1:B:337:ASN:N	2.09	0.51
1:A:389:SER:HB3	3:A:1126:HOH:O	2.10	0.51
1:B:90:VAL:O	1:B:90:VAL:HG13	2.11	0.51
1:B:154:ALA:O	1:B:160:GLN:HB2	2.11	0.51
1:B:286:VAL:HG21	1:B:335:ILE:CG2	2.41	0.50
1:B:243:ALA:N	1:B:296:ASN:HD22	2.08	0.50
1:A:347:THR:HG23	3:A:1106:HOH:O	2.11	0.50
1:B:93:CYS:HA	1:B:108:TRP:CE2	2.46	0.50
1:B:246:VAL:O	1:B:249:ILE:HG12	2.12	0.50
1:A:170:LEU:HD13	1:A:180:VAL:HG21	1.93	0.49
1:B:181:GLN:HA	1:B:236:TYR:O	2.11	0.49
1:A:64:PRO:HG3	3:A:1119:HOH:O	2.13	0.49
1:B:249:ILE:O	1:B:253:ARG:HG3	2.13	0.49
1:B:371:LYS:HG3	3:B:5065:HOH:O	2.12	0.49
1:B:186:ASN:O	1:B:190:LEU:HG	2.13	0.49
1:A:96:LYS:O	1:A:99:GLU:CB	2.57	0.49
1:A:71:ALA:HB3	1:A:413:VAL:HG22	1.95	0.49
1:A:190:LEU:CD1	1:A:212:ARG:HB3	2.37	0.48
1:A:181:GLN:HA	1:A:236:TYR:O	2.13	0.48
1:B:379:PHE:CG	1:B:380:PRO:HA	2.49	0.48
1:B:406:VAL:HG13	1:B:407:GLU:OE2	2.14	0.48
1:A:423:VAL:CG1	1:A:424:TYR:N	2.76	0.48
1:A:293:GLU:OE2	1:A:295:TRP:HZ3	1.96	0.48
1:B:203:THR:HB	1:B:331:ASP:HA	1.96	0.48
1:A:125:MET:HE3	1:A:159:PHE:HB3	1.94	0.48
1:B:90:VAL:HG13	1:B:123:HIS:NE2	2.29	0.47
1:A:322:ARG:NH1	1:A:322:ARG:HG3	2.28	0.47
1:B:212:ARG:HD2	3:B:5052:HOH:O	2.14	0.47
1:B:186:ASN:HB3	1:B:189:VAL:HG22	1.96	0.47
1:B:189:VAL:HG23	1:B:190:LEU:HD23	1.96	0.47
1:B:312:VAL:HG23	1:B:367:ILE:HG23	1.97	0.47
1:A:4:TRP:CH2	1:A:6:ARG:HD3	2.50	0.47
1:B:64:PRO:HG3	3:B:5114:HOH:O	2.13	0.47
1:A:249:ILE:O	1:A:253:ARG:HG3	2.15	0.47
1:B:351:SER:HB3	1:B:423:VAL:HG23	1.97	0.47
1:A:93:CYS:HA	1:A:108:TRP:CE2	2.50	0.47
1:A:346:LEU:HD22	1:A:364:PHE:CZ	2.50	0.46
1:B:140:VAL:O	1:B:144:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:HD23	1:B:140:VAL:HG21	1.96	0.46
1:B:156:LYS:O	1:B:157:ASN:HB2	2.14	0.46
1:A:97:LYS:HA	1:A:97:LYS:NZ	2.31	0.46
1:A:43:ILE:HD11	1:A:395:ILE:CD1	2.45	0.46
1:B:440:ASP:O	1:B:441:LYS:HB2	2.16	0.46
1:A:53:GLY:HA2	1:A:394:VAL:HG23	1.98	0.46
1:A:310:GLN:C	1:A:367:ILE:HD12	2.36	0.45
1:B:90:VAL:CG1	1:B:123:HIS:NE2	2.79	0.45
1:B:430:VAL:O	1:B:437:VAL:HG12	2.16	0.45
1:A:186:ASN:HB3	1:A:189:VAL:HG22	1.96	0.45
1:B:320:ASN:H	1:B:324:GLN:NE2	2.15	0.45
1:B:6:ARG:NH1	1:B:42:GLU:HB2	2.31	0.45
1:B:277:GLN:OE1	1:B:281:GLU:HG2	2.15	0.45
1:A:141:ILE:HD12	1:A:176:LEU:CD1	2.45	0.45
1:B:62:ASP:HB2	1:B:73:ASP:HA	1.99	0.45
1:B:190:LEU:O	1:B:194:THR:HG23	2.16	0.45
1:A:131:ASP:O	1:A:135:GLU:HG3	2.17	0.45
1:B:238:VAL:HG23	1:B:239:HIS:CE1	2.52	0.45
1:A:262:GLU:HB2	1:A:311:THR:OG1	2.17	0.45
1:B:423:VAL:HB	3:B:5105:HOH:O	2.17	0.44
1:A:423:VAL:HG12	1:A:424:TYR:N	2.31	0.44
1:A:182:VAL:O	1:A:238:VAL:HG22	2.16	0.44
1:A:6:ARG:NH1	1:A:6:ARG:HG3	2.32	0.44
1:B:11:VAL:HG21	1:B:361:LEU:HG	1.99	0.44
1:B:189:VAL:HG23	1:B:190:LEU:N	2.32	0.44
1:B:317:CYS:O	1:B:338:GLY:HA3	2.17	0.44
1:A:65:PHE:CE2	1:A:336:PRO:HB3	2.52	0.44
1:A:2:LYS:HA	1:A:23:ILE:O	2.17	0.44
1:B:253:ARG:HG2	3:B:5123:HOH:O	2.16	0.44
1:B:54:GLY:HA2	1:B:369:SER:HB3	1.99	0.44
1:B:378:MET:HE3	1:B:453:ILE:HD13	1.99	0.44
1:A:378:MET:CE	1:A:453:ILE:HD12	2.47	0.44
1:B:349:LEU:HA	1:B:349:LEU:HD12	1.90	0.44
1:B:392:ASP:HA	1:B:431:LEU:O	2.18	0.44
1:B:158:VAL:HG12	1:B:159:PHE:CD1	2.53	0.43
1:B:278:PRO:O	1:B:279:ASP:HB2	2.18	0.43
1:B:423:VAL:HG22	1:B:424:TYR:N	2.33	0.43
1:B:101:LEU:HD23	1:B:103:SER:HB3	1.99	0.43
1:A:166:LEU:HD13	1:A:227:LEU:HD12	2.00	0.43
1:A:431:LEU:HD23	1:A:436:PHE:HA	2.00	0.43
1:B:90:VAL:HG13	1:B:123:HIS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG21	1:A:252:ALA:HB2	1.98	0.43
1:B:63:MET:HA	1:B:64:PRO:HD3	1.79	0.43
1:A:101:LEU:O	1:A:105:ILE:HG13	2.19	0.43
1:B:351:SER:HB2	1:B:423:VAL:CG2	2.49	0.43
1:A:186:ASN:O	1:A:190:LEU:HG	2.19	0.42
1:A:63:MET:HA	1:A:64:PRO:HD3	1.87	0.42
1:B:330:GLY:O	1:B:331:ASP:HB3	2.20	0.42
1:B:316:HIS:CG	1:B:342:ILE:HB	2.54	0.42
1:A:348:ILE:O	1:A:352:GLU:HB2	2.19	0.42
1:B:378:MET:CE	1:B:453:ILE:HD13	2.49	0.42
1:B:90:VAL:CG1	1:B:123:HIS:HE2	2.33	0.42
1:B:2:LYS:HG2	1:B:40:ALA:CB	2.46	0.42
1:A:243:ALA:O	1:A:246:VAL:HG22	2.20	0.42
1:B:129:ALA:HB1	1:B:134:LEU:HD11	2.02	0.42
1:B:101:LEU:O	1:B:102:LYS:HB2	2.19	0.42
1:B:409:HIS:C	1:B:409:HIS:CD2	2.93	0.42
1:A:404:LEU:HD12	1:A:421:MET:HE3	2.02	0.42
1:A:191:ASP:OD1	1:A:195:LYS:HE2	2.19	0.42
1:A:352:GLU:O	1:A:358:ARG:NH1	2.53	0.42
1:B:113:ARG:HB3	1:B:113:ARG:HH11	1.83	0.42
1:B:253:ARG:NH2	3:B:5093:HOH:O	2.53	0.42
1:B:394:VAL:HG13	1:B:427:VAL:HG13	2.02	0.42
1:B:286:VAL:O	1:B:286:VAL:HG23	2.20	0.41
1:A:92:PHE:HE1	1:A:150:LYS:HB2	1.85	0.41
1:A:310:GLN:CD	1:A:310:GLN:N	2.73	0.41
1:B:148:SER:CB	1:B:455:ARG:HH22	2.24	0.41
1:A:238:VAL:HG23	1:A:239:HIS:CE1	2.55	0.41
1:B:97:LYS:HD3	1:B:97:LYS:HA	1.89	0.41
1:A:141:ILE:HG23	1:A:147:THR:HG22	2.01	0.41
1:A:126:ILE:HB	3:A:1134:HOH:O	2.19	0.41
1:A:322:ARG:NH1	1:A:326:GLU:OE1	2.54	0.41
1:A:355:ARG:HA	1:A:355:ARG:HD2	1.86	0.41
1:A:392:ASP:C	1:A:393:ILE:HD12	2.40	0.41
1:B:148:SER:HB2	1:B:455:ARG:NH2	2.23	0.41
1:A:409:HIS:C	1:A:409:HIS:ND1	2.74	0.41
1:B:101:LEU:N	1:B:101:LEU:HD23	2.33	0.41
1:A:246:VAL:HG23	1:A:247:GLN:N	2.35	0.41
1:A:65:PHE:CD2	1:A:336:PRO:HB3	2.55	0.41
1:A:272:VAL:HG22	1:A:292:ARG:O	2.21	0.41
1:B:213:PRO:HA	1:B:214:PRO:HD3	1.93	0.41
1:B:346:LEU:HD13	1:B:346:LEU:C	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ALA:HB3	1:B:413:VAL:HG22	2.03	0.40
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.86	0.40
1:B:225:ILE:HG21	1:B:252:ALA:HB2	2.04	0.40
1:B:339:GLY:C	1:B:341:LEU:HD22	2.42	0.40
1:B:140:VAL:HA	1:B:144:GLU:HG2	2.02	0.40
1:B:458:PHE:CG	1:B:459:GLU:N	2.88	0.40
1:B:78:THR:OG1	1:B:117:VAL:HG22	2.21	0.40
1:B:261:GLY:HA3	1:B:309:LEU:HD23	2.03	0.40
1:B:379:PHE:CD2	1:B:380:PRO:HA	2.56	0.40
1:A:97:LYS:CE	1:A:98:GLY:H	2.34	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	451/461 (98%)	426 (94%)	21 (5%)	4 (1%)	21	24
1	B	457/461 (99%)	425 (93%)	28 (6%)	4 (1%)	21	24
All	All	908/922 (98%)	851 (94%)	49 (5%)	8 (1%)	21	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASP
1	B	34	GLN
1	A	278	PRO
1	A	40	ALA
1	A	239	HIS
1	B	38	ASN
1	B	239	HIS
1	B	331	ASP

### 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	369/375 (98%)	344 (93%)	25 (7%)	20	25
1	B	373/375 (100%)	355 (95%)	18 (5%)	31	42
All	All	742/750 (99%)	699 (94%)	43 (6%)	25	33

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	97	LYS
1	A	108	TRP
1	A	124	LEU
1	A	134	LEU
1	A	166	LEU
1	A	170	LEU
1	A	172	LYS
1	A	179	LEU
1	A	206	ILE
1	A	212	ARG
1	A	263	THR
1	A	268	LEU
1	A	272	VAL
1	A	295	TRP
1	A	300	LEU
1	A	310	GLN
1	A	322	ARG
1	A	337	ASN
1	A	348	ILE
1	A	361	LEU
1	A	371	LYS
1	A	409	HIS
1	A	453	ILE
1	A	455	ARG
1	B	11	VAL
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	35	LEU
1	B	38	ASN
1	B	43	ILE
1	B	108	TRP
1	B	124	LEU
1	B	166	LEU
1	B	179	LEU
1	B	263	THR
1	B	268	LEU
1	B	272	VAL
1	B	348	ILE
1	B	355	ARG
1	B	356	GLN
1	B	381	ARG
1	B	409	HIS
1	B	412	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	181	GLN
1	A	247	GLN
1	A	258	ASN
1	A	277	GLN
1	A	296	ASN
1	A	306	ASN
1	A	337	ASN
1	B	38	ASN
1	B	132	GLN
1	B	157	ASN
1	B	160	GLN
1	B	258	ASN
1	B	296	ASN
1	B	306	ASN
1	B	320	ASN
1	B	324	GLN
1	B	337	ASN
1	B	356	GLN
1	B	363	GLN
1	B	412	ASN
1	B	446	GLN

### 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](#)

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 [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 ⓘ

### 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	455/461 (98%)	0.07	15 (3%) 50 59	10, 21, 37, 63	0
1	B	459/461 (99%)	0.17	25 (5%) 29 38	10, 21, 42, 67	0
All	All	914/922 (99%)	0.12	40 (4%) 38 47	10, 21, 40, 67	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LEU	10.8
1	B	99	GLU	8.9
1	A	39	GLY	6.5
1	A	99	GLU	6.2
1	B	38	ASN	6.1
1	B	37	VAL	5.6
1	B	35	LEU	5.5
1	B	34	GLN	5.4
1	A	33	HIS	5.1
1	A	278	PRO	4.8
1	B	98	GLY	4.1
1	A	34	GLN	4.0
1	A	40	ALA	3.9
1	B	278	PRO	3.3
1	B	97	LYS	3.2
1	B	18	GLN	3.2
1	B	40	ALA	3.2
1	B	279	ASP	3.2
1	A	279	ASP	3.1
1	B	100	SER	3.1
1	B	36	SER	2.9
1	B	39	GLY	2.8
1	B	4	TRP	2.8
1	A	4	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	460	GLN	2.6
1	A	202	ASN	2.6
1	A	27	ARG	2.5
1	B	202	ASN	2.4
1	B	67	GLY	2.4
1	B	329	ARG	2.4
1	A	330	GLY	2.2
1	A	18	GLN	2.2
1	B	330	GLY	2.2
1	A	97	LYS	2.2
1	A	198	LEU	2.1
1	B	96	LYS	2.1
1	B	33	HIS	2.1
1	A	322	ARG	2.1
1	B	207	TYR	2.1
1	B	331	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	A	471	1/1	0.99	0.09	-1.69	17,17,17,17	0
2	MN	B	471	1/1	0.99	0.09	-1.70	17,17,17,17	0
2	MN	B	472	1/1	0.99	0.08	-1.91	15,15,15,15	0
2	MN	A	472	1/1	0.99	0.09	-2.03	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.