



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:58 AM UTC

PDB ID : 1YNY / pdb_00001yny
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

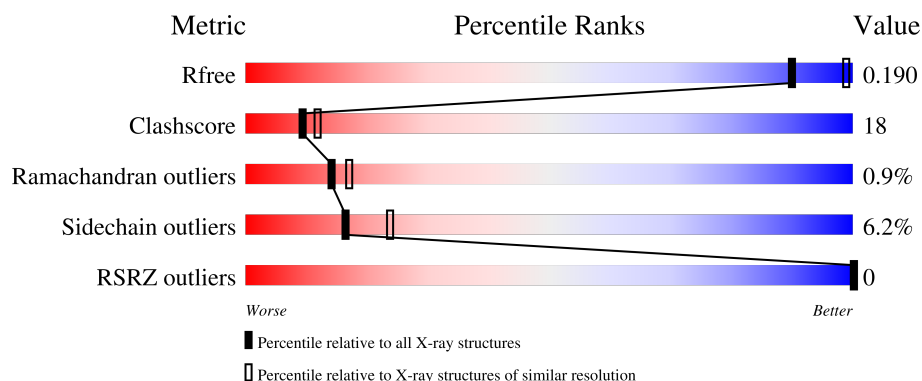
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	461	 66% 27% 5%
1	B	461	 65% 30% 5%

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 (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is water.

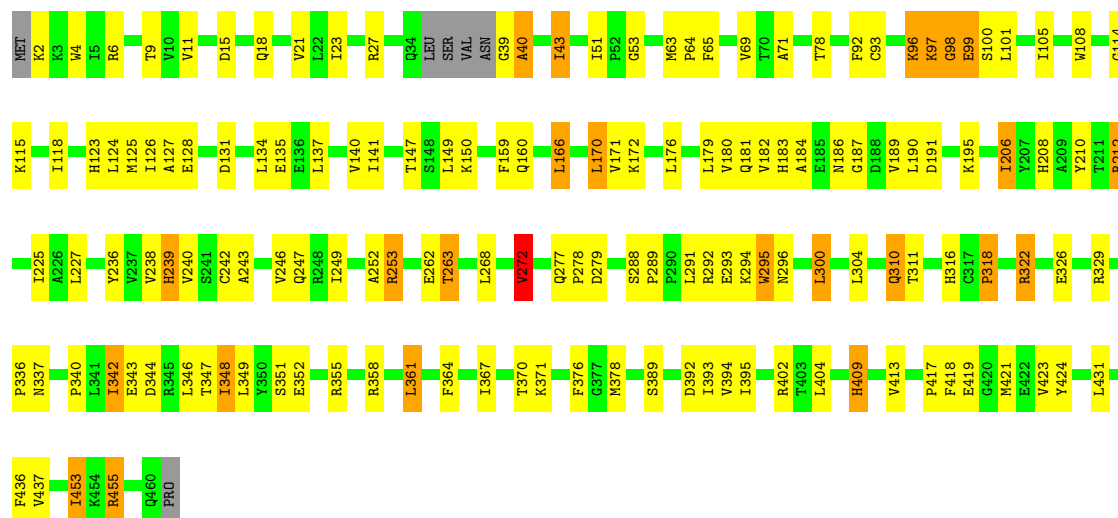
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	137	Total	O	0	0
			137	137		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

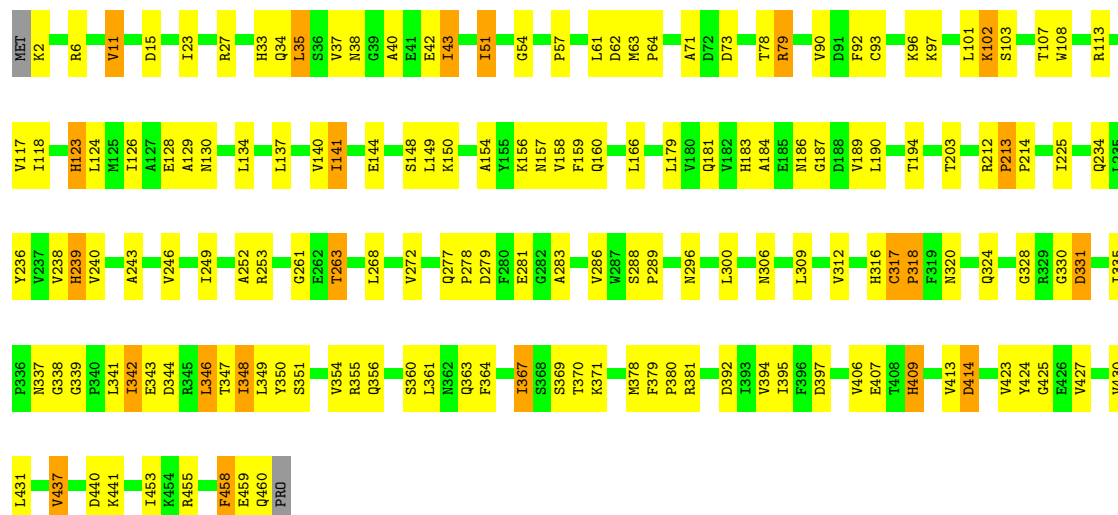
• Molecule 1: D-Hydantoinase

Chain A: 



• Molecule 1: D-Hydantoinase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	129.54Å 129.54Å 102.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.00-2.30) 98.5 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7333	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.40	0/3583	0.97	20/4855 (0.4%)
1	B	0.40	0/3613	0.96	20/4898 (0.4%)
All	All	0.40	0/7196	0.96	40/9753 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	VAL	N-CA-C	-12.96	101.24	112.12
1	A	437	VAL	N-CA-C	-11.85	102.30	111.90
1	A	98	GLY	N-CA-C	-8.76	99.87	114.76
1	A	183	HIS	N-CA-C	-7.49	96.35	108.41
1	B	458	PHE	N-CA-C	7.45	120.49	110.35
1	A	370	THR	N-CA-C	7.41	119.00	111.07
1	B	183	HIS	N-CA-C	-7.11	96.96	108.41
1	B	342	ILE	N-CA-C	6.79	119.54	111.05
1	B	102	LYS	N-CA-C	-6.41	104.65	113.56
1	A	27	ARG	N-CA-C	6.35	118.60	109.14
1	B	370	THR	N-CA-C	6.31	117.83	111.07
1	B	184	ALA	N-CA-C	6.30	119.80	107.57
1	B	123	HIS	N-CA-C	-6.29	100.39	110.14
1	B	317	CYS	CA-C-N	6.26	126.02	119.76
1	B	317	CYS	C-N-CA	6.26	126.02	119.76
1	A	184	ALA	N-CA-C	6.21	119.29	107.75
1	A	99	GLU	N-CA-C	6.06	119.39	109.76
1	A	277	GLN	CA-C-N	5.94	127.27	119.84
1	A	277	GLN	C-N-CA	5.94	127.27	119.84
1	A	242	CYS	N-CA-C	5.91	118.40	109.41
1	A	123	HIS	N-CA-C	-5.85	100.65	109.95
1	B	318	PRO	N-CA-C	5.84	120.36	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASP	N-CA-C	5.75	119.05	110.14
1	B	51	ILE	N-CA-C	5.69	114.15	107.84
1	A	294	LYS	N-CA-C	5.64	118.97	111.75
1	A	343	GLU	N-CA-C	5.47	118.42	111.69
1	B	343	GLU	N-CA-C	5.41	118.35	111.69
1	B	414	ASP	N-CA-C	5.33	119.49	113.15
1	B	306	ASN	N-CA-C	5.31	118.78	112.72
1	A	51	ILE	N-CA-C	5.25	113.66	107.84
1	A	208	HIS	N-CA-C	-5.24	105.64	111.36
1	A	318	PRO	N-CA-C	5.22	120.25	111.32
1	A	15	ASP	N-CA-C	5.22	118.51	110.42
1	B	213	PRO	CA-C-N	5.21	125.26	119.32
1	B	213	PRO	C-N-CA	5.21	125.26	119.32
1	B	354	VAL	N-CA-C	5.18	115.29	110.42
1	B	27	ARG	N-CA-C	5.17	118.01	109.85
1	A	342	ILE	N-CA-C	5.11	117.43	111.05
1	A	272	VAL	N-CA-C	5.09	118.20	111.17
1	A	100	SER	N-CA-C	-5.07	98.31	107.75

There are no chirality outliers.

There are no planarity outliers.

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	3509	0	3444	117	0
1	B	3538	0	3476	135	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
All	All	7333	0	6920	252	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 (252) 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:HD13	1:B:35:LEU:H	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:378:MET:HE3	1:A:453:ILE:HD12	1.63	0.78
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:378:MET:HE3	1:B:453:ILE:HD13	1.66	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:2:LYS:HG2	1:B:40:ALA:HB2	1.73	0.70
1:B:360:SER:H	1:B:363:GLN:HE21	1.38	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
1:B:101:LEU:H	1:B:101:LEU:HD23	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:43:ILE:C	1:B:43:ILE:HD13	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:O	1:B:140:VAL:HG22	1.97	0.65
1:B:367:ILE:HD11	3:B:5018:HOH:O	1.97	0.65
1:A:304:LEU:HD22	1:A:367:ILE:CD1	2.27	0.65
1:A:206:ILE:HD13	1:A:206:ILE:O	1.97	0.64
1:A:243:ALA:H	1:A:296:ASN:ND2	1.95	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:A:404:LEU:HD12	1:A:421:MET:HE2	1.79	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:HG3	1:A:322:ARG:HH11	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:A:115:LYS:HG2	3:A:1137:HOH:O	2.00	0.61
1:B:361:LEU:O	1:B:364:PHE:HB3	2.00	0.61
1:A:114:GLY:C	1:A:115:LYS:HD2	2.26	0.61
1:B:43:ILE:HD11	1:B:395:ILE:HD13	1.81	0.60
1:B:350:TYR:OH	1:B:355:ARG:NH1	2.34	0.60
1:B:35:LEU:H	1:B:35:LEU:CD1	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:A:78:THR:HB	1:A:118:ILE:HG12	1.84	0.59
1:A:288:SER:HA	1:A:289:PRO:C	2.27	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
1:B:288:SER:HA	1:B:289:PRO:C	2.28	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:HD12	1:B:141:ILE:C	2.29	0.58
1:A:97:LYS:HZ2	1:A:98:GLY:N	1.93	0.58
1:A:6:ARG:HG3	1:A:6:ARG:HH11	1.68	0.58
1:B:320:ASN:H	1:B:324:GLN:HE21	1.51	0.58
1:B:348:ILE:C	1:B:348:ILE:HD12	2.29	0.57
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:A:272:VAL:HG13	1:A:291:LEU:O	2.05	0.56
1:A:348:ILE:C	1:A:348:ILE:HD12	2.30	0.56
1:B:37:VAL:HG13	1:B:37:VAL:O	2.05	0.56
1:B:79:ARG:HB3	1:B:79:ARG:HH11	1.69	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:A:160:GLN:OE1	1:A:187:GLY:HA3	2.06	0.55
1:B:283:ALA:O	1:B:286:VAL:HG22	2.07	0.55
1:B:263:THR:HG21	1:B:300:LEU:HD13	1.87	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: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:378:MET:HE3	1:A:453:ILE:CD1	2.34	0.53
1:A:43:ILE:HG13	1:A:43:ILE:O	2.07	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:HA	1:A:97:LYS:HZ3	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: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:A:240:VAL:O	1:A:263:THR:HG23	2.10	0.52
1:B:43:ILE:HD13	1:B:43:ILE:O	2.10	0.52
1:B:78:THR:HB	1:B:118:ILE:HG12	1.91	0.51
1:B:35:LEU:HD13	1:B:35:LEU:N	2.18	0.51
1:A:206:ILE:HD12	1:A:210:TYR:CE2	2.45	0.51
1:B:328:GLY:HA3	1:B:335:ILE:CG1	2.41	0.51
1:B:126:ILE:HD11	1:B:149:LEU:HD22	1.91	0.51
1:A:389:SER:HB3	3:A:1126:HOH:O	2.10	0.51
1:A:455:ARG:HG2	1:A:455:ARG:HH11	1.76	0.51
1:B:337:ASN:N	1:B:337:ASN:HD22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:243:ALA:N	1:B:296:ASN:HD22	2.08	0.50
1:B:286:VAL:HG21	1:B:335:ILE:CG2	2.41	0.50
1:A:310:GLN:C	1:A:367:ILE:HD12	2.36	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:A:125:MET:HE1	1:A:159:PHE:CD1	2.48	0.49
1:B:186:ASN:O	1:B:190:LEU:HG	2.13	0.49
1:A:71:ALA:HB3	1:A:413:VAL:HG22	1.95	0.49
1:A:96:LYS:O	1:A:99:GLU:CB	2.57	0.49
1:A:181:GLN:HA	1:A:236:TYR:O	2.13	0.48
1:A:190:LEU:CD1	1:A:212:ARG:HB3	2.37	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:293:GLU:OE2	1:A:295:TRP:HZ3	1.96	0.48
1:A:423:VAL:CG1	1:A:424:TYR:N	2.76	0.48
1:B:203:THR:HB	1:B:331:ASP:HA	1.96	0.48
1:B:90:VAL:HG13	1:B:123:HIS:NE2	2.29	0.47
1:A:322:ARG:HG3	1:A:322:ARG:NH1	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:A:4:TRP:CH2	1:A:6:ARG:HD3	2.50	0.47
1:B:312:VAL:HG23	1:B:367:ILE:HG23	1.97	0.47
1:A:310:GLN:N	1:A:310:GLN:CD	2.73	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:A:93:CYS:HA	1:A:108:TRP:CE2	2.50	0.47
1:B:351:SER:HB3	1:B:423:VAL:HG23	1.97	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
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:392:ASP:C	1:A:393:ILE:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:HIS:C	1:B:409:HIS:CD2	2.93	0.46
1:A:97:LYS:NZ	1:A:97:LYS:HA	2.31	0.46
1:A:43:ILE:HD11	1:A:395:ILE:CD1	2.45	0.46
1:A:409:HIS:C	1:A:409:HIS:ND1	2.74	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: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:6:ARG:NH1	1:B:42:GLU:HB2	2.31	0.45
1:B:320:ASN:H	1:B:324:GLN:NE2	2.15	0.45
1:B:346:LEU:HD13	1:B:346:LEU:C	2.42	0.45
1:B:277:GLN:OE1	1:B:281:GLU:HG2	2.15	0.45
1:B:339:GLY:C	1:B:341:LEU:HD22	2.42	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:A:262:GLU:HB2	1:A:311:THR:OG1	2.17	0.45
1:B:238:VAL:HG23	1:B:239:HIS:CE1	2.52	0.45
1:A:6:ARG:HG3	1:A:6:ARG:NH1	2.32	0.44
1:A:182:VAL:O	1:A:238:VAL:HG22	2.16	0.44
1:A:423:VAL:HG12	1:A:424:TYR:N	2.31	0.44
1:B:423:VAL:HB	3:B:5105:HOH:O	2.17	0.44
1:B:11:VAL:HG21	1:B:361:LEU:HG	1.99	0.44
1:B:317:CYS:O	1:B:338:GLY:HA3	2.17	0.44
1:A:2:LYS:HA	1:A:23:ILE:O	2.17	0.44
1:A:65:PHE:CE2	1:A:336:PRO:HB3	2.52	0.44
1:B:54:GLY:HA2	1:B:369:SER:HB3	1.99	0.44
1:B:253:ARG:HG2	3:B:5123:HOH:O	2.16	0.44
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.90	0.44
1:B:189:VAL:HG23	1:B:190:LEU:N	2.32	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:101:LEU:HD23	1:B:103:SER:HB3	1.99	0.43
1:B:423:VAL:HG22	1:B:424:TYR:N	2.33	0.43
1:A:166:LEU:HD13	1:A:227:LEU:HD12	2.00	0.43
1:A:43:ILE:C	1:A:43:ILE:HD12	2.43	0.43
1:A:431:LEU:HD23	1:A:436:PHE:HA	2.00	0.43
1:A:225:ILE:HG21	1:A:252:ALA:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:HG22	1:A:292:ARG:C	2.44	0.43
1:A:295:TRP:CD1	1:A:295:TRP:C	2.95	0.43
1:B:90:VAL:HG13	1:B:123:HIS:HE2	1.84	0.43
1:A:101:LEU:O	1:A:105:ILE:HG13	2.19	0.43
1:B:63:MET:HA	1:B:64:PRO:HD3	1.79	0.43
1:A:418:PHE:O	1:A:419:GLU:C	2.62	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:316:HIS:CG	1:B:342:ILE:HB	2.54	0.42
1:B:330:GLY:O	1:B:331:ASP:HB3	2.20	0.42
1:A:348:ILE:O	1:A:352:GLU:HB2	2.19	0.42
1:A:243:ALA:O	1:A:246:VAL:HG22	2.20	0.42
1:B:2:LYS:HG2	1:B:40:ALA:CB	2.46	0.42
1:B:90:VAL:CG1	1:B:123:HIS:HE2	2.33	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: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:A:92:PHE:HE1	1:A:150:LYS:HB2	1.85	0.41
1:A:238:VAL:HG23	1:A:239:HIS:CE1	2.55	0.41
1:B:148:SER:CB	1:B:455:ARG:HH22	2.24	0.41
1:A:141:ILE:HG23	1:A:147:THR:HG22	2.01	0.41
1:B:97:LYS:HD3	1:B:97:LYS:HA	1.89	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:B:148:SER:HB2	1:B:455:ARG:NH2	2.23	0.41
1:A:65:PHE:CD2	1:A:336:PRO:HB3	2.55	0.41
1:A:246:VAL:HG23	1:A:247:GLN:N	2.35	0.41
1:B:101:LEU:HD23	1:B:101:LEU:N	2.33	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:71:ALA:HB3	1:B:413:VAL:HG22	2.03	0.40
1:A:97:LYS:HD3	1:A:97:LYS:C	2.46	0.40
1:B:6:ARG:HG2	1:B:6:ARG:HH11	1.86	0.40
1:B:225:ILE:HG21	1:B:252:ALA:HB2	2.04	0.40
1:B:78:THR:OG1	1:B:117:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HA	1:B:144:GLU:HG2	2.02	0.40
1:B:261:GLY:HA3	1:B:309:LEU:HD23	2.03	0.40
1:B:458:PHE:CG	1:B:459:GLU:N	2.88	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
1:B:286:VAL:O	1:B:286:VAL:HG23	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	451/461 (98%)	426 (94%)	21 (5%)	4 (1%)	14	17
1	B	457/461 (99%)	425 (93%)	28 (6%)	4 (1%)	14	17
All	All	908/922 (98%)	851 (94%)	49 (5%)	8 (1%)	14	17

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%)	342 (93%)	27 (7%)	13	18
1	B	373/375 (100%)	354 (95%)	19 (5%)	21	32
All	All	742/750 (99%)	696 (94%)	46 (6%)	16	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	43	ILE
1	A	96	LYS
1	A	97	LYS
1	A	124	LEU
1	A	134	LEU
1	A	166	LEU
1	A	170	LEU
1	A	171	VAL
1	A	172	LYS
1	A	179	LEU
1	A	206	ILE
1	A	212	ARG
1	A	253	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	348	ILE
1	A	349	LEU
1	A	361	LEU
1	A	409	HIS
1	A	453	ILE
1	A	455	ARG

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Mol	Chain	Res	Type
1	B	11	VAL
1	B	35	LEU
1	B	43	ILE
1	B	61	LEU
1	B	79	ARG
1	B	124	LEU
1	B	141	ILE
1	B	166	LEU
1	B	179	LEU
1	B	234	GLN
1	B	263	THR
1	B	268	LEU
1	B	272	VAL
1	B	346	LEU
1	B	348	ILE
1	B	356	GLN
1	B	367	ILE
1	B	381	ARG
1	B	409	HIS

Sometimes 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	208	HIS
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	A	363	GLN
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	337	ASN
1	B	356	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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 [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	455/461 (98%)	-1.63	0 100 100	10, 21, 37, 63	0
1	B	459/461 (99%)	-1.61	0 100 100	10, 21, 42, 66	0
All	All	914/922 (99%)	-1.62	0 100 100	10, 21, 40, 66	0

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
2	MN	A	471	1/1	1.00	0.01	17,17,17,17	0
2	MN	A	472	1/1	1.00	0.01	17,17,17,17	0
2	MN	B	471	1/1	1.00	0.01	17,17,17,17	0
2	MN	B	472	1/1	1.00	0.01	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.