



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:24 PM UTC

PDB ID : 2Q2W / pdb_00002q2w
Title : Structure of D-3-Hydroxybutyrate Dehydrogenase from Pseudomonas putida
Authors : Paithankar, K.S.; Feller, C.; Kuettner, E.B.; Keim, A.; Grunow, M.; Strater, N.
Deposited on : 2007-05-29
Resolution : 2.12 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

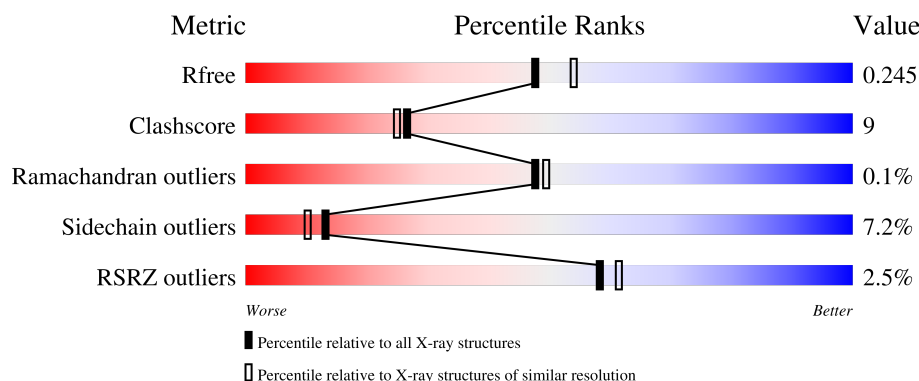
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 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	255	 75% 20% . ..
1	B	255	 75% 23% .
1	C	255	 74% 22% ...
1	D	255	 75% 19% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7712 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 Beta-D-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1859	1179	334	342	4			
1	B	255	Total	C	N	O	S	0	0	0
			1869	1185	336	344	4			
1	C	251	Total	C	N	O	S	0	0	0
			1840	1169	328	339	4			
1	D	248	Total	C	N	O	S	0	0	0
			1824	1161	325	334	4			

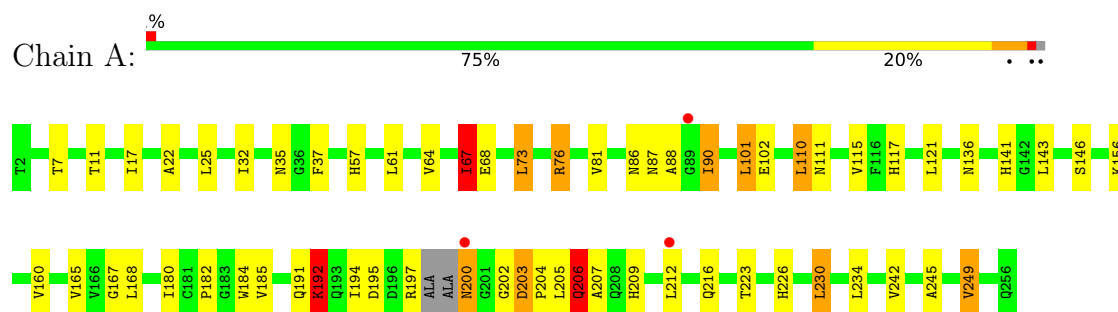
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	99	Total	O	0	0
			99	99		
2	C	75	Total	O	0	0
			75	75		
2	D	62	Total	O	0	0
			62	62		

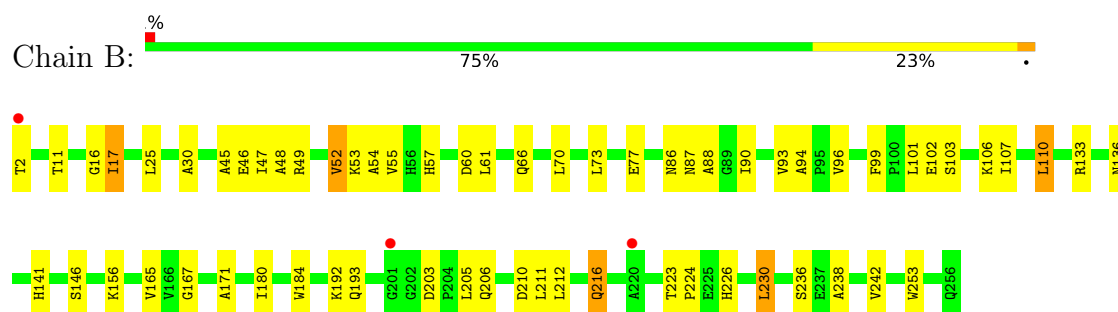
3 Residue-property plots [i](#)

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.

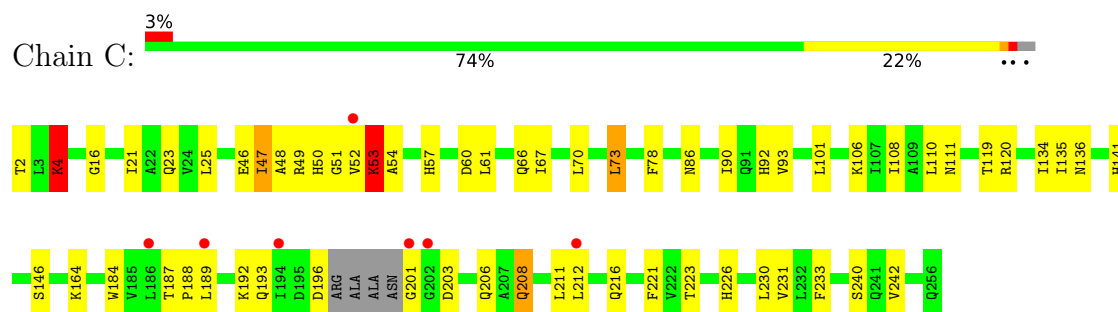
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase



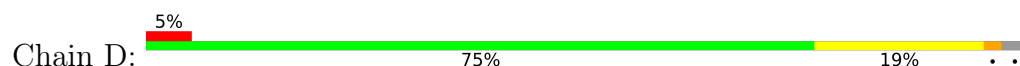
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

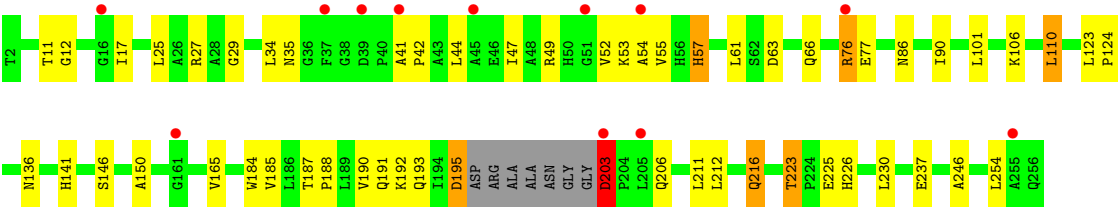


- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase



- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.68Å 58.81Å 119.46Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	30.00 – 2.12 30.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.12) 99.2 (30.00-2.12)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.247 0.180 , 0.245	Depositor DCC
R_{free} test set	2340 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7712	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 34.11 % 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 7.1842e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.81	20/1895 (1.1%)	1.38	11/2581 (0.4%)
1	B	1.53	11/1906 (0.6%)	1.35	13/2598 (0.5%)
1	C	1.49	12/1876 (0.6%)	1.24	3/2556 (0.1%)
1	D	1.50	11/1860 (0.6%)	1.31	7/2535 (0.3%)
All	All	1.59	54/7537 (0.7%)	1.32	34/10270 (0.3%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	ASP	CB-CG	15.23	1.90	1.52
1	A	202	GLY	C-O	15.03	1.38	1.23
1	A	203	ASP	CG-OD2	14.28	1.52	1.25
1	A	192	LYS	CE-NZ	13.40	1.89	1.49
1	A	195	ASP	CG-OD1	12.41	1.49	1.25
1	D	188	PRO	C-O	10.20	1.37	1.24
1	D	203	ASP	CG-OD1	9.08	1.42	1.25
1	A	203	ASP	CG-OD1	-8.81	1.08	1.25
1	C	196	ASP	C-O	8.75	1.41	1.23
1	D	195	ASP	CG-OD1	8.62	1.41	1.25
1	A	203	ASP	C-O	-7.56	1.15	1.24
1	A	67	ILE	CA-CB	7.23	1.63	1.54
1	A	165	VAL	CA-CB	7.20	1.62	1.54
1	A	168	LEU	C-O	-7.06	1.15	1.24
1	B	238	ALA	CA-CB	-7.03	1.40	1.53
1	C	201	GLY	N-CA	-6.92	1.34	1.45
1	A	32	ILE	CA-CB	6.88	1.64	1.54
1	D	203	ASP	CG-OD2	6.86	1.38	1.25
1	B	165	VAL	CA-CB	6.72	1.61	1.54
1	D	191	GLN	CD-OE1	6.72	1.36	1.23
1	B	242	VAL	CA-CB	6.58	1.61	1.54
1	A	245	ALA	CA-CB	6.54	1.64	1.53
1	B	253	TRP	C-O	6.54	1.31	1.24
1	A	202	GLY	C-N	6.41	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	GLY	N-CA	6.31	1.54	1.45
1	D	203	ASP	C-N	6.26	1.41	1.34
1	A	195	ASP	CG-OD2	6.22	1.37	1.25
1	C	201	GLY	C-N	6.22	1.41	1.33
1	A	249	VAL	CA-CB	6.16	1.60	1.53
1	C	4	LYS	CE-NZ	6.09	1.67	1.49
1	D	195	ASP	CG-OD2	6.02	1.36	1.25
1	B	236	SER	CA-C	5.95	1.61	1.53
1	D	165	VAL	CA-CB	5.91	1.60	1.54
1	D	49	ARG	N-CA	5.90	1.53	1.46
1	D	246	ALA	CA-CB	5.86	1.63	1.53
1	B	45	ALA	CA-CB	5.86	1.62	1.53
1	C	201	GLY	CA-C	5.66	1.62	1.52
1	B	48	ALA	CA-CB	5.62	1.62	1.53
1	B	203	ASP	CA-C	5.58	1.58	1.53
1	C	93	VAL	CA-CB	5.57	1.60	1.53
1	C	108	ILE	CB-CG2	5.57	1.71	1.52
1	C	242	VAL	CA-CB	5.44	1.59	1.53
1	D	150	ALA	CA-CB	5.38	1.61	1.53
1	B	30	ALA	CA-CB	5.33	1.62	1.53
1	A	115	VAL	CA-C	5.31	1.59	1.52
1	B	53	LYS	N-CA	5.25	1.52	1.46
1	C	51	GLY	C-N	5.25	1.40	1.33
1	C	53	LYS	CE-NZ	5.18	1.64	1.49
1	A	7	THR	C-O	-5.18	1.17	1.24
1	C	233	PHE	CA-C	5.16	1.59	1.52
1	C	189	LEU	CA-C	5.14	1.59	1.52
1	A	242	VAL	CA-CB	5.08	1.60	1.54
1	B	25	LEU	N-CA	5.04	1.52	1.46
1	A	81	VAL	C-O	-5.01	1.18	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	O-C-N	11.17	133.85	121.12
1	A	203	ASP	CA-C-O	-9.98	110.40	119.59
1	D	57	HIS	CA-C-N	7.37	128.34	120.83
1	D	57	HIS	C-N-CA	7.37	128.34	120.83
1	A	202	GLY	O-C-N	7.15	129.43	122.92
1	A	160	VAL	N-CA-C	-7.07	103.58	110.72
1	B	99	PHE	CA-C-N	-7.04	112.72	119.76
1	B	99	PHE	C-N-CA	-7.04	112.72	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	CA-CB-CG	-6.85	105.75	112.60
1	D	203	ASP	O-C-N	-6.68	112.31	123.00
1	B	94	ALA	N-CA-C	6.54	114.10	108.22
1	B	216	GLN	CA-C-N	6.17	126.36	119.32
1	B	216	GLN	C-N-CA	6.17	126.36	119.32
1	C	240	SER	N-CA-C	6.14	118.77	111.71
1	D	29	GLY	N-CA-C	5.85	123.68	115.43
1	A	203	ASP	CB-CG-OD1	5.78	131.69	118.40
1	A	67	ILE	N-CA-CB	5.71	118.30	110.54
1	D	254	LEU	N-CA-C	5.62	119.40	112.54
1	A	242	VAL	N-CA-C	-5.61	99.64	108.23
1	B	110	LEU	N-CA-C	5.57	117.43	111.36
1	B	17	ILE	N-CA-C	5.50	116.13	110.36
1	B	133	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	D	223	THR	CA-C-N	5.21	124.83	119.05
1	D	223	THR	C-N-CA	5.21	124.83	119.05
1	A	64	VAL	N-CA-C	5.20	115.41	110.42
1	B	16	GLY	N-CA-C	5.20	120.54	111.50
1	A	22	ALA	N-CA-C	5.19	117.61	111.33
1	B	167	GLY	N-CA-C	-5.13	106.43	112.64
1	A	206	GLN	CB-CA-C	5.13	120.15	109.95
1	C	21	ILE	N-CA-C	5.10	115.31	110.42
1	B	52	VAL	N-CA-CB	-5.08	103.94	112.47
1	C	73	LEU	N-CA-C	5.03	117.41	111.33
1	B	171	ALA	N-CA-C	5.01	117.39	111.33
1	B	93	VAL	N-CA-C	5.00	115.05	107.80

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	1859	0	1877	45	1
1	B	1869	0	1888	27	0
1	C	1840	0	1858	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1824	0	1848	33	0
2	A	84	0	0	2	0
2	B	99	0	0	3	1
2	C	75	0	0	1	0
2	D	62	0	0	3	0
All	All	7712	0	7471	138	1

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 9.

All (138) 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:4:LYS:CE	1:C:4:LYS:NZ	1.67	1.56
1:A:203:ASP:CB	1:A:203:ASP:CG	1.90	1.42
1:A:192:LYS:CE	1:A:192:LYS:NZ	1.89	1.34
1:C:184:TRP:H	1:C:216:GLN:HE22	1.07	0.97
1:D:184:TRP:H	1:D:216:GLN:HE22	1.16	0.94
1:A:184:TRP:H	1:A:216:GLN:HE22	1.15	0.91
1:D:76:ARG:HH11	1:D:76:ARG:HG3	1.40	0.87
1:C:86:ASN:HD22	1:C:136:ASN:ND2	1.80	0.79
1:A:86:ASN:HD22	1:A:136:ASN:ND2	1.81	0.78
1:B:86:ASN:HD22	1:B:136:ASN:ND2	1.80	0.78
1:B:184:TRP:H	1:B:216:GLN:HE22	1.32	0.77
1:C:86:ASN:HD22	1:C:136:ASN:HD21	1.33	0.76
1:D:27:ARG:NH1	2:D:302:HOH:O	2.19	0.75
1:A:76:ARG:HB2	1:A:76:ARG:HH11	1.54	0.73
1:D:34:LEU:HD12	1:D:44:LEU:HD23	1.69	0.73
1:A:141:HIS:HE1	1:A:146:SER:OG	1.73	0.71
1:B:86:ASN:HD22	1:B:136:ASN:HD21	1.38	0.71
1:B:156:LYS:NZ	2:B:260:HOH:O	2.23	0.70
1:D:76:ARG:HH11	1:D:76:ARG:CG	2.04	0.69
1:A:90:ILE:H	1:A:111:ASN:HD21	1.41	0.68
1:B:49:ARG:HD3	2:B:330:HOH:O	1.94	0.67
1:D:86:ASN:HD22	1:D:136:ASN:HD21	1.42	0.67
1:B:90:ILE:HG12	1:B:110:LEU:HD13	1.76	0.67
1:C:90:ILE:CD1	1:C:106:LYS:HG3	2.24	0.67
1:C:57:HIS:HB3	1:C:70:LEU:HD13	1.75	0.66
1:C:184:TRP:N	1:C:216:GLN:HE22	1.89	0.66
1:D:86:ASN:HD22	1:D:136:ASN:ND2	1.93	0.66
1:A:37:PHE:HE2	2:A:301:HOH:O	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:HG12	1:B:230:LEU:HD13	1.79	0.64
1:B:103:SER:O	1:B:107:ILE:HG12	1.98	0.64
1:B:60:ASP:H	1:B:66:GLN:NE2	1.95	0.63
1:A:68:GLU:HG2	1:A:121:LEU:HD11	1.79	0.63
1:D:12:GLY:H	1:D:35:ASN:HD22	1.46	0.63
1:B:57:HIS:HB3	1:B:70:LEU:HD13	1.80	0.62
1:B:110:LEU:C	1:B:110:LEU:HD23	2.24	0.62
1:A:184:TRP:N	1:A:216:GLN:HE22	1.93	0.62
1:D:86:ASN:HB2	1:D:136:ASN:HD22	1.65	0.61
1:A:67:ILE:HD11	1:A:121:LEU:HD12	1.82	0.61
1:A:192:LYS:NZ	1:A:192:LYS:CD	2.62	0.61
1:D:90:ILE:CD1	1:D:106:LYS:HG3	2.30	0.61
1:C:47:ILE:CG2	1:C:54:ALA:HB2	2.31	0.61
1:C:223:THR:H	1:C:226:HIS:CD2	2.19	0.60
1:B:46:GLU:HG3	2:B:318:HOH:O	2.02	0.60
1:D:190:VAL:O	1:D:193:GLN:HB2	2.03	0.59
1:A:86:ASN:HD22	1:A:136:ASN:HD21	1.49	0.59
1:A:184:TRP:H	1:A:216:GLN:NE2	1.94	0.59
1:D:47:ILE:HG21	1:D:54:ALA:HB2	1.85	0.59
1:A:76:ARG:HH11	1:A:76:ARG:CB	2.16	0.58
1:D:184:TRP:H	1:D:216:GLN:NE2	1.96	0.57
1:C:47:ILE:HG21	1:C:54:ALA:HB2	1.86	0.56
1:D:90:ILE:HG12	1:D:110:LEU:HG	1.85	0.56
1:D:90:ILE:HD11	1:D:106:LYS:HG3	1.87	0.56
1:B:17:ILE:HA	1:B:224:PRO:HB3	1.87	0.56
1:B:206:GLN:NE2	1:B:210:ASP:OD1	2.39	0.56
1:A:76:ARG:HB2	1:A:76:ARG:NH1	2.20	0.56
1:B:11:THR:HB	1:B:61:LEU:HD11	1.88	0.56
1:B:141:HIS:HE1	1:B:146:SER:OG	1.89	0.56
1:A:184:TRP:CD1	1:A:212:LEU:HD22	2.41	0.55
1:A:197:ARG:C	1:A:200:ASN:N	2.64	0.55
1:D:41:ALA:HB3	1:D:42:PRO:HD3	1.88	0.55
1:C:187:THR:HB	1:C:188:PRO:HD2	1.89	0.54
1:C:184:TRP:H	1:C:216:GLN:NE2	1.91	0.54
1:B:90:ILE:HD12	1:B:107:ILE:HD13	1.88	0.54
1:A:57:HIS:HB2	1:A:73:LEU:HD12	1.89	0.54
1:D:11:THR:HB	1:D:61:LEU:HD11	1.89	0.53
1:C:135:ILE:HD13	1:C:231:VAL:HG13	1.90	0.53
1:A:143:LEU:O	1:C:164:LYS:NZ	2.43	0.52
1:A:180:ILE:HG12	1:A:230:LEU:HD13	1.90	0.52
1:D:203:ASP:HB2	2:D:305:HOH:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ASP:H	1:C:66:GLN:NE2	2.07	0.52
1:C:23:GLN:NE2	1:C:46:GLU:HG3	2.24	0.52
1:C:23:GLN:HE22	1:C:46:GLU:HG3	1.75	0.52
1:C:53:LYS:HG3	1:C:78:PHE:HE1	1.75	0.52
1:C:119:THR:HG23	1:C:134:ILE:HD13	1.92	0.51
1:A:197:ARG:HE	1:A:207:ALA:HB2	1.75	0.51
1:C:92:HIS:HE1	2:C:302:HOH:O	1.94	0.51
1:B:184:TRP:CG	1:B:212:LEU:HD22	2.46	0.51
1:C:90:ILE:H	1:C:111:ASN:HD21	1.57	0.51
1:A:203:ASP:CG	1:A:203:ASP:CA	2.77	0.50
1:B:110:LEU:HD23	1:B:110:LEU:O	2.11	0.50
1:A:67:ILE:HD12	1:A:117:HIS:HB3	1.93	0.50
1:D:17:ILE:HG12	1:D:185:VAL:HG11	1.94	0.49
1:A:141:HIS:CE1	1:A:146:SER:OG	2.61	0.48
1:D:63:ASP:CG	1:D:66:GLN:HG3	2.38	0.48
1:B:47:ILE:HG21	1:B:54:ALA:HB2	1.95	0.47
1:D:35:ASN:HA	1:D:57:HIS:O	2.14	0.47
1:B:223:THR:H	1:B:226:HIS:CD2	2.32	0.47
1:D:184:TRP:N	1:D:216:GLN:HE22	1.97	0.47
1:B:55:VAL:HG11	1:B:77:GLU:HG2	1.98	0.46
1:A:87:ASN:O	1:A:88:ALA:C	2.58	0.46
1:A:206:GLN:HA	1:A:209:HIS:HB2	1.96	0.46
1:C:141:HIS:HE1	1:C:146:SER:OG	1.99	0.46
1:C:46:GLU:O	1:C:49:ARG:HB2	2.15	0.46
1:B:184:TRP:H	1:B:216:GLN:NE2	2.08	0.46
1:C:110:LEU:C	1:C:110:LEU:HD13	2.41	0.45
1:D:55:VAL:HG11	1:D:77:GLU:HG2	1.98	0.45
1:D:223:THR:H	1:D:226:HIS:CD2	2.34	0.45
1:A:223:THR:H	1:A:226:HIS:CD2	2.33	0.45
1:A:61:LEU:HB2	1:A:110:LEU:CD2	2.46	0.45
1:A:76:ARG:CB	1:A:76:ARG:NH1	2.79	0.45
1:C:47:ILE:HG22	1:C:54:ALA:HB2	1.98	0.45
1:B:87:ASN:O	1:B:88:ALA:C	2.60	0.45
1:B:192:LYS:O	1:B:193:GLN:C	2.59	0.45
1:C:90:ILE:HD11	1:C:106:LYS:HG3	1.97	0.45
1:D:27:ARG:NH2	2:D:277:HOH:O	2.36	0.45
1:A:11:THR:O	1:A:87:ASN:HB3	2.16	0.44
1:C:16:GLY:HA2	1:C:188:PRO:HD3	1.99	0.44
1:A:197:ARG:HE	1:A:207:ALA:CB	2.31	0.44
1:C:23:GLN:HE22	1:C:46:GLU:CG	2.30	0.44
1:A:101:LEU:HD11	1:C:120:ARG:CZ	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HB2	1:C:110:LEU:CD2	2.48	0.43
1:D:123:LEU:HB3	1:D:124:PRO:HD3	1.99	0.43
1:A:156:LYS:NZ	2:A:269:HOH:O	2.45	0.43
1:A:192:LYS:HZ2	1:A:192:LYS:HA	1.83	0.43
1:B:90:ILE:CD1	1:B:107:ILE:HD13	2.48	0.43
1:A:203:ASP:OD2	1:A:205:LEU:HB3	2.18	0.43
1:A:192:LYS:NZ	1:A:192:LYS:HA	2.33	0.43
1:C:61:LEU:O	1:C:67:ILE:HD11	2.19	0.43
1:A:184:TRP:CG	1:A:212:LEU:HD22	2.52	0.43
1:B:11:THR:O	1:B:87:ASN:HB3	2.18	0.42
1:A:203:ASP:HA	1:A:204:PRO:HD2	1.89	0.42
1:D:76:ARG:HG3	1:D:76:ARG:NH1	2.20	0.42
1:C:61:LEU:HB2	1:C:110:LEU:HD23	2.01	0.42
1:C:208:GLN:HG3	1:C:221:PHE:CE1	2.55	0.41
1:D:187:THR:OG1	1:D:190:VAL:HG23	2.20	0.41
1:A:67:ILE:CD1	1:A:121:LEU:HD12	2.49	0.41
1:D:12:GLY:H	1:D:35:ASN:ND2	2.15	0.41
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.95	0.41
1:A:35:ASN:HA	1:A:57:HIS:O	2.20	0.41
1:C:184:TRP:CD1	1:C:212:LEU:HD23	2.56	0.41
1:D:47:ILE:CG2	1:D:54:ALA:HB2	2.50	0.41
1:D:63:ASP:HB3	1:D:66:GLN:HG3	2.02	0.41
1:D:34:LEU:HD12	1:D:44:LEU:CD2	2.47	0.40
1:C:48:ALA:C	1:C:50:HIS:N	2.80	0.40
1:A:182:PRO:HA	1:A:249:VAL:O	2.20	0.40
1:A:17:ILE:HG12	1:A:185:VAL:HG11	2.03	0.40
1:A:67:ILE:CD1	1:A:117:HIS:HB3	2.50	0.40
1:D:141:HIS:HE1	1:D:146:SER:OG	2.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:CD2	2:B:307:HOH:O[1_565]	1.87	0.33

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	249/255 (98%)	241 (97%)	8 (3%)	0	100	100
1	B	253/255 (99%)	243 (96%)	9 (4%)	1 (0%)	30	28
1	C	247/255 (97%)	237 (96%)	10 (4%)	0	100	100
1	D	244/255 (96%)	230 (94%)	14 (6%)	0	100	100
All	All	993/1020 (97%)	951 (96%)	41 (4%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	VAL

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	189/189 (100%)	175 (93%)	14 (7%)	13	10
1	B	189/189 (100%)	180 (95%)	9 (5%)	23	22
1	C	187/189 (99%)	172 (92%)	15 (8%)	11	8
1	D	186/189 (98%)	170 (91%)	16 (9%)	10	7
All	All	751/756 (99%)	697 (93%)	54 (7%)	13	10

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	67	ILE
1	A	73	LEU
1	A	76	ARG
1	A	90	ILE
1	A	101	LEU
1	A	102	GLU
1	A	110	LEU
1	A	191	GLN
1	A	192	LYS
1	A	194	ILE
1	A	200	ASN
1	A	206	GLN
1	A	230	LEU
1	B	2	THR
1	B	52	VAL
1	B	73	LEU
1	B	101	LEU
1	B	102	GLU
1	B	106	LYS
1	B	205	LEU
1	B	211	LEU
1	B	230	LEU
1	C	2	THR
1	C	4	LYS
1	C	25	LEU
1	C	47	ILE
1	C	52	VAL
1	C	53	LYS
1	C	73	LEU
1	C	101	LEU
1	C	192	LYS
1	C	193	GLN
1	C	203	ASP
1	C	206	GLN
1	C	208	GLN
1	C	211	LEU
1	C	230	LEU
1	D	25	LEU
1	D	52	VAL
1	D	53	LYS
1	D	76	ARG
1	D	101	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	110	LEU
1	D	192	LYS
1	D	195	ASP
1	D	203	ASP
1	D	206	GLN
1	D	211	LEU
1	D	212	LEU
1	D	216	GLN
1	D	225	GLU
1	D	230	LEU
1	D	237	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	66	GLN
1	A	91	GLN
1	A	136	ASN
1	A	141	HIS
1	A	191	GLN
1	A	200	ASN
1	A	216	GLN
1	A	226	HIS
1	B	35	ASN
1	B	56	HIS
1	B	66	GLN
1	B	136	ASN
1	B	141	HIS
1	B	216	GLN
1	B	226	HIS
1	B	256	GLN
1	C	23	GLN
1	C	35	ASN
1	C	66	GLN
1	C	92	HIS
1	C	111	ASN
1	C	136	ASN
1	C	141	HIS
1	C	193	GLN
1	C	216	GLN
1	C	226	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	256	GLN
1	D	31	ASN
1	D	35	ASN
1	D	66	GLN
1	D	98	GLN
1	D	136	ASN
1	D	141	HIS
1	D	209	HIS
1	D	216	GLN
1	D	256	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](#)

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 ⓘ

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, 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	253/255 (99%)	0.20	3 (1%) 76 79	25, 31, 43, 52	0
1	B	255/255 (100%)	0.25	3 (1%) 76 79	26, 31, 39, 46	0
1	C	251/255 (98%)	0.41	7 (2%) 55 58	27, 31, 43, 52	0
1	D	248/255 (97%)	0.62	12 (4%) 35 38	26, 32, 41, 48	0
All	All	1007/1020 (98%)	0.37	25 (2%) 58 61	25, 31, 41, 52	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202	GLY	3.6
1	A	89	GLY	3.2
1	D	37	PHE	3.0
1	B	201	GLY	2.9
1	D	51	GLY	2.9
1	C	201	GLY	2.8
1	C	212	LEU	2.7
1	D	54	ALA	2.6
1	D	39	ASP	2.4
1	D	203	ASP	2.4
1	D	255	ALA	2.4
1	A	200	ASN	2.4
1	D	41	ALA	2.4
1	C	52	VAL	2.3
1	B	2	THR	2.2
1	C	186	LEU	2.2
1	C	194	ILE	2.1
1	D	45	ALA	2.1
1	D	76	ARG	2.1
1	B	220	ALA	2.1
1	D	161	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	212	LEU	2.0
1	C	189	LEU	2.0
1	D	205	LEU	2.0
1	D	16	GLY	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 oligosaccharides 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.