Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2021 – 12:11 PM EST

PDB ID	:	1WVI
Title	:	Crystal structure of putative phosphatase from Streptococcus mutans UA159
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-12-15
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

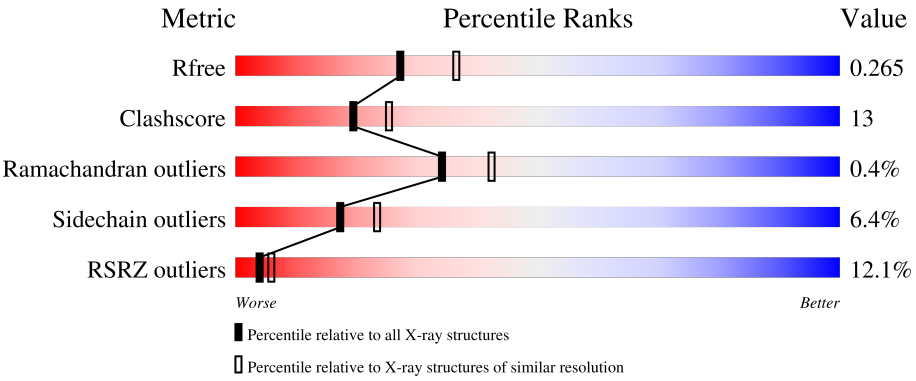
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	257	12% 74% 22%
1	B	257	6% 72% 24%
1	C	257	24% 71% 25%
1	D	257	5% 73% 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7840 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 putative phosphatases involved in N-acetyl-glucosamine catabolism.

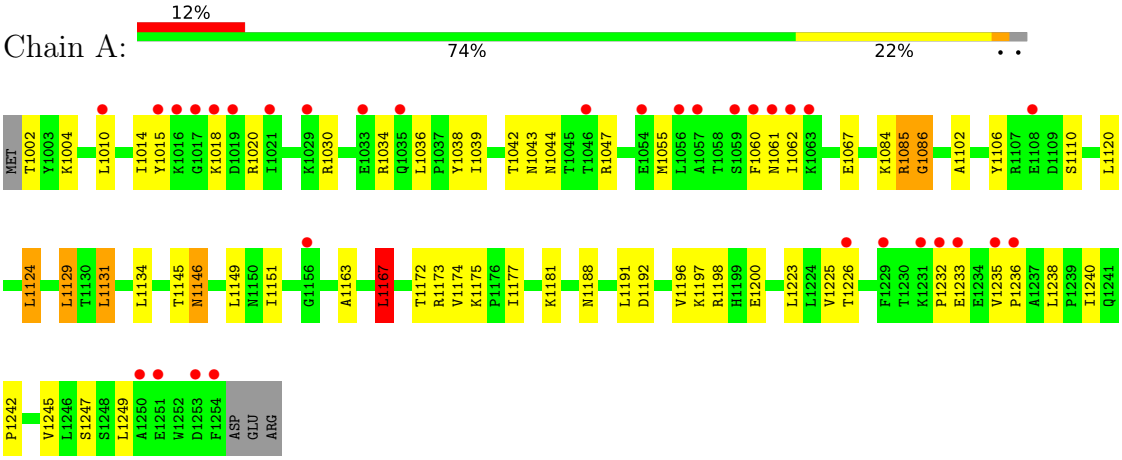
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1960	1259	320	375	6			
1	B	253	Total	C	N	O	S	0	0	0
			1960	1259	320	375	6			
1	C	253	Total	C	N	O	S	0	0	0
			1960	1259	320	375	6			
1	D	253	Total	C	N	O	S	0	0	0
			1960	1259	320	375	6			

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.

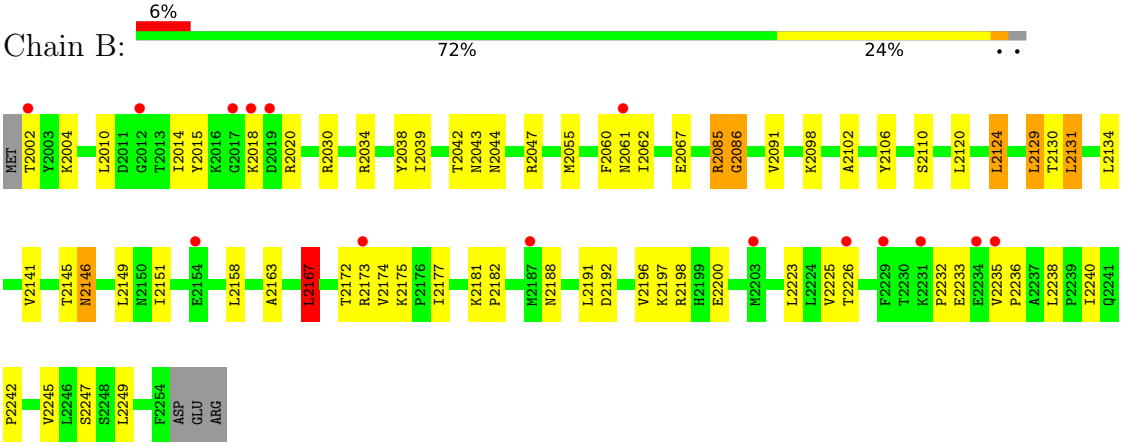
• Molecule 1: putative phosphatases involved in N-acetyl-glucosamine catabolism

Chain A:



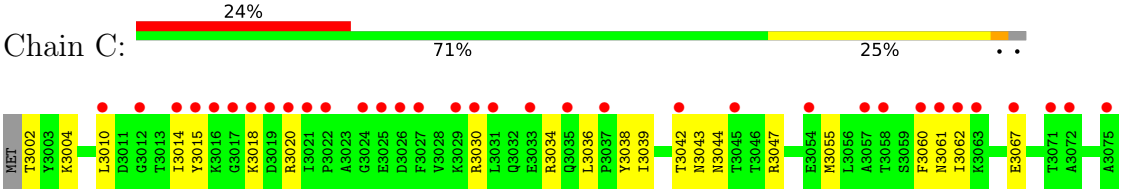
• Molecule 1: putative phosphatases involved in N-acetyl-glucosamine catabolism

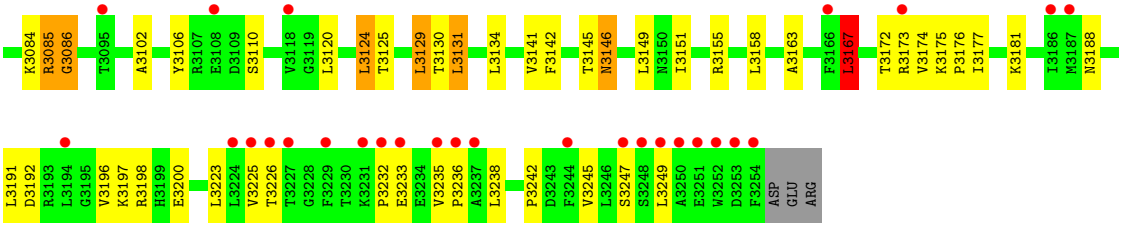
Chain B:



• Molecule 1: putative phosphatases involved in N-acetyl-glucosamine catabolism

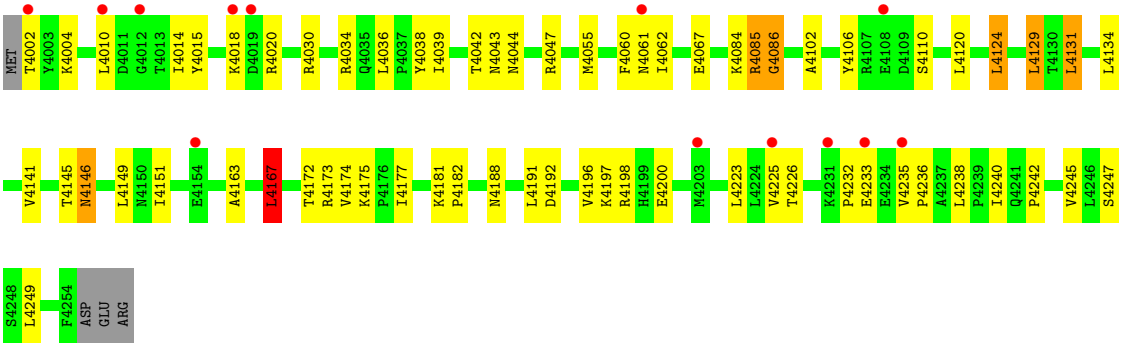
Chain C:





• Molecule 1: putative phosphatases involved in N-acetyl-glucosamine catabolism

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.64Å 107.42Å 81.94Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 29.72 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-2.30) 98.4 (29.72-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.41 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.264 0.248 , 0.265	Depositor DCC
R_{free} test set	2395 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.5	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	0.91	EDS
Total number of atoms	7840	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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	0.39	0/1994	0.65	1/2711 (0.0%)
1	B	0.38	0/1994	0.65	1/2711 (0.0%)
1	C	0.39	0/1994	0.65	1/2711 (0.0%)
1	D	0.39	0/1994	0.65	1/2711 (0.0%)
All	All	0.39	0/7976	0.65	4/10844 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4167	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	1167	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	2167	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	3167	LEU	CA-CB-CG	5.15	127.14	115.30

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	1960	0	2021	53	0
1	B	1960	0	2021	55	0
1	C	1960	0	2021	54	0
1	D	1960	0	2021	53	0
All	All	7840	0	8084	203	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 13.

All (203) 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:A:1043:ASN:HD21	1:A:1181:LYS:H	1.25	0.82
1:B:2043:ASN:HD21	1:B:2181:LYS:H	1.27	0.82
1:C:3196:VAL:HG13	1:C:3200:GLU:HB2	1.63	0.81
1:D:4043:ASN:HD21	1:D:4181:LYS:H	1.28	0.81
1:D:4044:ASN:HD21	1:D:4047:ARG:H	1.29	0.80
1:A:1196:VAL:HG13	1:A:1200:GLU:HB2	1.62	0.80
1:B:2044:ASN:HD21	1:B:2047:ARG:H	1.28	0.80
1:C:3043:ASN:HD21	1:C:3181:LYS:H	1.29	0.80
1:B:2196:VAL:HG13	1:B:2200:GLU:HB2	1.62	0.79
1:D:4196:VAL:HG13	1:D:4200:GLU:HB2	1.63	0.79
1:A:1044:ASN:HD21	1:A:1047:ARG:H	1.28	0.78
1:C:3044:ASN:HD21	1:C:3047:ARG:H	1.29	0.78
1:C:3196:VAL:CG1	1:C:3200:GLU:HB2	2.15	0.76
1:A:1196:VAL:CG1	1:A:1200:GLU:HB2	2.16	0.75
1:B:2163:ALA:HB1	1:C:3167:LEU:HD13	1.69	0.74
1:B:2196:VAL:CG1	1:B:2200:GLU:HB2	2.18	0.73
1:D:4196:VAL:CG1	1:D:4200:GLU:HB2	2.20	0.71
1:B:2130:THR:HG23	1:C:3158:LEU:HG	1.73	0.70
1:B:2167:LEU:HD13	1:C:3163:ALA:HB1	1.73	0.70
1:C:3188:ASN:ND2	1:C:3198:ARG:HH22	1.92	0.68
1:D:4002:THR:HB	1:D:4004:LYS:NZ	2.09	0.68
1:D:4188:ASN:ND2	1:D:4198:ARG:HH22	1.94	0.65
1:B:2188:ASN:ND2	1:B:2198:ARG:HH22	1.93	0.65
1:A:1002:THR:HB	1:A:1004:LYS:NZ	2.12	0.65
1:A:1188:ASN:ND2	1:A:1198:ARG:HH22	1.95	0.64
1:C:3002:THR:HB	1:C:3004:LYS:NZ	2.12	0.64
1:B:2002:THR:HB	1:B:2004:LYS:NZ	2.13	0.64
1:D:4235:VAL:HG22	1:D:4236:PRO:HD3	1.80	0.64
1:B:2235:VAL:CG2	1:B:2236:PRO:HD3	2.28	0.63
1:D:4235:VAL:CG2	1:D:4236:PRO:HD3	2.28	0.63
1:A:1235:VAL:HG22	1:A:1236:PRO:HD3	1.80	0.63
1:C:3235:VAL:HG22	1:C:3236:PRO:HD3	1.81	0.63
1:D:4225:VAL:HG11	1:D:4249:LEU:HD22	1.81	0.62
1:B:2225:VAL:HG11	1:B:2249:LEU:HD22	1.81	0.62
1:A:1225:VAL:HG11	1:A:1249:LEU:HD22	1.81	0.61
1:B:2141:VAL:HG13	1:D:4240:ILE:HD12	1.81	0.61
1:B:2235:VAL:HG22	1:B:2236:PRO:HD3	1.79	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3225:VAL:HG11	1:C:3249:LEU:HD22	1.82	0.61
1:B:2158:LEU:HG	1:C:3130:THR:HG23	1.82	0.60
1:A:1235:VAL:CG2	1:A:1236:PRO:HD3	2.31	0.60
1:C:3235:VAL:CG2	1:C:3236:PRO:HD3	2.31	0.60
1:A:1020:ARG:HH12	1:A:1061:ASN:HD22	1.52	0.57
1:C:3030:ARG:O	1:C:3034:ARG:HG2	2.05	0.57
1:A:1030:ARG:O	1:A:1034:ARG:HG2	2.04	0.56
1:B:2240:ILE:HD12	1:D:4141:VAL:HG13	1.87	0.56
1:D:4030:ARG:O	1:D:4034:ARG:HG2	2.05	0.56
1:C:3020:ARG:HH12	1:C:3061:ASN:HD22	1.54	0.56
1:B:2044:ASN:ND2	1:B:2047:ARG:H	2.03	0.55
1:D:4020:ARG:HH12	1:D:4061:ASN:HD22	1.54	0.55
1:B:2030:ARG:O	1:B:2034:ARG:HG2	2.07	0.55
1:C:3226:THR:OG1	1:C:3247:SER:HA	2.07	0.55
1:A:1002:THR:HB	1:A:1004:LYS:HZ1	1.71	0.55
1:B:2020:ARG:HH12	1:B:2061:ASN:HD22	1.55	0.54
1:A:1043:ASN:HD21	1:A:1181:LYS:N	2.02	0.54
1:A:1044:ASN:ND2	1:A:1047:ARG:H	2.03	0.54
1:A:1226:THR:OG1	1:A:1247:SER:HA	2.08	0.54
1:C:3002:THR:HB	1:C:3004:LYS:HZ1	1.72	0.53
1:D:4226:THR:OG1	1:D:4247:SER:HA	2.09	0.53
1:B:2226:THR:OG1	1:B:2247:SER:HA	2.09	0.53
1:B:2002:THR:HB	1:B:2004:LYS:HZ1	1.73	0.52
1:B:2043:ASN:HD21	1:B:2181:LYS:N	2.03	0.52
1:B:2131:LEU:HD13	1:C:3155:ARG:NH2	2.25	0.51
1:D:4002:THR:HB	1:D:4004:LYS:HZ2	1.76	0.51
1:A:1240:ILE:HD12	1:C:3141:VAL:HG13	1.92	0.50
1:D:4044:ASN:ND2	1:D:4047:ARG:H	2.04	0.50
1:A:1067:GLU:CD	1:A:1067:GLU:H	2.15	0.50
1:D:4232:PRO:O	1:D:4235:VAL:HG22	2.12	0.50
1:C:3014:ILE:HG13	1:C:3015:TYR:HD1	1.77	0.49
1:C:3044:ASN:ND2	1:C:3047:ARG:H	2.05	0.49
1:D:4149:LEU:HD22	1:D:4149:LEU:N	2.26	0.49
1:A:1235:VAL:HA	1:A:1238:LEU:HG	1.95	0.49
1:D:4067:GLU:CD	1:D:4067:GLU:H	2.16	0.49
1:B:2067:GLU:H	1:B:2067:GLU:CD	2.16	0.49
1:C:3018:LYS:N	1:C:3018:LYS:HD2	2.27	0.49
1:B:2149:LEU:HD22	1:B:2149:LEU:N	2.27	0.49
1:C:3067:GLU:H	1:C:3067:GLU:CD	2.16	0.49
1:A:1149:LEU:HD22	1:A:1149:LEU:N	2.29	0.48
1:B:2151:ILE:HG23	1:B:2151:ILE:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4124:LEU:HD21	1:D:4129:LEU:HD13	1.95	0.48
1:A:1014:ILE:HG13	1:A:1015:TYR:HD1	1.79	0.48
1:C:3047:ARG:NH1	1:C:3055:MET:SD	2.86	0.48
1:C:3151:ILE:HG23	1:C:3151:ILE:O	2.12	0.48
1:C:3232:PRO:O	1:C:3235:VAL:HG22	2.13	0.48
1:D:4014:ILE:HG13	1:D:4015:TYR:HD1	1.79	0.48
1:C:3235:VAL:HA	1:C:3238:LEU:HG	1.94	0.48
1:D:4018:LYS:HD2	1:D:4018:LYS:N	2.29	0.48
1:C:3010:LEU:HD12	1:C:3042:THR:HB	1.95	0.48
1:B:2014:ILE:HG13	1:B:2015:TYR:HD1	1.79	0.48
1:B:2232:PRO:O	1:B:2235:VAL:HG22	2.14	0.48
1:A:1020:ARG:HB3	1:A:1060:PHE:HD1	1.79	0.47
1:B:2235:VAL:HA	1:B:2238:LEU:HG	1.96	0.47
1:A:1232:PRO:O	1:A:1235:VAL:HG22	2.14	0.47
1:D:4043:ASN:HD21	1:D:4181:LYS:N	2.05	0.47
1:A:1242:PRO:HG2	1:A:1245:VAL:HG22	1.97	0.47
1:C:3196:VAL:CG1	1:C:3197:LYS:N	2.78	0.47
1:D:4151:ILE:HG23	1:D:4151:ILE:O	2.15	0.47
1:A:1124:LEU:HD21	1:A:1129:LEU:HD13	1.96	0.47
1:B:2242:PRO:HG2	1:B:2245:VAL:HG22	1.96	0.47
1:A:1151:ILE:HG23	1:A:1151:ILE:O	2.15	0.47
1:D:4020:ARG:HB3	1:D:4060:PHE:HD1	1.80	0.47
1:D:4110:SER:HB2	1:D:4131:LEU:HG	1.97	0.47
1:C:3242:PRO:HG2	1:C:3245:VAL:HG22	1.96	0.47
1:D:4235:VAL:HA	1:D:4238:LEU:HG	1.96	0.47
1:B:2020:ARG:HB3	1:B:2060:PHE:HD1	1.79	0.47
1:A:1018:LYS:N	1:A:1018:LYS:HD2	2.29	0.47
1:C:3020:ARG:HB3	1:C:3060:PHE:HD1	1.80	0.47
1:A:1010:LEU:HD12	1:A:1042:THR:HB	1.96	0.46
1:B:2018:LYS:N	1:B:2018:LYS:HD2	2.29	0.46
1:C:3145:THR:OG1	1:C:3146:ASN:ND2	2.48	0.46
1:D:4002:THR:HB	1:D:4004:LYS:HZ1	1.78	0.46
1:A:1047:ARG:NH1	1:A:1055:MET:SD	2.88	0.46
1:A:1110:SER:HB2	1:A:1131:LEU:HG	1.97	0.46
1:B:2149:LEU:HD22	1:B:2149:LEU:H	1.81	0.46
1:B:2233:GLU:O	1:B:2236:PRO:HD2	2.16	0.46
1:C:3110:SER:HB2	1:C:3131:LEU:HG	1.97	0.46
1:A:1233:GLU:O	1:A:1236:PRO:HD2	2.16	0.46
1:C:3043:ASN:HD21	1:C:3181:LYS:N	2.05	0.46
1:D:4233:GLU:O	1:D:4236:PRO:HD2	2.16	0.46
1:A:1167:LEU:C	1:A:1167:LEU:CD1	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2124:LEU:HD21	1:B:2129:LEU:HD13	1.98	0.45
1:D:4060:PHE:O	1:D:4062:ILE:HG13	2.16	0.45
1:C:3149:LEU:N	1:C:3149:LEU:HD22	2.30	0.45
1:D:4149:LEU:HD22	1:D:4149:LEU:H	1.81	0.45
1:C:3167:LEU:CD1	1:C:3167:LEU:C	2.85	0.45
1:C:3233:GLU:O	1:C:3236:PRO:HD2	2.16	0.45
1:B:2167:LEU:C	1:B:2167:LEU:CD1	2.85	0.45
1:B:2038:TYR:C	1:B:2039:ILE:HD12	2.36	0.45
1:D:4047:ARG:NH1	1:D:4055:MET:SD	2.89	0.44
1:D:4102:ALA:HA	1:D:4106:TYR:O	2.17	0.44
1:B:2010:LEU:HD12	1:B:2042:THR:HB	1.98	0.44
1:B:2047:ARG:NH1	1:B:2055:MET:SD	2.90	0.44
1:C:3124:LEU:HD21	1:C:3129:LEU:HD13	1.99	0.44
1:D:4038:TYR:C	1:D:4039:ILE:HD12	2.37	0.44
1:D:4085:ARG:O	1:D:4086:GLY:O	2.35	0.44
1:A:1085:ARG:O	1:A:1086:GLY:C	2.56	0.44
1:C:3142:PHE:CE1	1:C:3176:PRO:HB3	2.53	0.44
1:C:3196:VAL:HG12	1:C:3197:LYS:O	2.18	0.43
1:D:4196:VAL:CG1	1:D:4197:LYS:N	2.81	0.43
1:A:1149:LEU:H	1:A:1149:LEU:HD22	1.83	0.43
1:B:2145:THR:OG1	1:B:2146:ASN:ND2	2.51	0.43
1:A:1167:LEU:HB2	1:D:4167:LEU:HB2	2.00	0.43
1:B:2196:VAL:HG12	1:B:2197:LYS:O	2.18	0.43
1:B:2110:SER:HB2	1:B:2131:LEU:HG	2.00	0.43
1:D:4196:VAL:HG12	1:D:4197:LYS:O	2.17	0.43
1:A:1196:VAL:CG1	1:A:1197:LYS:N	2.80	0.43
1:A:1167:LEU:HD13	1:D:4163:ALA:HB1	2.01	0.43
1:B:2196:VAL:CG1	1:B:2197:LYS:N	2.81	0.43
1:D:4085:ARG:O	1:D:4086:GLY:C	2.56	0.43
1:A:1085:ARG:O	1:A:1086:GLY:O	2.37	0.43
1:B:2060:PHE:O	1:B:2062:ILE:HG13	2.19	0.43
1:D:4010:LEU:HD12	1:D:4042:THR:HB	2.00	0.43
1:D:4010:LEU:HD23	1:D:4014:ILE:HD11	2.01	0.43
1:D:4020:ARG:NH1	1:D:4061:ASN:HD22	2.17	0.43
1:A:1020:ARG:NH1	1:A:1061:ASN:HD22	2.15	0.42
1:C:3038:TYR:C	1:C:3039:ILE:HD12	2.39	0.42
1:D:4242:PRO:HG2	1:D:4245:VAL:HG22	2.00	0.42
1:A:1102:ALA:HA	1:A:1106:TYR:O	2.20	0.42
1:A:1223:LEU:HD23	1:A:1223:LEU:C	2.39	0.42
1:C:3085:ARG:O	1:C:3086:GLY:C	2.57	0.42
1:D:4167:LEU:C	1:D:4167:LEU:CD1	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:LEU:C	1:A:1167:LEU:HD12	2.39	0.42
1:A:1172:THR:O	1:A:1173:ARG:HB2	2.20	0.42
1:B:2223:LEU:HD23	1:B:2223:LEU:C	2.40	0.42
1:D:4010:LEU:CD2	1:D:4014:ILE:HD11	2.50	0.42
1:A:1038:TYR:C	1:A:1039:ILE:HD12	2.40	0.42
1:B:2085:ARG:O	1:B:2086:GLY:O	2.38	0.42
1:A:1010:LEU:CD2	1:A:1014:ILE:HD11	2.50	0.42
1:C:3085:ARG:O	1:C:3086:GLY:O	2.37	0.42
1:A:1163:ALA:HB1	1:D:4167:LEU:HD13	2.02	0.42
1:B:2124:LEU:O	1:C:3125:THR:HA	2.20	0.42
1:C:3060:PHE:O	1:C:3062:ILE:HG13	2.20	0.42
1:C:3146:ASN:HD22	1:C:3146:ASN:N	2.17	0.42
1:B:2172:THR:O	1:B:2173:ARG:HB2	2.20	0.42
1:C:3167:LEU:C	1:C:3167:LEU:HD12	2.41	0.42
1:D:4145:THR:OG1	1:D:4146:ASN:ND2	2.51	0.42
1:B:2010:LEU:CD2	1:B:2014:ILE:HD11	2.50	0.42
1:D:4172:THR:O	1:D:4173:ARG:HB2	2.20	0.42
1:A:1145:THR:OG1	1:A:1146:ASN:ND2	2.53	0.41
1:C:3034:ARG:HB2	1:C:3036:LEU:HG	2.02	0.41
1:A:1060:PHE:O	1:A:1062:ILE:HG13	2.20	0.41
1:A:1225:VAL:HG11	1:A:1249:LEU:CD2	2.50	0.41
1:B:2146:ASN:N	1:B:2146:ASN:HD22	2.19	0.41
1:B:2167:LEU:HD12	1:B:2167:LEU:C	2.39	0.41
1:C:3223:LEU:C	1:C:3223:LEU:HD23	2.41	0.41
1:D:4034:ARG:HB2	1:D:4036:LEU:HG	2.02	0.41
1:A:1084:LYS:HG3	1:A:1084:LYS:O	2.20	0.41
1:A:1146:ASN:HD22	1:A:1146:ASN:N	2.19	0.41
1:B:2010:LEU:HD23	1:B:2014:ILE:HD11	2.03	0.41
1:B:2085:ARG:O	1:B:2086:GLY:C	2.56	0.41
1:D:4084:LYS:HG3	1:D:4084:LYS:O	2.20	0.41
1:D:4181:LYS:HE3	1:D:4181:LYS:HB2	1.89	0.41
1:C:3102:ALA:HA	1:C:3106:TYR:O	2.21	0.41
1:B:2102:ALA:HA	1:B:2106:TYR:O	2.21	0.41
1:D:4223:LEU:HD23	1:D:4223:LEU:C	2.41	0.41
1:C:3149:LEU:HD22	1:C:3149:LEU:H	1.86	0.41
1:C:3172:THR:O	1:C:3173:ARG:HB2	2.21	0.41
1:C:3084:LYS:O	1:C:3084:LYS:HG3	2.21	0.40
1:A:1010:LEU:HD23	1:A:1014:ILE:HD11	2.02	0.40
1:A:1085:ARG:HG2	1:A:1085:ARG:HH11	1.86	0.40
1:A:1034:ARG:HB2	1:A:1036:LEU:HG	2.03	0.40
1:B:2091:VAL:HB	1:B:2098:LYS:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2225:VAL:HG11	1:B:2249:LEU:CD2	2.51	0.40
1:C:3181:LYS:HB2	1:C:3181:LYS:HE3	1.91	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	251/257 (98%)	243 (97%)	7 (3%)	1 (0%)	34	42
1	B	251/257 (98%)	243 (97%)	7 (3%)	1 (0%)	34	42
1	C	251/257 (98%)	243 (97%)	7 (3%)	1 (0%)	34	42
1	D	251/257 (98%)	243 (97%)	7 (3%)	1 (0%)	34	42
All	All	1004/1028 (98%)	972 (97%)	28 (3%)	4 (0%)	34	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4086	GLY
1	A	1086	GLY
1	B	2086	GLY
1	C	3086	GLY

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	212/216 (98%)	199 (94%)	13 (6%)	18	25
1	B	212/216 (98%)	198 (93%)	14 (7%)	16	22
1	C	212/216 (98%)	199 (94%)	13 (6%)	18	25
1	D	212/216 (98%)	198 (93%)	14 (7%)	16	22
All	All	848/864 (98%)	794 (94%)	54 (6%)	17	23

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

Mol	Chain	Res	Type
1	A	1085	ARG
1	A	1120	LEU
1	A	1124	LEU
1	A	1129	LEU
1	A	1131	LEU
1	A	1134	LEU
1	A	1146	ASN
1	A	1167	LEU
1	A	1174	VAL
1	A	1175	LYS
1	A	1177	ILE
1	A	1191	LEU
1	A	1192	ASP
1	B	2085	ARG
1	B	2120	LEU
1	B	2124	LEU
1	B	2129	LEU
1	B	2131	LEU
1	B	2134	LEU
1	B	2146	ASN
1	B	2167	LEU
1	B	2174	VAL
1	B	2175	LYS
1	B	2177	ILE
1	B	2182	PRO
1	B	2191	LEU
1	B	2192	ASP
1	C	3085	ARG
1	C	3120	LEU
1	C	3124	LEU
1	C	3129	LEU
1	C	3131	LEU
1	C	3134	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3146	ASN
1	C	3167	LEU
1	C	3174	VAL
1	C	3175	LYS
1	C	3177	ILE
1	C	3191	LEU
1	C	3192	ASP
1	D	4085	ARG
1	D	4120	LEU
1	D	4124	LEU
1	D	4129	LEU
1	D	4131	LEU
1	D	4134	LEU
1	D	4146	ASN
1	D	4167	LEU
1	D	4174	VAL
1	D	4175	LYS
1	D	4177	ILE
1	D	4182	PRO
1	D	4191	LEU
1	D	4192	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1032	GLN
1	A	1043	ASN
1	A	1044	ASN
1	A	1061	ASN
1	A	1137	GLN
1	A	1146	ASN
1	A	1188	ASN
1	B	2032	GLN
1	B	2043	ASN
1	B	2044	ASN
1	B	2061	ASN
1	B	2137	GLN
1	B	2146	ASN
1	B	2188	ASN
1	C	3032	GLN
1	C	3043	ASN
1	C	3044	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3061	ASN
1	C	3137	GLN
1	C	3146	ASN
1	C	3150	ASN
1	C	3188	ASN
1	D	4032	GLN
1	D	4043	ASN
1	D	4044	ASN
1	D	4061	ASN
1	D	4137	GLN
1	D	4146	ASN
1	D	4150	ASN
1	D	4188	ASN

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	253/257 (98%)	0.79	32 (12%) 3 5	16, 37, 59, 70	0
1	B	253/257 (98%)	0.42	15 (5%) 22 28	12, 26, 55, 63	0
1	C	253/257 (98%)	1.32	62 (24%) 0 0	16, 41, 62, 70	0
1	D	253/257 (98%)	0.35	13 (5%) 28 35	12, 26, 54, 62	0
All	All	1012/1028 (98%)	0.72	122 (12%) 4 6	12, 34, 58, 70	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3250	ALA	7.0
1	C	3029	LYS	6.7
1	C	3022	PRO	6.4
1	C	3254	PHE	6.4
1	C	3016	LYS	5.6
1	C	3063	LYS	5.3
1	C	3061	ASN	5.2
1	C	3235	VAL	5.0
1	C	3057	ALA	4.9
1	C	3017	GLY	4.9
1	A	1017	GLY	4.8
1	C	3019	ASP	4.6
1	C	3253	ASP	4.6
1	C	3014	ILE	4.5
1	C	3018	LYS	4.4
1	A	1019	ASP	4.2
1	C	3021	ILE	4.1
1	A	1033	GLU	4.0
1	D	4154	GLU	4.0
1	A	1236	PRO	4.0
1	C	3035	GLN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2235	VAL	3.7
1	C	3058	THR	3.7
1	C	3247	SER	3.6
1	A	1062	ILE	3.5
1	C	3027	PHE	3.5
1	C	3249	LEU	3.5
1	C	3248	SER	3.5
1	A	1253	ASP	3.5
1	A	1059	SER	3.5
1	A	1233	GLU	3.4
1	C	3033	GLU	3.4
1	C	3010	LEU	3.4
1	A	1054	GLU	3.3
1	C	3236	PRO	3.2
1	A	1029	LYS	3.2
1	A	1229	PHE	3.2
1	C	3020	ARG	3.2
1	A	1063	LYS	3.2
1	A	1015	TYR	3.2
1	C	3067	GLU	3.1
1	C	3251	GLU	3.1
1	D	4002	THR	3.1
1	B	2187	MET	3.1
1	A	1010	LEU	3.1
1	B	2154	GLU	3.0
1	D	4018	LYS	3.0
1	B	2061	ASN	3.0
1	C	3024	GLY	3.0
1	A	1061	ASN	3.0
1	C	3012	GLY	2.9
1	A	1231	LYS	2.9
1	C	3229	PHE	2.9
1	D	4061	ASN	2.9
1	C	3231	LYS	2.9
1	C	3225	VAL	2.9
1	C	3031	LEU	2.9
1	C	3252	TRP	2.9
1	C	3233	GLU	2.8
1	C	3026	ASP	2.8
1	B	2203	MET	2.8
1	A	1254	PHE	2.8
1	A	1251	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	3015	TYR	2.8
1	A	1018	LYS	2.7
1	C	3042	THR	2.7
1	B	2229	PHE	2.7
1	B	2231	LYS	2.7
1	C	3062	ILE	2.7
1	D	4019	ASP	2.7
1	C	3226	THR	2.7
1	C	3227	THR	2.7
1	C	3232	PRO	2.6
1	B	2002	THR	2.6
1	C	3030	ARG	2.6
1	A	1060	PHE	2.6
1	D	4108	GLU	2.6
1	B	2234	GLU	2.6
1	C	3108	GLU	2.6
1	A	1056	LEU	2.6
1	C	3224	LEU	2.6
1	C	3037	PRO	2.5
1	C	3060	PHE	2.5
1	A	1035	GLN	2.5
1	C	3237	ALA	2.5
1	B	2018	LYS	2.5
1	C	3071	THR	2.5
1	A	1021	ILE	2.5
1	D	4225	VAL	2.5
1	A	1250	ALA	2.5
1	B	2017	GLY	2.5
1	A	1057	ALA	2.4
1	B	2019	ASP	2.4
1	C	3054	GLU	2.4
1	A	1016	LYS	2.4
1	B	2012	GLY	2.4
1	C	3045	THR	2.4
1	D	4233	GLU	2.4
1	D	4235	VAL	2.4
1	C	3244	PHE	2.4
1	A	1108	GLU	2.4
1	B	2226	THR	2.3
1	C	3194	LEU	2.3
1	A	1156	GLY	2.3
1	C	3187	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1235	VAL	2.3
1	A	1226	THR	2.2
1	D	4010	LEU	2.2
1	D	4012	GLY	2.2
1	C	3072	ALA	2.2
1	A	1046	THR	2.2
1	D	4203	MET	2.2
1	B	2173	ARG	2.1
1	C	3173	ARG	2.1
1	C	3075	ALA	2.1
1	C	3186	ILE	2.1
1	C	3166	PHE	2.1
1	C	3025	GLU	2.0
1	D	4231	LYS	2.0
1	A	1232	PRO	2.0
1	C	3095	THR	2.0
1	C	3118	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.