Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 09:14 PM EDT

PDB ID	:	2Q2W
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:

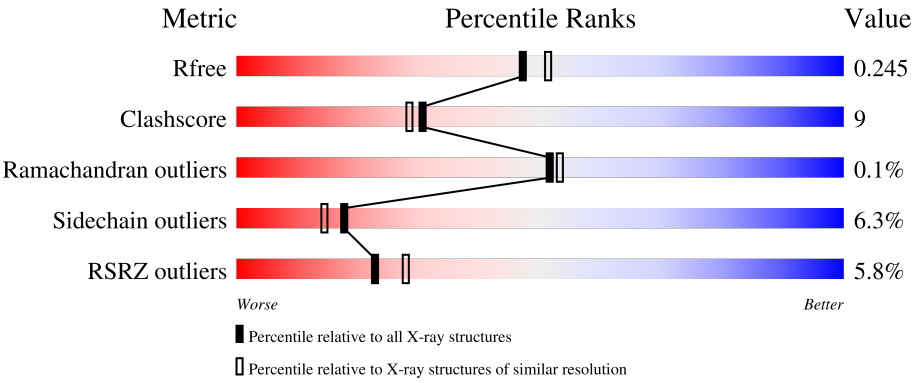
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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 <=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	6% 77% 17%
1	B	255	4% 80% 19%
1	C	255	7% 75% 22%
1	D	255	5% 76% 19%

2 Entry composition (i)

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.

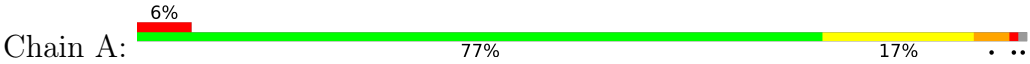
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	99	Total	O	0	0
			99	99		
2	C	75	Total	O	0	0
			75	75		
2	D	62	Total	O	0	0
			62	62		

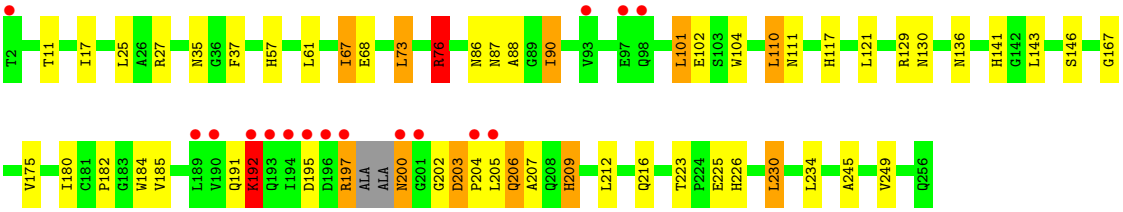
3 Residue-property plots (i)

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

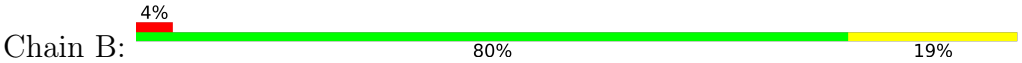
Chain A:

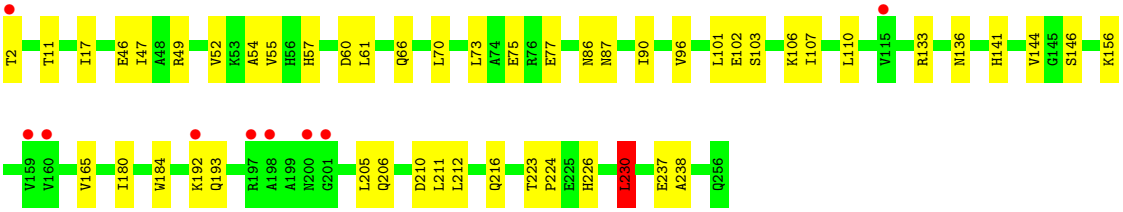




• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

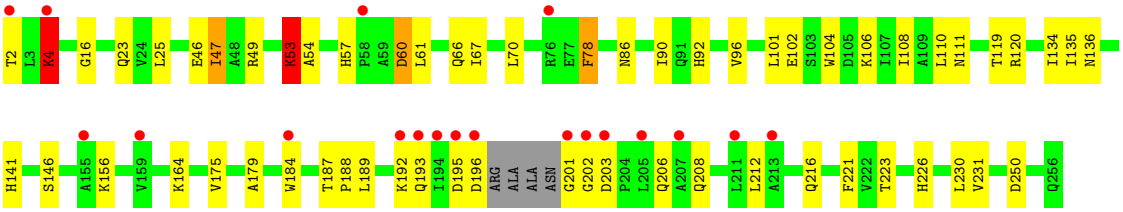
Chain B:





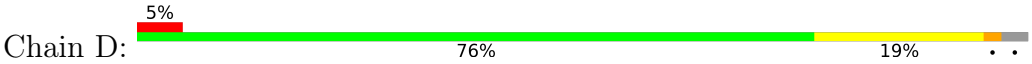
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

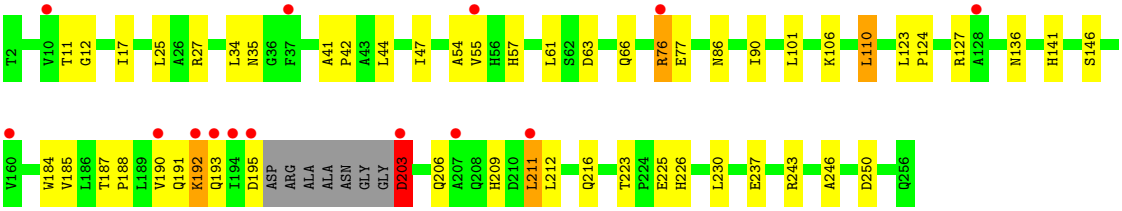
Chain C:



• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain D:




T2
V10
T11
G12
I17
L25
A26
R27
L34
N35
G36
F37
A41
P42
A43
L44
I47
A54
V55
H56
H57
L61
S62
D63
Q66
R76
E77
N86
I90
L101
K106
L110
L123
P124
R127
A128
N136
H141
S146
V160
W184
V185
L186
T187
P188
L189
V190
Q191
K192
Q193
I194
D195
ASP
ARG
ALA
ALA
ASN
GLY
GLY
D203
Q206
A207
Q208
H209
D210
L211
L212
Q216
T223
P224
E225
H226
L230
E237
R243
A246
D250
Q256

4 Data and refinement statistics (i)

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 29.80 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.12) 99.0 (29.80-2.12)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.05%)	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 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.52	14/1895 (0.7%)	1.11	8/2581 (0.3%)
1	B	1.21	6/1906 (0.3%)	0.98	2/2598 (0.1%)
1	C	1.24	12/1876 (0.6%)	0.92	4/2556 (0.2%)
1	D	1.20	9/1860 (0.5%)	1.00	6/2535 (0.2%)
All	All	1.30	41/7537 (0.5%)	1.01	20/10270 (0.2%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	ASP	CB-CG	18.28	1.90	1.51
1	A	192	LYS	CE-NZ	16.20	1.89	1.49
1	A	203	ASP	CG-OD2	11.80	1.52	1.25
1	A	195	ASP	CG-OD1	10.25	1.49	1.25
1	A	202	GLY	C-O	9.40	1.38	1.23
1	C	196	ASP	C-O	9.31	1.41	1.23
1	C	201	GLY	N-CA	-7.71	1.34	1.46
1	D	203	ASP	CG-OD1	7.50	1.42	1.25
1	C	4	LYS	CE-NZ	7.42	1.67	1.49
1	D	188	PRO	C-O	7.28	1.37	1.23
1	A	203	ASP	CG-OD1	-7.28	1.08	1.25
1	D	195	ASP	CG-OD1	7.12	1.41	1.25
1	B	237	GLU	CG-CD	7.08	1.62	1.51
1	C	104	TRP	CB-CG	6.91	1.62	1.50
1	B	75	GLU	CB-CG	6.78	1.65	1.52
1	A	225	GLU	CG-CD	6.75	1.62	1.51
1	C	201	GLY	CA-C	6.49	1.62	1.51
1	C	53	LYS	CE-NZ	6.34	1.64	1.49
1	A	104	TRP	CB-CG	6.26	1.61	1.50
1	C	108	ILE	CB-CG2	5.83	1.71	1.52
1	C	175	VAL	CB-CG2	5.76	1.65	1.52
1	D	203	ASP	CG-OD2	5.66	1.38	1.25
1	A	167	GLY	N-CA	5.64	1.54	1.46
1	D	191	GLN	CD-OE1	5.62	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	GLY	N-CA	5.59	1.54	1.46
1	B	238	ALA	CA-CB	-5.51	1.40	1.52
1	B	144	VAL	CB-CG1	5.51	1.64	1.52
1	A	245	ALA	CA-CB	5.46	1.64	1.52
1	D	225	GLU	CG-CD	5.45	1.60	1.51
1	C	96	VAL	CB-CG1	5.30	1.64	1.52
1	A	175	VAL	CB-CG2	5.29	1.64	1.52
1	B	75	GLU	CG-CD	5.25	1.59	1.51
1	D	203	ASP	CB-CG	5.21	1.62	1.51
1	B	165	VAL	CB-CG1	5.18	1.63	1.52
1	A	130	ASN	CB-CG	5.14	1.62	1.51
1	A	195	ASP	CG-OD2	5.14	1.37	1.25
1	C	102	GLU	CG-CD	5.10	1.59	1.51
1	A	197	ARG	CZ-NH1	5.08	1.39	1.33
1	C	179	ALA	CA-CB	5.08	1.63	1.52
1	D	246	ALA	CA-CB	5.03	1.63	1.52
1	D	192	LYS	CE-NZ	5.02	1.61	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	ASP	CB-CG-OD1	14.88	131.69	118.30
1	B	133	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	A	27	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	27	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	76	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	D	250	ASP	CB-CG-OD2	6.88	124.50	118.30
1	A	129	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	203	ASP	O-C-N	6.71	133.85	121.10
1	C	189	LEU	CB-CG-CD2	-6.35	100.21	111.00
1	B	230	LEU	CB-CG-CD1	6.33	121.77	111.00
1	A	203	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	192	LYS	CD-CE-NZ	-6.18	97.49	111.70
1	D	211	LEU	CA-CB-CG	6.12	129.38	115.30
1	D	243	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	250	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	D	195	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	C	60	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	195	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	C	250	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	127	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	1859	0	1877	44	1
1	B	1869	0	1888	26	0
1	C	1840	0	1858	35	0
1	D	1824	0	1848	33	0
2	A	84	0	0	1	0
2	B	99	0	0	3	1
2	C	75	0	0	2	0
2	D	62	0	0	3	0
All	All	7712	0	7471	136	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 (136) 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	1.39
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:156:LYS:NZ	2:B:260:HOH:O	2.23	0.66
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
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: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:B:110:LEU:C	1:B:110:LEU:HD23	2.24	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:197:ARG:C	1:A:200:ASN:N	2.64	0.51
1:C:90:ILE:H	1:C:111:ASN:HD21	1.57	0.51
1:C:156:LYS:NZ	2:C:285:HOH:O	2.44	0.51
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: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: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:A:203:ASP:CG	1:A:203:ASP:CA	2.77	0.46
1:B:184:TRP:H	1:B:216:GLN:NE2	2.08	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:D:63:ASP:CG	1:D:66:GLN:HG3	2.38	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:A:87:ASN:O	1:A:88:ALA:C	2.58	0.41
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:110:LEU:C	1:C:110:LEU:HD13	2.41	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: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:B:192:LYS:O	1:B:193:GLN:C	2.59	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 (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	249/255 (98%)	241 (97%)	8 (3%)	0	100 100
1	B	253/255 (99%)	243 (96%)	9 (4%)	1 (0%)	34 32
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%)	51 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	189/189 (100%)	175 (93%)	14 (7%)	13 10
1	B	189/189 (100%)	180 (95%)	9 (5%)	25 23
1	C	187/189 (99%)	175 (94%)	12 (6%)	17 14
1	D	186/189 (98%)	174 (94%)	12 (6%)	17 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	751/756 (99%)	704 (94%)	47 (6%)	18 14

All (47) 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	200	ASN
1	A	206	GLN
1	A	209	HIS
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	53	LYS
1	C	78	PHE
1	C	101	LEU
1	C	192	LYS
1	C	193	GLN
1	C	203	ASP
1	C	206	GLN
1	C	230	LEU
1	D	25	LEU
1	D	76	ARG

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Mol	Chain	Res	Type
1	D	101	LEU
1	D	110	LEU
1	D	192	LYS
1	D	203	ASP
1	D	206	GLN
1	D	209	HIS
1	D	211	LEU
1	D	212	LEU
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	35	ASN
1	A	66	GLN
1	A	111	ASN
1	A	136	ASN
1	A	141	HIS
1	A	191	GLN
1	A	200	ASN
1	A	206	GLN
1	A	216	GLN
1	A	226	HIS
1	B	23	GLN
1	B	35	ASN
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

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Mol	Chain	Res	Type
1	C	226	HIS
1	C	256	GLN
1	D	35	ASN
1	D	66	GLN
1	D	136	ASN
1	D	141	HIS
1	D	216	GLN
1	D	226	HIS
1	D	256	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.28	16 (6%)	20	24	25, 31, 43, 52	0
1	B	255/255 (100%)	0.13	9 (3%)	44	50	26, 31, 39, 46	0
1	C	251/255 (98%)	0.24	19 (7%)	13	17	27, 31, 43, 52	0
1	D	248/255 (97%)	0.32	14 (5%)	24	29	26, 32, 41, 48	0
All	All	1007/1020 (98%)	0.24	58 (5%)	23	28	25, 31, 41, 52	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	194	ILE	5.1
1	D	203	ASP	4.9
1	A	195	ASP	4.8
1	A	192	LYS	4.7
1	A	194	ILE	4.7
1	A	190	VAL	4.0
1	D	76	ARG	3.9
1	B	201	GLY	3.7
1	C	201	GLY	3.7
1	A	197	ARG	3.5
1	A	196	ASP	3.5
1	A	189	LEU	3.5
1	A	200	ASN	3.4
1	A	93	VAL	3.4
1	A	98	GLN	3.3
1	C	202	GLY	3.3
1	B	197	ARG	3.1
1	D	207	ALA	3.0
1	B	200	ASN	2.9
1	D	211	LEU	2.9
1	D	194	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	192	LYS	2.7
1	A	97	GLU	2.7
1	C	184	TRP	2.7
1	A	193	GLN	2.6
1	B	115	VAL	2.5
1	D	193	GLN	2.5
1	D	190	VAL	2.5
1	C	193	GLN	2.5
1	A	201	GLY	2.5
1	D	128	ALA	2.5
1	C	192	LYS	2.4
1	D	37	PHE	2.4
1	A	2	THR	2.4
1	A	205	LEU	2.4
1	C	159	VAL	2.4
1	B	2	THR	2.4
1	C	195	ASP	2.4
1	C	207	ALA	2.3
1	D	195	ASP	2.3
1	B	192	LYS	2.3
1	C	205	LEU	2.3
1	C	196	ASP	2.3
1	B	160	VAL	2.3
1	C	4	LYS	2.3
1	B	198	ALA	2.3
1	B	159	VAL	2.2
1	C	58	PRO	2.2
1	C	211	LEU	2.2
1	A	204	PRO	2.2
1	D	55	VAL	2.1
1	D	160	VAL	2.1
1	C	203	ASP	2.0
1	C	2	THR	2.0
1	C	155	ALA	2.0
1	C	213	ALA	2.0
1	C	76	ARG	2.0
1	D	10	VAL	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 monosaccharides 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.