Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 07:04 am BST

PDB ID	:	6TQ8
Title	:	Alcohol dehydrogenase from Candida magnoliae DSMZ 70638 (ADHA): thermostable 10fold mutant
Authors	:	Rovida, S.; Aalbers, F.S.; Fraaije, M.W.; Mattevi, A.
Deposited on	:	2019-12-16
Resolution	:	2.50 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.50 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	Percentile Ranks	Value
Rfree		0.296
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		7.0%
RSRZ outliers		5.9%

Worse ← → Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
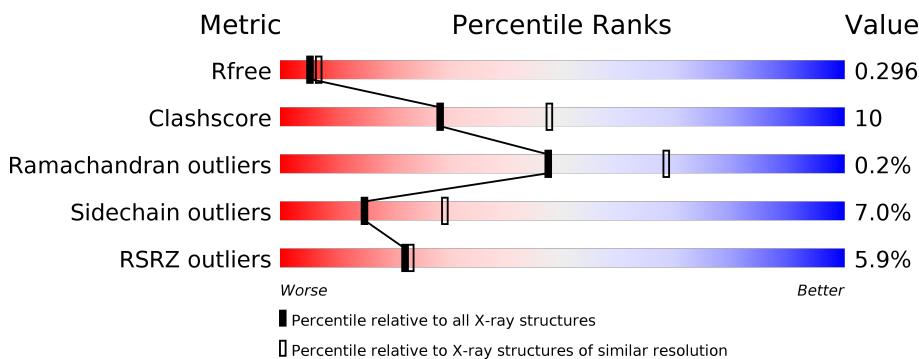
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	246	6% / 79% / 20% / •
1	B	246	6% / 78% / 17% / • •
1	C	246	7% / 72% / 25% / • •
1	D	246	5% / 73% / 22% / • •
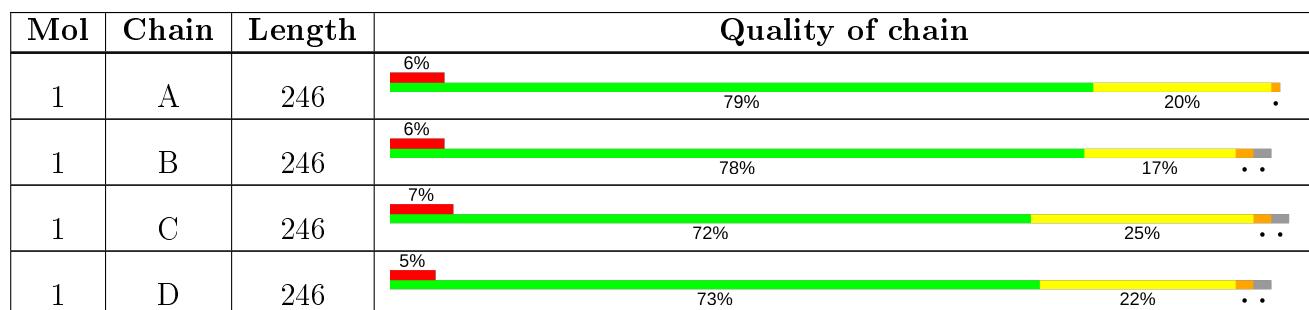
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7253 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 enzyme subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1808	1141	307	352	8			
1	B	241	Total	C	N	O	S	0	0	0
			1775	1121	304	343	7			
1	C	241	Total	C	N	O	S	0	0	0
			1758	1109	300	343	6			
1	D	240	Total	C	N	O	S	0	0	0
			1775	1123	304	341	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	33	Total	O	0	0
			33	33		
2	C	29	Total	O	0	0
			29	29		
2	D	33	Total	O	0	0
			33	33		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: enzyme subunit
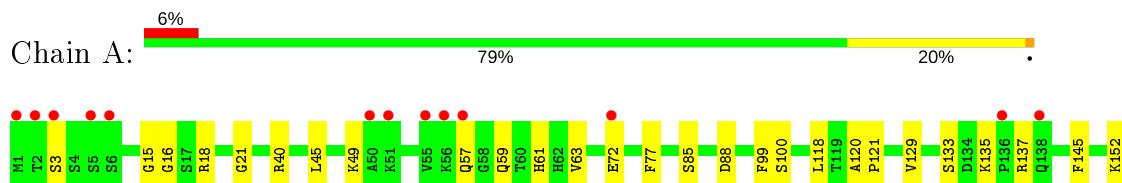
- Molecule 1: enzyme subunit
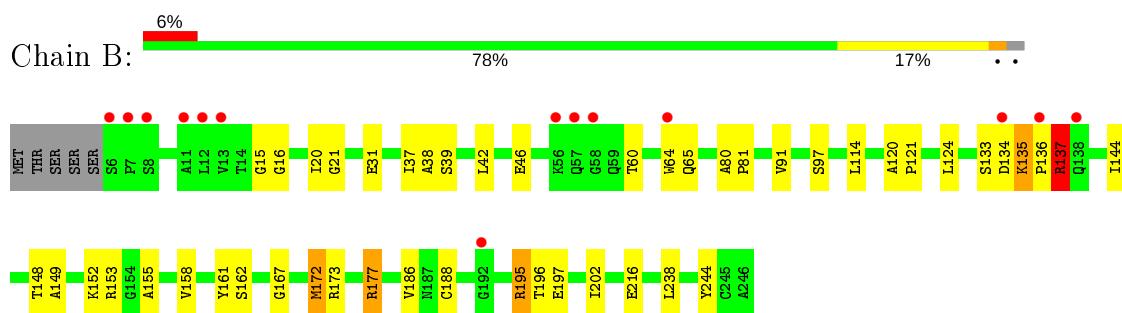
- Molecule 1: enzyme subunit
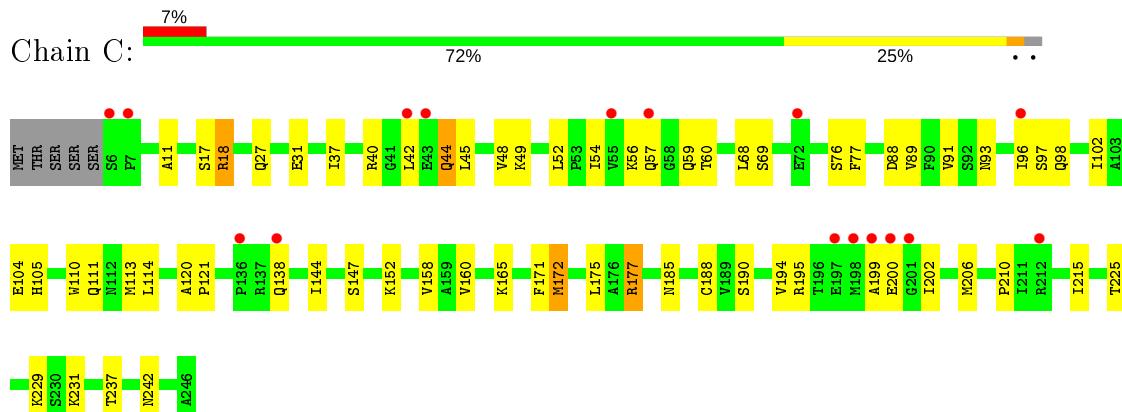
- Molecule 1: enzyme subunit
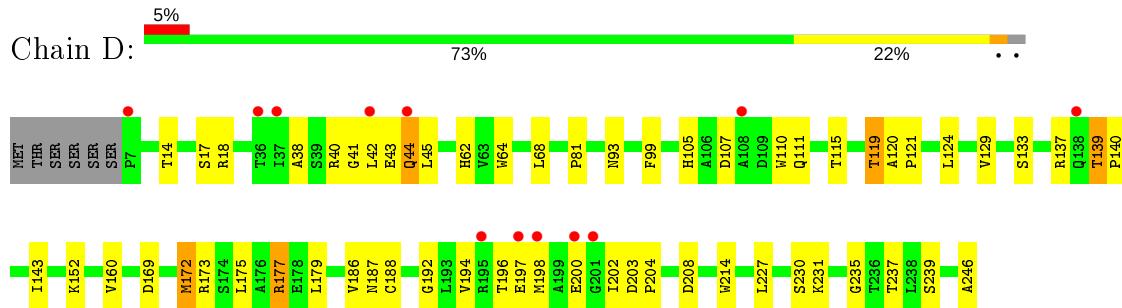
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.67Å 86.52Å 102.75Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	19.90 – 2.50 19.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.90-2.50) 95.4 (19.90-2.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.189 , 0.288 0.202 , 0.296	Depositor DCC
R_{free} test set	842 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.7	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	7253	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.52	0/1843	0.65	0/2506
1	B	0.52	0/1808	0.65	0/2457
1	C	0.48	0/1792	0.65	0/2442
1	D	0.48	0/1810	0.66	0/2460
All	All	0.50	0/7253	0.65	0/9865

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	173	ARG	Sidechain
1	B	177	ARG	Sidechain
1	C	177	ARG	Sidechain
1	C	18	ARG	Sidechain
1	D	137	ARG	Sidechain

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	1808	0	1820	33	0
1	B	1775	0	1779	31	0
1	C	1758	0	1750	42	0
1	D	1775	0	1793	39	0
2	A	42	0	0	2	0
2	B	33	0	0	1	0
2	C	29	0	0	2	0
2	D	33	0	0	2	0
All	All	7253	0	7142	140	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 10.

All (140) 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:202:ILE:HD12	1:C:206:MET:SD	1.93	1.06
1:A:246:ALA:O	1:D:177:ARG:NH1	2.03	0.91
1:C:18:ARG:HB3	1:C:44:GLN:HE22	1.37	0.88
1:A:195:ARG:O	1:A:196:THR:HG22	1.74	0.88
1:D:196:THR:HG21	2:D:330:HOH:O	1.79	0.82
1:C:105:HIS:CE1	1:C:110:TRP:HB3	2.17	0.80
1:A:177:ARG:NH2	1:D:246:ALA:O	2.16	0.79
1:C:202:ILE:CD1	1:C:206:MET:SD	2.72	0.77
1:A:172:MET:HE1	1:A:186:VAL:O	1.87	0.75
1:B:136:PRO:C	1:B:137:ARG:N	2.43	0.72
1:C:97:SER:HA	1:C:113:MET:HE2	1.73	0.71
1:C:98:GLN:N	1:C:113:MET:HE1	2.06	0.70
1:D:152:LYS:HE2	1:D:237:THR:HG21	1.75	0.69
1:B:172:MET:HG2	1:B:188:CYS:SG	2.33	0.67
1:B:195:ARG:NE	1:B:216:GLU:OE2	2.27	0.67
1:D:200:GLU:N	1:D:200:GLU:OE1	2.28	0.66
1:A:99:PHE:CE2	1:A:199:ALA:O	2.49	0.66
1:D:172:MET:HG2	1:D:188:CYS:SG	2.36	0.66
1:C:120:ALA:HB3	1:C:121:PRO:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PHE:CZ	1:C:175:LEU:HD11	2.34	0.62
1:C:44:GLN:HB2	2:C:309:HOH:O	1.99	0.62
1:D:129:VAL:O	1:D:133:SER:OG	2.16	0.62
1:B:135:LYS:HE2	1:B:135:LYS:N	2.15	0.61
1:D:120:ALA:HB3	1:D:121:PRO:HD3	1.82	0.60
1:A:169:ASP:O	1:A:172:MET:HG3	2.02	0.59
1:A:45:LEU:HD13	1:A:63:VAL:HG13	1.84	0.59
1:A:49:LYS:NZ	2:A:303:HOH:O	2.36	0.58
1:D:194:VAL:O	1:D:196:THR:HG22	2.02	0.58
1:B:64:TRP:CE2	1:B:80:ALA:HB2	2.38	0.58
1:C:76:SER:O	1:C:77:PHE:HB2	2.02	0.58
1:D:139:THR:HG23	1:D:140:PRO:O	2.04	0.58
1:C:42:LEU:HA	1:C:45:LEU:HD12	1.86	0.58
1:C:40:ARG:HD2	1:C:68:LEU:HD12	1.87	0.56
1:D:143:ILE:O	1:D:186:VAL:HA	2.05	0.56
1:B:158:VAL:HG23	1:B:162:SER:HG	1.73	0.54
1:B:15:GLY:O	1:B:21:GLY:HA3	2.07	0.54
1:A:172:MET:CE	1:A:186:VAL:O	2.56	0.54
1:B:195:ARG:O	1:B:196:THR:OG1	2.17	0.54
1:C:147:SER:HA	1:C:165:LYS:HD2	1.89	0.53
1:C:185:ASN:ND2	1:C:231:LYS:O	2.41	0.53
1:D:38:ALA:HA	1:D:64:TRP:O	2.08	0.53
1:C:88:ASP:OD1	2:C:301:HOH:O	2.18	0.52
1:A:85:SER:O	1:A:135:LYS:NZ	2.35	0.52
1:B:135:LYS:CE	1:B:135:LYS:N	2.73	0.52
1:B:148:THR:HG21	1:B:161:TYR:CE2	2.45	0.52
1:C:202:ILE:HG23	1:C:202:ILE:O	2.08	0.51
1:A:59:GLN:HE21	1:A:61:HIS:CE1	2.28	0.51
1:C:31:GLU:OE1	1:C:229:LYS:NZ	2.40	0.51
1:A:172:MET:CE	1:A:187:ASN:HA	2.40	0.51
1:A:59:GLN:HE21	1:A:61:HIS:HE1	1.59	0.51
1:C:48:VAL:O	1:C:52:LEU:HG	2.11	0.51
1:D:227:LEU:O	1:D:230:SER:OG	2.23	0.51
1:A:210:PRO:HG2	1:A:243:GLY:HA3	1.92	0.50
1:B:155:ALA:O	1:B:158:VAL:HG22	2.11	0.50
1:A:246:ALA:HB2	1:D:235:GLY:HA3	1.94	0.50
1:D:152:LYS:CE	1:D:237:THR:HG21	2.42	0.49
1:D:44:GLN:HA	1:D:44:GLN:HE21	1.77	0.49
1:C:97:SER:HA	1:C:113:MET:CE	2.40	0.49
1:B:64:TRP:CZ2	1:B:80:ALA:HB2	2.48	0.49
1:D:115:THR:HA	1:D:119:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:MET:HE1	1:A:187:ASN:HA	1.94	0.48
1:C:171:PHE:CE2	1:C:175:LEU:HD11	2.47	0.48
1:C:210:PRO:HD2	1:C:242:ASN:O	2.14	0.48
1:D:169:ASP:O	1:D:172:MET:HG3	2.13	0.48
1:D:40:ARG:HH21	1:D:68:LEU:HD12	1.77	0.48
1:D:62:HIS:HB3	1:D:81:PRO:HG3	1.95	0.48
1:D:139:THR:HG22	2:D:321:HOH:O	2.13	0.48
1:D:172:MET:CE	1:D:187:ASN:HA	2.44	0.48
1:B:91:VAL:HA	1:B:144:ILE:O	2.14	0.47
1:D:14:THR:O	1:D:93:ASN:HB3	2.14	0.47
1:B:135:LYS:HD3	1:B:135:LYS:HA	1.55	0.47
1:B:149:ALA:HB1	1:B:244:TYR:HD2	1.79	0.47
1:A:172:MET:HG2	1:A:188:CYS:SG	2.54	0.47
1:B:120:ALA:N	1:B:121:PRO:HD2	2.30	0.47
1:A:180:GLY:N	1:A:181:PRO:CD	2.77	0.47
1:C:110:TRP:HB2	1:C:160:VAL:HG11	1.96	0.47
1:B:172:MET:HB2	1:B:186:VAL:HG12	1.97	0.46
1:D:172:MET:HB2	1:D:186:VAL:HG12	1.97	0.46
1:A:194:VAL:HB	1:A:215:ILE:O	2.15	0.46
1:D:204:PRO:HD2	1:D:214:TRP:CZ2	2.51	0.46
1:D:107:ASP:HB3	1:D:111:GLN:OE1	2.15	0.45
1:C:93:ASN:CG	1:C:93:ASN:O	2.55	0.45
1:A:15:GLY:O	1:A:21:GLY:HA3	2.16	0.45
1:A:172:MET:HE3	1:A:172:MET:HB2	1.77	0.45
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.81	0.45
1:A:145:PHE:O	1:A:188:CYS:HA	2.17	0.45
1:B:42:LEU:O	1:B:46:GLU:HG2	2.16	0.44
1:D:169:ASP:HB3	1:D:173:ARG:HH21	1.81	0.44
1:C:194:VAL:HG22	1:C:215:ILE:HB	1.99	0.44
1:D:172:MET:CE	1:D:186:VAL:O	2.65	0.44
1:D:41:GLY:O	1:D:45:LEU:HG	2.18	0.44
1:A:163:ALA:O	1:B:167:GLY:HA2	2.17	0.44
1:C:18:ARG:HB3	1:C:44:GLN:NE2	2.18	0.44
1:A:129:VAL:O	1:A:133:SER:OG	2.24	0.44
1:D:99:PHE:CE1	1:D:202:ILE:HD13	2.53	0.44
1:C:27:GLN:NE2	1:C:225:THR:OG1	2.51	0.44
1:C:194:VAL:HG13	1:C:215:ILE:O	2.19	0.43
1:A:16:GLY:HA2	1:A:21:GLY:HA3	1.99	0.43
1:C:96:ILE:O	1:C:113:MET:HE2	2.18	0.43
1:C:172:MET:HG2	1:C:188:CYS:SG	2.59	0.43
1:C:37:ILE:HG13	1:C:45:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLY:O	1:D:194:VAL:HG23	2.18	0.43
1:C:152:LYS:HE2	1:C:237:THR:HG21	2.00	0.43
1:C:114:LEU:HD23	1:D:119:THR:HG23	2.01	0.42
1:B:158:VAL:HG23	1:B:162:SER:OG	2.19	0.42
1:B:136:PRO:O	1:B:137:ARG:N	2.53	0.42
1:C:98:GLN:N	1:C:113:MET:CE	2.81	0.42
1:B:64:TRP:CG	1:B:80:ALA:HA	2.54	0.42
1:D:172:MET:HE1	1:D:187:ASN:HA	2.01	0.42
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.85	0.42
1:A:175:LEU:HD22	1:A:179:LEU:HD11	2.01	0.41
1:B:134:ASP:C	1:B:135:LYS:HE2	2.39	0.41
1:C:104:GLU:HG2	1:C:104:GLU:O	2.19	0.41
1:C:11:ALA:HA	1:C:89:VAL:O	2.20	0.41
1:A:99:PHE:HB3	2:A:328:HOH:O	2.20	0.41
1:B:16:GLY:HA3	1:B:37:ILE:HG22	2.02	0.41
1:A:188:CYS:O	1:A:237:THR:HA	2.21	0.41
1:B:64:TRP:CD2	1:B:80:ALA:HB2	2.55	0.41
1:B:64:TRP:HB2	1:B:81:PRO:HD3	2.03	0.41
1:A:152:LYS:HE3	1:A:237:THR:HG21	2.02	0.41
1:C:158:VAL:O	1:C:158:VAL:HG23	2.21	0.41
1:C:194:VAL:HA	1:C:215:ILE:O	2.21	0.41
1:B:97:SER:HA	1:B:161:TYR:CD1	2.55	0.41
1:D:172:MET:HE1	1:D:186:VAL:O	2.20	0.41
1:D:175:LEU:HD22	1:D:179:LEU:HD11	2.03	0.41
1:C:91:VAL:HA	1:C:144:ILE:O	2.21	0.41
1:A:120:ALA:HB3	1:A:121:PRO:HD3	2.03	0.40
1:D:105:HIS:CD2	1:D:110:TRP:HB3	2.56	0.40
1:A:216:GLU:HA	1:A:217:PRO:HD3	1.95	0.40
1:C:152:LYS:HZ1	1:C:190:SER:CB	2.35	0.40
1:C:17:SER:O	1:C:44:GLN:NE2	2.54	0.40
1:D:110:TRP:HB2	1:D:160:VAL:HG11	2.01	0.40
1:D:143:ILE:HB	1:D:186:VAL:HG22	2.02	0.40
1:A:118:LEU:C	1:A:121:PRO:HD2	2.41	0.40
1:B:153:ARG:HB3	1:B:244:TYR:CE2	2.56	0.40
1:B:195:ARG:HA	2:B:326:HOH:O	2.20	0.40
1:B:38:ALA:HA	1:B:64:TRP:O	2.20	0.40
1:C:54:ILE:HA	1:C:59:GLN:OE1	2.22	0.40
1:B:20:ILE:HD12	1:B:197:GLU:HG3	2.04	0.40
1:D:42:LEU:O	1:D:43:GLU:C	2.60	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	244/246 (99%)	230 (94%)	13 (5%)	1 (0%)	34	54
1	B	237/246 (96%)	220 (93%)	17 (7%)	0	100	100
1	C	239/246 (97%)	220 (92%)	18 (8%)	1 (0%)	34	54
1	D	238/246 (97%)	222 (93%)	16 (7%)	0	100	100
All	All	958/984 (97%)	892 (93%)	64 (7%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	ALA
1	A	100	SER

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	194/195 (100%)	183 (94%)	11 (6%)	20	39
1	B	188/195 (96%)	173 (92%)	15 (8%)	12	23
1	C	185/195 (95%)	172 (93%)	13 (7%)	15	29
1	D	189/195 (97%)	175 (93%)	14 (7%)	13	27
All	All	756/780 (97%)	703 (93%)	53 (7%)	15	29

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	18	ARG
1	A	57	GLN
1	A	72	GLU
1	A	77	PHE
1	A	88	ASP
1	A	172	MET
1	A	177	ARG
1	A	195	ARG
1	A	202	ILE
1	A	218	ASP
1	B	31	GLU
1	B	39	SER
1	B	60	THR
1	B	65	GLN
1	B	114	LEU
1	B	124	LEU
1	B	133	SER
1	B	135	LYS
1	B	137	ARG
1	B	152	LYS
1	B	172	MET
1	B	177	ARG
1	B	195	ARG
1	B	202	ILE
1	B	238	LEU
1	C	44	GLN
1	C	49	LYS
1	C	56	LYS
1	C	57	GLN
1	C	60	THR
1	C	69	SER
1	C	102	ILE
1	C	111	GLN
1	C	138	GLN
1	C	172	MET
1	C	177	ARG
1	C	195	ARG
1	C	200	GLU
1	D	17	SER
1	D	18	ARG
1	D	44	GLN
1	D	119	THR

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Mol	Chain	Res	Type
1	D	124	LEU
1	D	139	THR
1	D	172	MET
1	D	177	ARG
1	D	197	GLU
1	D	198	MET
1	D	203	ASP
1	D	208	ASP
1	D	231	LYS
1	D	239	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	GLN
1	C	105	HIS
1	D	44	GLN
1	D	232	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

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5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	136:PRO	C	137:ARG	N	2.43

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	246/246 (100%)	0.01	15 (6%)	21 22	35, 51, 80, 114	0
1	B	241/246 (97%)	0.10	14 (5%)	23 24	38, 55, 86, 117	0
1	C	241/246 (97%)	0.25	16 (6%)	18 19	40, 60, 89, 128	0
1	D	240/246 (97%)	0.09	12 (5%)	28 30	37, 60, 92, 132	0
All	All	968/984 (98%)	0.11	57 (5%)	22 23	35, 56, 87, 132	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	ALA	7.7
1	C	6	SER	5.4
1	B	6	SER	5.3
1	A	1	MET	5.1
1	C	212	ARG	4.6
1	C	197	GLU	4.6
1	B	11	ALA	4.0
1	C	57	GLN	4.0
1	B	7	PRO	3.8
1	D	7	PRO	3.7
1	C	138	GLN	3.6
1	A	50	ALA	3.6
1	D	37	ILE	3.4
1	D	44	GLN	3.4
1	B	138	GLN	3.3
1	D	108	ALA	3.3
1	A	57	GLN	3.2
1	D	197	GLU	3.2
1	A	6	SER	3.1
1	C	42	LEU	3.1
1	D	201	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	136	PRO	3.1
1	C	7	PRO	3.0
1	C	96	ILE	2.9
1	A	2	THR	2.9
1	C	200	GLU	2.9
1	A	196	THR	2.9
1	B	56	LYS	2.8
1	D	195	ARG	2.8
1	C	43	GLU	2.7
1	A	5	SER	2.7
1	D	198	MET	2.6
1	B	57	GLN	2.5
1	C	201	GLY	2.5
1	B	134	ASP	2.4
1	A	138	GLN	2.4
1	C	55	VAL	2.4
1	A	3	SER	2.4
1	C	136	PRO	2.3
1	D	200	GLU	2.3
1	B	12	LEU	2.3
1	D	138	GLN	2.3
1	B	58	GLY	2.3
1	A	72	GLU	2.3
1	A	56	LYS	2.2
1	B	13	VAL	2.2
1	B	192	GLY	2.2
1	A	200	GLU	2.2
1	B	64	TRP	2.2
1	C	72	GLU	2.2
1	D	36	THR	2.1
1	C	198	MET	2.1
1	B	8	SER	2.1
1	D	42	LEU	2.1
1	A	136	PRO	2.1
1	A	55	VAL	2.0
1	A	51	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.