Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 05:08 PM EST

PDB ID	:	1CZD
Title	:	CRYSTAL STRUCTURE OF THE PROCESSIVITY CLAMP GP45 FROM BACTERIOPHAGE T4
Authors	:	Moarefi, I.; Jeruzalmi, D.; Turner, J.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	1999-09-02
Resolution	:	2.45 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:

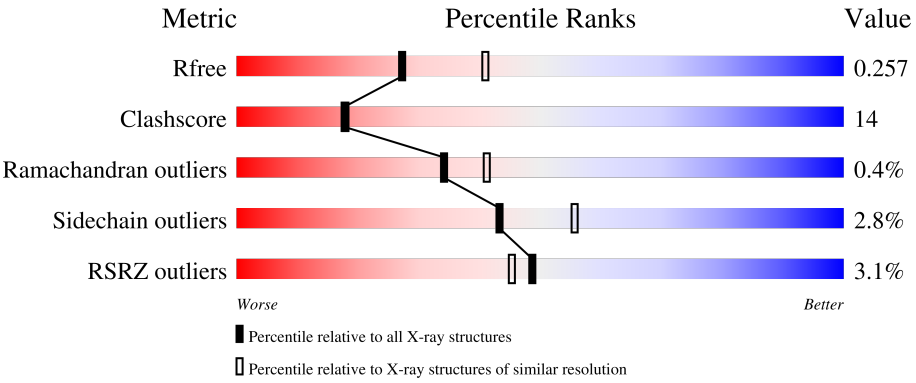
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

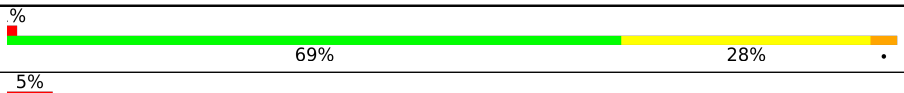
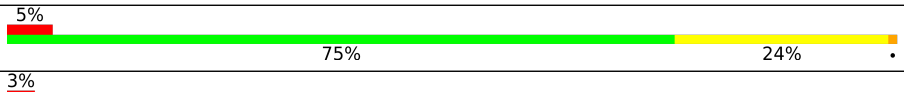
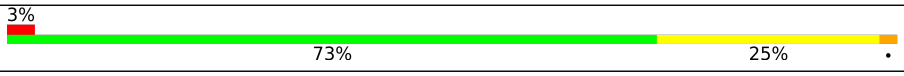
The reported resolution of this entry is 2.45 Å.

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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	228	
1	B	228	
1	C	228	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5250 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 DNA POLYMERASE ACCESSORY PROTEIN G45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
1	B	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
1	C	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			

There are 3 discrepancies between the modelled and reference sequences:

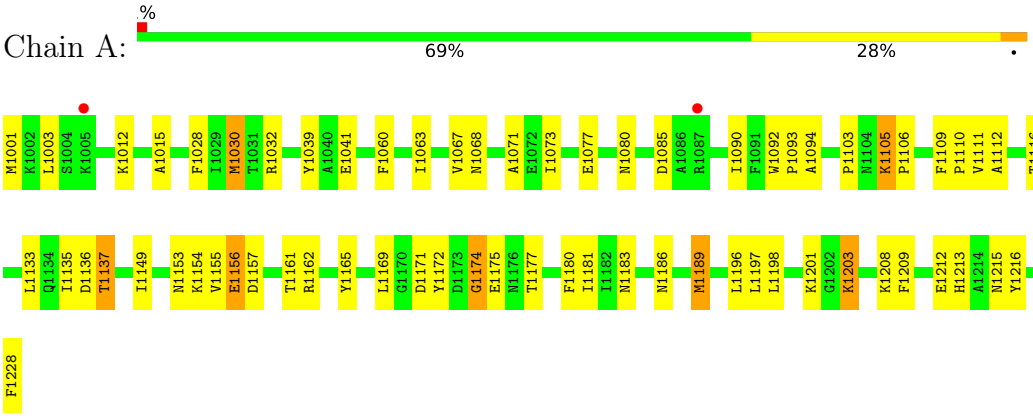
Chain	Residue	Modelled	Actual	Comment	Reference
A	1093	PRO	ARG	conflict	UNP P04525
B	2093	PRO	ARG	conflict	UNP P04525
C	3093	PRO	ARG	conflict	UNP P04525

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.

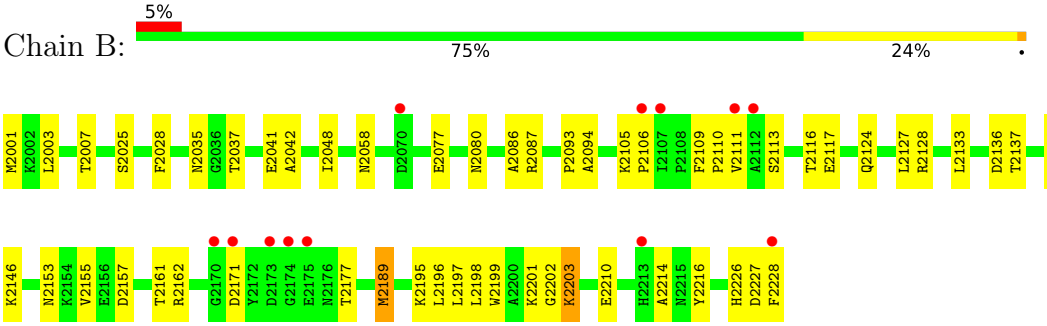
• Molecule 1: DNA POLYMERASE ACCESSORY PROTEIN G45

Chain A:



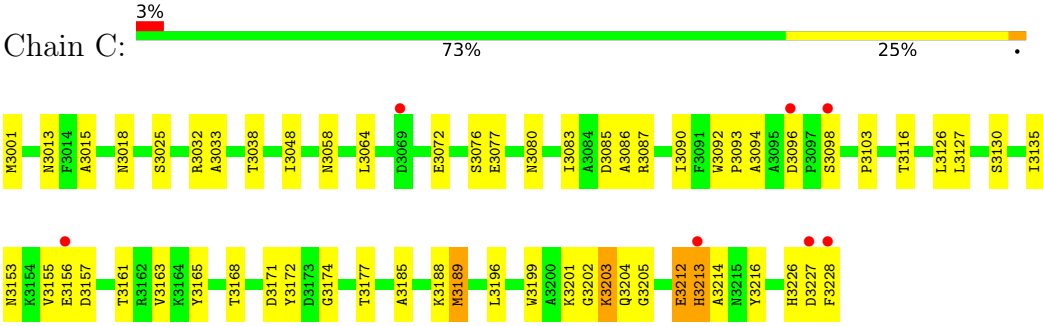
• Molecule 1: DNA POLYMERASE ACCESSORY PROTEIN G45

Chain B:



• Molecule 1: DNA POLYMERASE ACCESSORY PROTEIN G45

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.18Å 93.94Å 141.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.45 56.60 – 2.44	Depositor EDS
% Data completeness (in resolution range)	92.5 (100.00-2.45) 95.6 (56.60-2.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.76 (at 2.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.259 0.240 , 0.257	Depositor DCC
R_{free} test set	1127 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5250	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.47	2/1779 (0.1%)	0.79	6/2410 (0.2%)
1	B	0.41	0/1779	0.65	0/2410
1	C	0.43	0/1779	0.73	2/2410 (0.1%)
All	All	0.44	2/5337 (0.0%)	0.73	8/7230 (0.1%)

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	2
1	C	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1156	GLU	C-N	-8.94	1.13	1.34
1	A	1112	ALA	C-N	6.51	1.49	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3213	HIS	N-CA-CB	-14.83	83.91	110.60
1	A	1156	GLU	O-C-N	-12.63	102.48	122.70
1	A	1157	ASP	N-CA-CB	-11.18	90.47	110.60
1	A	1111	VAL	N-CA-CB	10.35	134.27	111.50
1	A	1156	GLU	C-N-CA	9.76	146.09	121.70
1	C	3212	GLU	O-C-N	-7.71	110.37	122.70
1	A	1111	VAL	CB-CA-C	-7.69	96.79	111.40
1	A	1156	GLU	CA-C-N	7.42	133.53	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1156	GLU	Mainchain,Peptide
1	C	3212	GLU	Mainchain,Peptide

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	1750	0	1751	56	0
1	B	1750	0	1752	44	0
1	C	1750	0	1752	46	0
All	All	5250	0	5255	143	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 (143) 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:3203:LYS:HD3	1:C:3203:LYS:H	1.16	1.07
1:C:3080:ASN:HD22	1:C:3094:ALA:H	1.02	0.96
1:A:1080:ASN:HD22	1:A:1093:PRO:HA	1.32	0.95
1:C:3213:HIS:CD2	1:C:3214:ALA:H	1.93	0.86
1:C:3203:LYS:HD3	1:C:3203:LYS:N	1.89	0.84
1:A:1080:ASN:ND2	1:A:1093:PRO:HA	1.91	0.84
1:A:1136:ASP:OD1	1:A:1137:THR:HG22	1.81	0.80
1:A:1030:MET:HE3	1:A:1106:PRO:HG3	1.64	0.78
1:C:3203:LYS:H	1:C:3203:LYS:CD	1.97	0.74
1:C:3177:THR:HG22	1:C:3227:ASP:OD2	1.88	0.72
1:C:3213:HIS:CG	1:C:3214:ALA:H	2.08	0.72
1:A:1030:MET:CE	1:A:1106:PRO:HG3	2.20	0.71
1:A:1201:LYS:NZ	1:A:1201:LYS:HB3	2.05	0.71
1:C:3213:HIS:ND1	1:C:3213:HIS:N	2.36	0.70
1:B:2109:PHE:CD1	1:B:2110:PRO:HD2	2.27	0.69
1:B:2080:ASN:HD22	1:B:2094:ALA:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:LEU:HD11	1:C:3090:ILE:HG23	1.75	0.69
1:A:1197:LEU:HD12	1:A:1208:LYS:HD3	1.75	0.68
1:B:2201:LYS:NZ	1:B:2201:LYS:HB3	2.08	0.68
1:A:1001:MET:HG3	1:A:1073:ILE:HG23	1.75	0.67
1:A:1105:LYS:HD2	1:A:1105:LYS:O	1.95	0.65
1:A:1153:ASN:OD1	1:A:1155:VAL:HG22	1.96	0.65
1:A:1226:HIS:HD2	1:A:1228:PHE:HB2	1.60	0.65
1:C:3147:ILE:HD11	1:C:3172:TYR:CD1	2.32	0.64
1:B:2080:ASN:HD22	1:B:2093:PRO:HA	1.62	0.64
1:C:3213:HIS:CD2	1:C:3214:ALA:N	2.63	0.64
1:B:2157:ASP:OD1	1:B:2161:THR:HG22	2.01	0.61
1:A:1203:LYS:H	1:A:1203:LYS:HD3	1.65	0.61
1:B:2077:GLU:H	1:B:2077:GLU:CD	2.05	0.60
1:B:2203:LYS:H	1:B:2203:LYS:HD3	1.65	0.60
1:C:3080:ASN:ND2	1:C:3094:ALA:H	1.87	0.59
1:B:2197:LEU:HD11	1:B:2210:GLU:OE2	2.03	0.59
1:B:2035:ASN:OD1	1:B:2037:THR:HG23	2.02	0.59
1:B:2001:MET:CE	1:B:2003:LEU:HD21	2.33	0.59
1:A:1203:LYS:H	1:A:1203:LYS:CD	2.16	0.58
1:B:2111:VAL:O	1:B:2199:TRP:CD1	2.57	0.58
1:A:1201:LYS:HB3	1:A:1201:LYS:HZ3	1.69	0.58
1:A:1137:THR:HG21	1:A:1154:LYS:HB2	1.86	0.56
1:C:3032:ARG:HG2	1:C:3103:PRO:HD3	1.87	0.56
1:B:2195:LYS:HE2	1:B:2197:LEU:HD21	1.88	0.56
1:C:3013:ASN:ND2	1:C:3216:TYR:OH	2.39	0.55
1:B:2109:PHE:CG	1:B:2110:PRO:HD2	2.41	0.55
1:A:1067:VAL:HG12	1:A:1068:ASN:N	2.20	0.55
1:C:3153:ASN:OD1	1:C:3155:VAL:HG22	2.07	0.54
1:B:2136:ASP:OD1	1:B:2137:THR:HG23	2.08	0.54
1:C:3172:TYR:CZ	1:C:3174:GLY:HA3	2.41	0.54
1:B:2111:VAL:O	1:B:2199:TRP:HD1	1.91	0.54
1:A:1226:HIS:CD2	1:A:1228:PHE:HB2	2.42	0.53
1:B:2028:PHE:CZ	1:B:2041:GLU:HB2	2.43	0.53
1:A:1067:VAL:HG12	1:A:1071:ALA:HB2	1.91	0.53
1:A:1137:THR:CG2	1:A:1154:LYS:HB2	2.39	0.52
1:B:2202:GLY:O	1:B:2226:HIS:HE1	1.92	0.52
1:A:1165:TYR:HD1	1:C:3090:ILE:HG12	1.74	0.52
1:B:2201:LYS:HB3	1:B:2201:LYS:HZ2	1.72	0.52
1:A:1077:GLU:H	1:A:1077:GLU:CD	2.12	0.52
1:B:2153:ASN:OD1	1:B:2155:VAL:HG22	2.09	0.52
1:C:3076:SER:HB3	1:C:3080:ASN:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2110:PRO:HG2	1:B:2199:TRP:CG	2.44	0.51
1:C:3226:HIS:CD2	1:C:3228:PHE:HB2	2.45	0.51
1:C:3130:SER:HA	1:C:3135:ILE:HB	1.92	0.51
1:A:1109:PHE:CD1	1:A:1110:PRO:HD2	2.46	0.51
1:B:2042:ALA:HB2	1:B:2214:ALA:HB2	1.92	0.51
1:C:3201:LYS:O	1:C:3204:GLN:HB2	2.11	0.51
1:C:3226:HIS:HD2	1:C:3228:PHE:HB2	1.75	0.50
1:C:3157:ASP:OD1	1:C:3161:THR:HG22	2.10	0.50
1:A:1030:MET:HE2	1:A:1039:TYR:OH	2.11	0.50
1:C:3033:ALA:HB2	1:C:3038:THR:HG22	1.95	0.49
1:A:1030:MET:CE	1:A:1039:TYR:OH	2.60	0.49
1:A:1068:ASN:ND2	1:A:1085:ASP:OD2	2.45	0.49
1:C:3077:GLU:H	1:C:3077:GLU:CD	2.15	0.49
1:B:2116:THR:HG23	1:B:2196:LEU:HB3	1.93	0.49
1:B:2042:ALA:HB2	1:B:2214:ALA:CB	2.42	0.49
1:C:3213:HIS:CG	1:C:3214:ALA:N	2.68	0.49
1:B:2124:GLN:O	1:B:2128:ARG:HG2	2.12	0.48
1:B:2080:ASN:ND2	1:B:2093:PRO:HA	2.29	0.48
1:B:2189:MET:HA	1:B:2216:TYR:CZ	2.49	0.48
1:A:1001:MET:CG	1:A:1073:ILE:HG23	2.42	0.47
1:A:1041:GLU:HG3	1:A:1215:ASN:HB2	1.95	0.47
1:C:3096:ASP:OD1	1:C:3098:SER:HB2	2.14	0.47
1:B:2087:ARG:HG3	1:B:2087:ARG:HH11	1.80	0.47
1:A:1060:PHE:HZ	1:A:1073:ILE:HD12	1.79	0.47
1:B:2177:THR:HB	1:B:2227:ASP:OD2	2.14	0.47
1:A:1172:TYR:CZ	1:A:1174:GLY:HA3	2.50	0.47
1:A:1177:THR:HB	1:A:1227:ASP:OD2	2.15	0.47
1:C:3153:ASN:HB3	1:C:3156:GLU:HG2	1.96	0.46
1:A:1032:ARG:HG2	1:A:1103:PRO:HD3	1.98	0.46
1:A:1161:THR:HG23	1:A:1162:ARG:HG3	1.97	0.46
1:A:1028:PHE:CE2	1:A:1030:MET:HE3	2.50	0.46
1:A:1063:ILE:HG13	1:A:1092:TRP:CZ3	2.51	0.46
1:A:1149:ILE:HD11	1:A:1169:LEU:HD11	1.98	0.46
1:B:2140:ILE:HG21	1:B:2198:LEU:HD11	1.97	0.46
1:C:3064:LEU:HD23	1:C:3083:ILE:HD13	1.98	0.46
1:A:1130:SER:HA	1:A:1135:ILE:HB	1.98	0.46
1:B:2113:SER:HB3	1:B:2228:PHE:CG	2.51	0.45
1:A:1181:ILE:HD12	1:A:1223:ASP:HB2	1.99	0.45
1:C:3015:ALA:HA	1:C:3018:ASN:O	2.16	0.45
1:A:1063:ILE:HG13	1:A:1092:TRP:HZ3	1.82	0.45
1:B:2035:ASN:OD1	1:B:2035:ASN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2080:ASN:ND2	1:B:2094:ALA:H	2.11	0.45
1:A:1028:PHE:HE2	1:A:1030:MET:HE3	1.81	0.45
1:C:3001:MET:N	1:C:3072:GLU:OE2	2.50	0.45
1:A:1067:VAL:HG12	1:A:1068:ASN:H	1.81	0.44
1:A:1067:VAL:HG13	1:A:1085:ASP:CG	2.38	0.44
1:A:1196:LEU:HD13	1:A:1209:PHE:CE2	2.52	0.44
1:B:2162:ARG:HH11	1:B:2162:ARG:HG3	1.82	0.44
1:C:3146:LYS:HA	1:C:3171:ASP:HA	1.99	0.44
1:A:1067:VAL:CG1	1:A:1071:ALA:HB2	2.48	0.44
1:B:2003:LEU:HD22	1:B:2007:THR:HG21	1.98	0.44
1:A:1080:ASN:ND2	1:A:1094:ALA:H	2.15	0.44
1:A:1116:THR:HG23	1:A:1196:LEU:HB3	2.00	0.44
1:C:3227:ASP:OD1	1:C:3227:ASP:C	2.56	0.44
1:C:3116:THR:HG23	1:C:3196:LEU:HB3	1.99	0.43
1:A:1183:ASN:HB3	1:A:1186:ASN:ND2	2.33	0.43
1:B:2001:MET:HE2	1:B:2003:LEU:HD21	2.01	0.43
1:C:3092:TRP:CG	1:C:3093:PRO:HD2	2.54	0.43
1:C:3126:LEU:HD13	1:C:3165:TYR:HE2	1.83	0.43
1:C:3087:ARG:HH11	1:C:3087:ARG:HG3	1.84	0.43
1:C:3226:HIS:HD2	1:C:3228:PHE:H	1.65	0.43
1:B:2001:MET:HE3	1:B:2003:LEU:HD21	2.00	0.42
1:A:1030:MET:HE2	1:A:1030:MET:HB2	1.86	0.42
1:C:3199:TRP:O	1:C:3205:GLY:HA2	2.18	0.42
1:C:3202:GLY:O	1:C:3226:HIS:HE1	2.03	0.42
1:B:2025:SER:HA	1:B:2048:ILE:O	2.20	0.42
1:C:3085:ASP:OD1	1:C:3086:ALA:N	2.52	0.42
1:A:1012:LYS:O	1:A:1015:ALA:HB3	2.18	0.42
1:B:2195:LYS:HB3	1:B:2210:GLU:HB3	2.00	0.42
1:B:2116:THR:OG1	1:B:2117:GLU:N	2.52	0.42
1:B:2146:LYS:HG2	1:B:2171:ASP:HA	2.02	0.42
1:C:3189:MET:HA	1:C:3216:TYR:CZ	2.53	0.42
1:A:1180:PHE:CD1	1:A:1198:LEU:HD13	2.55	0.42
1:C:3146:LYS:HD3	1:C:3168:THR:HG21	2.01	0.42
1:A:1189:MET:HA	1:A:1216:TYR:CZ	2.55	0.42
1:A:1189:MET:HA	1:A:1216:TYR:CE2	2.55	0.42
1:C:3025:SER:HA	1:C:3048:ILE:O	2.20	0.41
1:A:1212:GLU:HG3	1:A:1213:HIS:ND1	2.35	0.41
1:B:2105:LYS:HA	1:B:2106:PRO:HD3	1.84	0.41
1:C:3126:LEU:HD13	1:C:3165:TYR:CE2	2.56	0.41
1:A:1090:ILE:HG23	1:B:2133:LEU:HD11	2.02	0.41
1:C:3185:ALA:O	1:C:3188:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:TRP:CG	1:A:1093:PRO:HD2	2.56	0.41
1:A:1001:MET:CE	1:A:1003:LEU:HD21	2.51	0.40
1:B:2226:HIS:HD2	1:B:2228:PHE:HB2	1.86	0.40
1:B:2142:VAL:HA	1:B:2146:LYS:O	2.21	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	226/228 (99%)	214 (95%)	10 (4%)	2 (1%)	17 19
1	B	226/228 (99%)	217 (96%)	8 (4%)	1 (0%)	34 41
1	C	226/228 (99%)	215 (95%)	11 (5%)	0	100 100
All	All	678/684 (99%)	646 (95%)	29 (4%)	3 (0%)	34 41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1175	GLU
1	A	1174	GLY
1	B	2086	ALA

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%)	182 (96%)	7 (4%)	34 45
1	B	189/189 (100%)	185 (98%)	4 (2%)	53 66
1	C	189/189 (100%)	184 (97%)	5 (3%)	46 58
All	All	567/567 (100%)	551 (97%)	16 (3%)	43 56

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1030	MET
1	A	1105	LYS
1	A	1126	LEU
1	A	1137	THR
1	A	1171	ASP
1	A	1189	MET
1	A	1203	LYS
1	B	2058	ASN
1	B	2127	LEU
1	B	2189	MET
1	B	2203	LYS
1	C	3058	ASN
1	C	3127	LEU
1	C	3163	VAL
1	C	3189	MET
1	C	3203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1075	GLN
1	A	1080	ASN
1	A	1104	ASN
1	A	1190	GLN
1	A	1215	ASN
1	A	1226	HIS
1	B	2043	ASN
1	B	2058	ASN
1	B	2080	ASN
1	B	2134	GLN
1	B	2190	GLN
1	B	2215	ASN
1	B	2226	HIS

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Mol	Chain	Res	Type
1	C	3013	ASN
1	C	3080	ASN
1	C	3176	ASN
1	C	3204	GLN
1	C	3215	ASN
1	C	3226	HIS

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1156:GLU	C	1157:ASP	N	1.13

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	228/228 (100%)	0.40	2 (0%) 84 85	27, 43, 64, 79	0
1	B	228/228 (100%)	0.50	12 (5%) 26 23	28, 46, 70, 85	0
1	C	228/228 (100%)	0.45	7 (3%) 49 45	26, 41, 64, 82	0
All	All	684/684 (100%)	0.45	21 (3%) 49 45	26, 43, 67, 85	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2173	ASP	3.7
1	C	3156	GLU	3.4
1	B	2106	PRO	3.4
1	B	2175	GLU	3.2
1	B	2111	VAL	3.0
1	C	3227	ASP	2.9
1	A	1005	LYS	2.9
1	B	2112	ALA	2.8
1	C	3228	PHE	2.7
1	C	3213	HIS	2.6
1	B	2171	ASP	2.5
1	B	2213	HIS	2.4
1	B	2228	PHE	2.3
1	C	3098	SER	2.3
1	B	2170	GLY	2.3
1	B	2174	GLY	2.3
1	B	2107	ILE	2.2
1	B	2070	ASP	2.2
1	A	1087	ARG	2.2
1	C	3096	ASP	2.1
1	C	3069	ASP	2.1

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.