Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 07:34 AM EDT

PDB ID	:	1G24
Title	:	THE CRYSTAL STRUCTURE OF EXOENZYME C3 FROM CLOSTRIDIUM BOTULINUM
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Deposited on	:	2000-10-16
Resolution	:	1.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

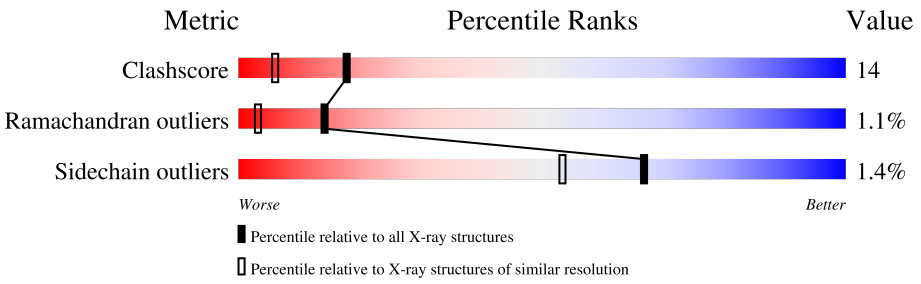
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.70 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))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	78% 20% •
1	B	211	81% 18% •
1	C	211	71% 28%
1	D	211	74% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7493 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 EXOENZYME C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	1656	1053	282	314	7	0	0	0
1	B	211	1656	1053	282	314	7	0	0	0
1	C	211	1656	1053	282	314	7	0	0	0
1	D	211	1656	1053	282	314	7	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	202	202	202	0	0
2	B	224	224	224	0	0
2	C	221	221	221	0	0
2	D	222	222	222	0	0

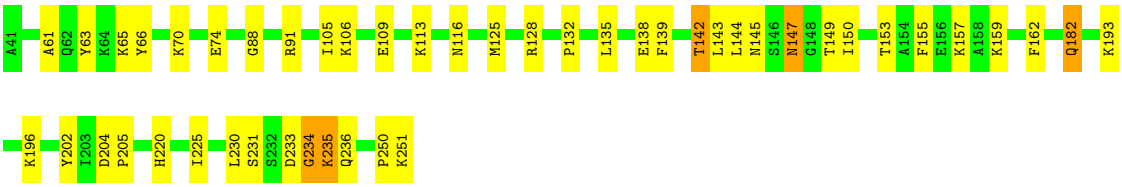
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

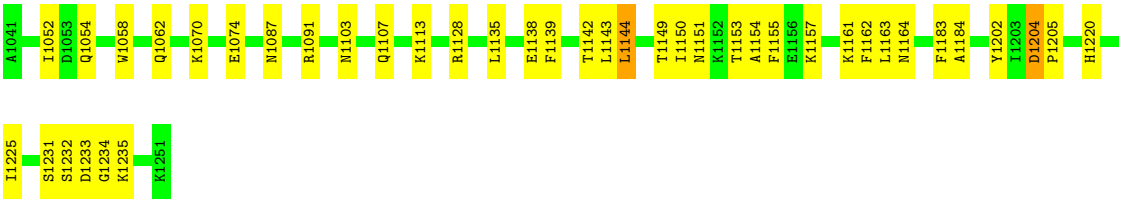
• Molecule 1: EXOENZYME C3

Chain A:



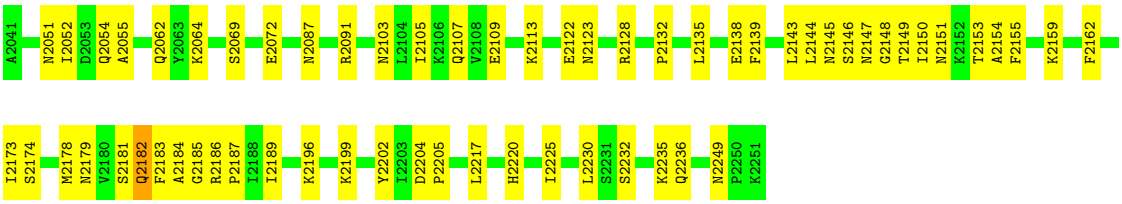
• Molecule 1: EXOENZYME C3

Chain B:



• Molecule 1: EXOENZYME C3

Chain C:



• Molecule 1: EXOENZYME C3

Chain D:

N3151
K3152
T3153
A3154
F3155
K3159
F3162
Y3172
Q3182
K3193
K3196
L3213
I3225
L3230
K3235
Q3236
I3237
K3251

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	233.75Å 73.76Å 73.75Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70	Depositor
% Data completeness (in resolution range)	9.4 (30.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	5.70	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

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	0.30	0/1686	0.58	0/2266
1	B	0.31	0/1686	0.58	0/2266
1	C	0.32	0/1686	0.59	0/2266
1	D	0.31	0/1686	0.57	0/2266
All	All	0.31	0/6744	0.58	0/9064

There are no bond length outliers.

There are no bond angle outliers.

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	1656	0	1677	43	0
1	B	1656	0	1677	28	0
1	C	1656	0	1677	66	0
1	D	1656	0	1677	44	0
2	A	202	0	0	3	0
2	B	224	0	0	1	0
2	C	221	0	0	6	0
2	D	222	0	0	5	0
All	All	7493	0	6708	181	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 14.

All (181) 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:2052:ILE:HA	1:C:2178:MET:HE1	1.29	1.14
1:A:135:LEU:HD12	1:A:143:LEU:HD11	1.43	0.99
1:A:149:THR:HB	1:A:235:LYS:HD2	1.44	0.97
1:C:2150:ILE:HG12	1:C:2235:LYS:HB3	1.53	0.89
1:A:150:ILE:HG12	1:A:235:LYS:HB3	1.55	0.86
1:B:1151:ASN:HD21	1:B:1153:THR:HB	1.44	0.82
1:D:3066:TYR:HB3	1:D:3068:LEU:HD13	1.62	0.81
1:A:61:ALA:O	1:A:65:LYS:HD3	1.83	0.79
1:D:3135:LEU:HD12	1:D:3143:LEU:HD11	1.64	0.78
1:A:113:LYS:HE3	1:A:251:LYS:HE3	1.64	0.78
1:B:1052:ILE:HD12	1:B:1052:ILE:H	1.49	0.77
1:C:2182:GLN:HG2	2:C:4154:HOH:O	1.84	0.77
1:B:1162:PHE:HB3	1:B:1225:ILE:HD12	1.67	0.76
1:C:2183:PHE:O	1:C:2186:ARG:HG3	1.85	0.76
1:A:153:THR:HG22	1:A:157:LYS:HE3	1.70	0.73
1:D:3151:ASN:HD21	1:D:3153:THR:HB	1.51	0.73
1:C:2135:LEU:HD12	1:C:2143:LEU:HD11	1.69	0.72
1:A:150:ILE:HD11	1:A:230:LEU:HD22	1.70	0.72
1:A:196:LYS:HE3	2:A:4660:HOH:O	1.91	0.71
1:D:3149:THR:HA	1:D:3235:LYS:HB3	1.74	0.69
1:A:138:GLU:HG3	1:A:139:PHE:CD1	2.27	0.68
1:D:3150:ILE:HG21	1:D:3230:LEU:HD22	1.76	0.68
1:B:1138:GLU:HG3	1:B:1139:PHE:CD1	2.28	0.68
1:A:139:PHE:HB3	1:A:143:LEU:HG	1.76	0.66
1:A:231:SER:OG	1:A:236:GLN:HB3	1.95	0.66
1:C:2052:ILE:CA	1:C:2178:MET:HE1	2.19	0.65
1:C:2181:SER:C	1:C:2183:PHE:H	2.00	0.65
1:C:2150:ILE:HB	1:C:2235:LYS:HD2	1.79	0.65
1:A:250:PRO:O	1:A:251:LYS:HB2	1.96	0.63
1:C:2162:PHE:HB3	1:C:2225:ILE:HD12	1.81	0.63
1:D:3151:ASN:ND2	1:D:3153:THR:HB	2.14	0.63
1:B:1151:ASN:ND2	1:B:1153:THR:HB	2.13	0.63
1:D:3151:ASN:ND2	1:D:3154:ALA:H	1.97	0.62
1:C:2181:SER:O	1:C:2183:PHE:N	2.33	0.62
1:B:1150:ILE:HD13	1:B:1155:PHE:HB2	1.81	0.62
1:B:1052:ILE:HD12	1:B:1052:ILE:N	2.13	0.62
1:D:3145:ASN:HB3	1:D:3147:ASN:OD1	2.00	0.61
1:C:2147:ASN:HD21	1:C:2149:THR:HG23	1.66	0.61
1:C:2199:LYS:NZ	1:C:2249:ASN:HD22	1.99	0.60
1:D:3151:ASN:HD22	1:D:3154:ALA:H	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2151:ASN:HD21	1:C:2153:THR:HB	1.66	0.60
1:A:230:LEU:HA	1:A:236:GLN:O	2.02	0.60
1:C:2150:ILE:H	1:C:2235:LYS:CG	2.16	0.59
1:C:2149:THR:CB	1:C:2235:LYS:HG3	2.32	0.59
1:C:2230:LEU:HD13	1:C:2235:LYS:NZ	2.17	0.59
1:B:1150:ILE:O	1:B:1150:ILE:HD12	2.04	0.58
1:B:1052:ILE:H	1:B:1052:ILE:CD1	2.15	0.58
1:C:2183:PHE:CE2	1:C:2189:ILE:HD11	2.39	0.58
1:A:162:PHE:HB3	1:A:225:ILE:HD12	1.84	0.57
1:D:3151:ASN:O	1:D:3152:LYS:HB3	2.05	0.57
1:A:155:PHE:CE2	1:A:159:LYS:HE3	2.39	0.57
1:D:3144:LEU:HD12	1:D:3144:LEU:N	2.20	0.56
1:C:2149:THR:CA	1:C:2235:LYS:HG3	2.36	0.56
1:A:88:GLY:HA2	1:A:91:ARG:NH1	2.20	0.56
1:D:3162:PHE:HB3	1:D:3225:ILE:HD12	1.87	0.56
1:D:3150:ILE:HD11	1:D:3155:PHE:HB2	1.87	0.56
1:C:2149:THR:HB	1:C:2235:LYS:HG3	1.88	0.55
1:B:1113:LYS:HD3	2:B:4748:HOH:O	2.06	0.55
1:C:2155:PHE:CZ	1:C:2159:LYS:HD2	2.42	0.55
1:D:3056:LYS:HG2	1:D:3213:LEU:HD21	1.89	0.54
1:C:2149:THR:HA	1:C:2235:LYS:HB2	1.89	0.54
1:D:3155:PHE:CZ	1:D:3159:LYS:HD3	2.43	0.54
1:C:2122:GLU:HA	1:C:2196:LYS:HG2	1.89	0.54
1:A:132:PRO:HB3	1:A:143:LEU:HD12	1.90	0.54
1:C:2128:ARG:HD3	2:C:4541:HOH:O	2.07	0.54
1:B:1070:LYS:O	1:B:1074:GLU:HG3	2.08	0.54
1:D:3139:PHE:HB3	1:D:3143:LEU:HG	1.90	0.52
1:C:2155:PHE:CE2	1:C:2159:LYS:HD2	2.44	0.52
1:B:1128:ARG:HA	1:B:1183:PHE:CZ	2.45	0.52
1:B:1233:ASP:C	1:B:1235:LYS:H	2.13	0.52
1:C:2199:LYS:HZ1	1:C:2249:ASN:HD22	1.58	0.52
1:A:250:PRO:O	1:A:251:LYS:CB	2.59	0.51
1:B:1163:LEU:HG	1:B:1164:ASN:ND2	2.25	0.51
1:C:2230:LEU:HD13	1:C:2235:LYS:HZ2	1.74	0.51
1:A:149:THR:HB	1:A:235:LYS:CD	2.31	0.51
1:C:2149:THR:HA	1:C:2235:LYS:HG3	1.91	0.51
1:C:2054:GLN:HA	1:C:2054:GLN:OE1	2.11	0.51
1:A:150:ILE:O	1:A:235:LYS:HD3	2.11	0.50
1:D:3132:PRO:HA	1:D:3143:LEU:HD12	1.93	0.50
1:B:1135:LEU:HD12	1:B:1143:LEU:HD11	1.93	0.50
1:C:2087:ASN:O	1:C:2091:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2151:ASN:ND2	1:C:2154:ALA:H	2.10	0.49
1:D:3150:ILE:CD1	1:D:3155:PHE:HB2	2.43	0.49
1:A:144:LEU:N	1:A:144:LEU:HD12	2.27	0.49
1:B:1202:TYR:CE2	1:B:1205:PRO:HD3	2.48	0.48
1:D:3122:GLU:HA	1:D:3196:LYS:HG2	1.94	0.48
1:D:3105:ILE:O	1:D:3109:GLU:HG3	2.12	0.48
1:D:3149:THR:CA	1:D:3235:LYS:HB3	2.43	0.48
1:A:116:ASN:HD22	1:A:251:LYS:CE	2.26	0.48
1:A:116:ASN:HD22	1:A:251:LYS:HE3	1.79	0.48
1:A:116:ASN:ND2	1:A:251:LYS:HD2	2.29	0.48
1:D:3111:LEU:HD23	1:D:3172:TYR:CZ	2.49	0.48
1:A:153:THR:O	1:A:157:LYS:HG3	2.13	0.48
1:C:2064:LYS:HG2	2:C:4782:HOH:O	2.13	0.48
1:D:3148:GLY:C	1:D:3235:LYS:HD3	2.34	0.48
1:B:1103:ASN:O	1:B:1107:GLN:HG3	2.13	0.47
1:C:2150:ILE:H	1:C:2235:LYS:HD2	1.79	0.47
1:B:1150:ILE:HD12	1:B:1150:ILE:C	2.34	0.47
1:D:3144:LEU:C	1:D:3146:SER:H	2.18	0.47
1:C:2055:ALA:CB	1:C:2178:MET:HE3	2.45	0.47
1:C:2183:PHE:C	1:C:2185:GLY:H	2.18	0.47
1:C:2150:ILE:H	1:C:2235:LYS:CD	2.28	0.47
1:B:1142:THR:HG22	1:B:1154:ALA:HB2	1.97	0.47
1:C:2181:SER:C	1:C:2183:PHE:N	2.68	0.47
1:C:2151:ASN:HD22	1:C:2154:ALA:H	1.63	0.46
1:A:65:LYS:N	1:A:65:LYS:HD2	2.30	0.46
1:C:2147:ASN:ND2	1:C:2149:THR:HG23	2.30	0.46
1:C:2183:PHE:C	1:C:2185:GLY:N	2.67	0.46
1:D:3138:GLU:HG3	1:D:3139:PHE:CD1	2.51	0.46
1:C:2147:ASN:CG	1:C:2148:GLY:H	2.19	0.46
1:A:202:TYR:CE2	1:A:205:PRO:HD3	2.50	0.46
1:C:2232:SER:HA	2:C:4834:HOH:O	2.16	0.46
1:D:3087:ASN:O	1:D:3091:ARG:HG3	2.16	0.46
1:A:105:ILE:O	1:A:109:GLU:HG3	2.16	0.46
1:B:1144:LEU:HD12	1:B:1144:LEU:N	2.31	0.46
1:C:2183:PHE:HE2	1:C:2189:ILE:HD11	1.79	0.46
1:C:2113:LYS:HB3	2:C:4081:HOH:O	2.15	0.45
1:A:231:SER:CB	1:A:236:GLN:HB3	2.46	0.45
1:D:3123:ASN:OD1	1:D:3196:LYS:HG3	2.16	0.45
1:D:3150:ILE:HD12	1:D:3237:ILE:CG1	2.46	0.45
1:C:2151:ASN:ND2	1:C:2153:THR:HB	2.31	0.45
1:D:3145:ASN:O	1:D:3145:ASN:OD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLY:O	1:A:235:LYS:HB2	2.17	0.45
1:B:1204:ASP:N	1:B:1205:PRO:HD2	2.31	0.44
1:C:2144:LEU:HD12	1:C:2144:LEU:N	2.33	0.44
1:C:2202:TYR:CE2	1:C:2205:PRO:HD3	2.52	0.44
1:D:3046:TYR:CD2	1:D:3123:ASN:HB3	2.52	0.44
1:A:65:LYS:N	1:A:65:LYS:CD	2.81	0.44
1:C:2128:ARG:NH1	1:C:2174:SER:O	2.50	0.44
1:A:113:LYS:HE3	1:A:251:LYS:CE	2.41	0.44
1:C:2183:PHE:HE2	1:C:2236:GLN:HE22	1.64	0.44
1:D:3078:SER:HB2	1:D:3107:GLN:NE2	2.33	0.44
1:D:3182:GLN:HG3	2:D:4712:HOH:O	2.17	0.44
1:C:2055:ALA:CB	1:C:2178:MET:CE	2.96	0.43
1:B:1153:THR:O	1:B:1157:LYS:HG3	2.18	0.43
1:C:2145:ASN:ND2	1:C:2146:SER:H	2.16	0.43
1:D:3054:GLN:HA	1:D:3054:GLN:OE1	2.19	0.43
1:C:2055:ALA:HB2	1:C:2178:MET:CE	2.49	0.43
1:C:2204:ASP:N	1:C:2205:PRO:HD2	2.33	0.43
1:C:2173:ILE:HB	1:C:2217:LEU:HB2	2.00	0.43
1:A:150:ILE:CD1	1:A:230:LEU:HD22	2.45	0.43
1:C:2069:SER:OG	1:C:2072:GLU:HG3	2.19	0.43
1:A:155:PHE:CZ	1:A:159:LYS:HE3	2.54	0.43
1:C:2183:PHE:O	1:C:2184:ALA:HB3	2.18	0.43
1:C:2179:ASN:HD21	1:C:2183:PHE:HZ	1.66	0.43
1:B:1161:LYS:HD3	1:B:1162:PHE:CE2	2.54	0.42
1:D:3041:ALA:HB1	2:D:4763:HOH:O	2.18	0.42
1:D:3106:LYS:HD3	2:D:4259:HOH:O	2.19	0.42
1:A:143:LEU:C	1:A:144:LEU:HD12	2.40	0.42
1:B:1231:SER:O	1:B:1232:SER:C	2.58	0.42
1:B:1058:TRP:O	1:B:1062:GLN:HG2	2.20	0.41
1:D:3113:LYS:HB3	2:D:4143:HOH:O	2.19	0.41
1:A:70:LYS:O	1:A:74:GLU:HG3	2.20	0.41
1:C:2052:ILE:HD13	1:C:2178:MET:SD	2.61	0.41
1:D:3150:ILE:HD13	1:D:3230:LEU:HD21	2.02	0.41
1:D:3069:SER:OG	1:D:3072:GLU:HG3	2.20	0.41
1:D:3070:LYS:O	1:D:3074:GLU:HG3	2.21	0.41
1:A:145:ASN:HB2	1:A:147:ASN:OD1	2.21	0.41
1:D:3150:ILE:HG12	1:D:3152:LYS:H	1.86	0.41
1:A:142:THR:O	1:A:142:THR:HG22	2.20	0.41
1:B:1087:ASN:O	1:B:1091:ARG:HG3	2.21	0.41
1:C:2149:THR:HA	1:C:2235:LYS:CB	2.49	0.41
1:D:3078:SER:CB	1:D:3107:GLN:NE2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1054:GLN:HA	1:B:1054:GLN:OE1	2.20	0.41
1:C:2105:ILE:O	1:C:2109:GLU:HG3	2.19	0.41
1:C:2204:ASP:HB3	1:C:2205:PRO:HD3	2.02	0.41
1:A:182:GLN:HG3	2:A:4351:HOH:O	2.21	0.41
1:B:1149:THR:HA	1:B:1234:GLY:O	2.21	0.41
1:C:2103:ASN:O	1:C:2107:GLN:HG3	2.21	0.41
1:C:2138:GLU:HG3	1:C:2139:PHE:CD1	2.56	0.41
1:A:106:LYS:HG3	2:A:4267:HOH:O	2.21	0.41
1:A:125:MET:SD	1:A:193:LYS:HG2	2.61	0.41
1:C:2123:ASN:OD1	1:C:2196:LYS:HG3	2.21	0.41
1:C:2132:PRO:HD3	1:C:2187:PRO:HG3	2.03	0.40
1:C:2183:PHE:HB3	1:C:2185:GLY:H	1.86	0.40
1:D:3125:MET:SD	1:D:3193:LYS:HG2	2.61	0.40
1:D:3041:ALA:O	1:D:3042:TYR:HB2	2.21	0.40
1:D:3116:ASN:ND2	2:D:4179:HOH:O	2.55	0.40
1:A:63:TYR:HA	1:A:66:TYR:CD2	2.56	0.40
1:A:150:ILE:H	1:A:235:LYS:HB3	1.86	0.40
1:C:2062:GLN:HB3	2:C:4781:HOH:O	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	209/211 (99%)	197 (94%)	7 (3%)	5 (2%)	6 1
1	B	209/211 (99%)	200 (96%)	7 (3%)	2 (1%)	15 4
1	C	209/211 (99%)	199 (95%)	9 (4%)	1 (0%)	29 13
1	D	209/211 (99%)	197 (94%)	11 (5%)	1 (0%)	29 13
All	All	836/844 (99%)	793 (95%)	34 (4%)	9 (1%)	14 3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	B	1184	ALA
1	C	2182	GLN
1	A	233	ASP
1	B	1144	LEU
1	A	234	GLY
1	A	142	THR
1	D	3142	THR
1	A	235	LYS

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	179/179 (100%)	175 (98%)	4 (2%)	52	34
1	B	179/179 (100%)	177 (99%)	2 (1%)	73	63
1	C	179/179 (100%)	177 (99%)	2 (1%)	73	63
1	D	179/179 (100%)	177 (99%)	2 (1%)	73	63
All	All	716/716 (100%)	706 (99%)	10 (1%)	67	53

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	182	GLN
1	A	204	ASP
1	A	220	HIS
1	B	1204	ASP
1	B	1220	HIS
1	C	2051	ASN
1	C	2220	HIS
1	D	3068	LEU
1	D	3119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	140	GLN
1	A	164	ASN
1	A	182	GLN
1	B	1047	GLN
1	B	1140	GLN
1	B	1151	ASN
1	B	1164	ASN
1	C	2051	ASN
1	C	2060	ASN
1	C	2092	GLN
1	C	2140	GLN
1	C	2151	ASN
1	C	2164	ASN
1	C	2182	GLN
1	C	2249	ASN
1	D	3047	GLN
1	D	3051	ASN
1	D	3060	ASN
1	D	3107	GLN
1	D	3116	ASN
1	D	3140	GLN
1	D	3145	ASN
1	D	3151	ASN
1	D	3164	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.