



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

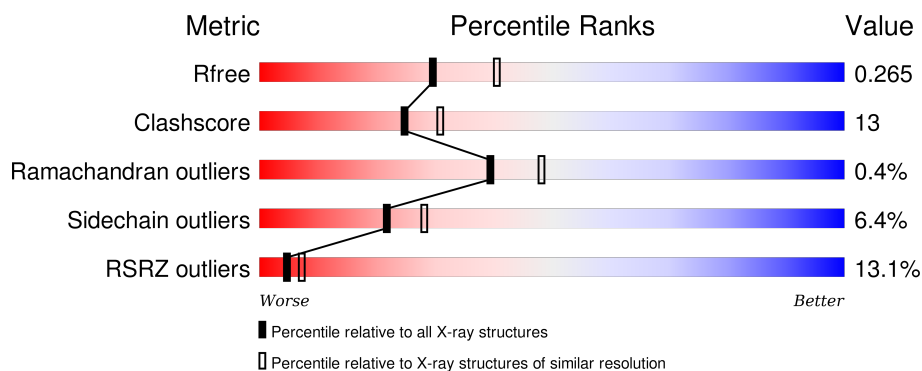
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	<div> <div>13%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	B	257	<div> <div>6%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
1	C	257	<div> <div>26%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	D	257	<div> <div>6%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>

## 2 Entry composition

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.

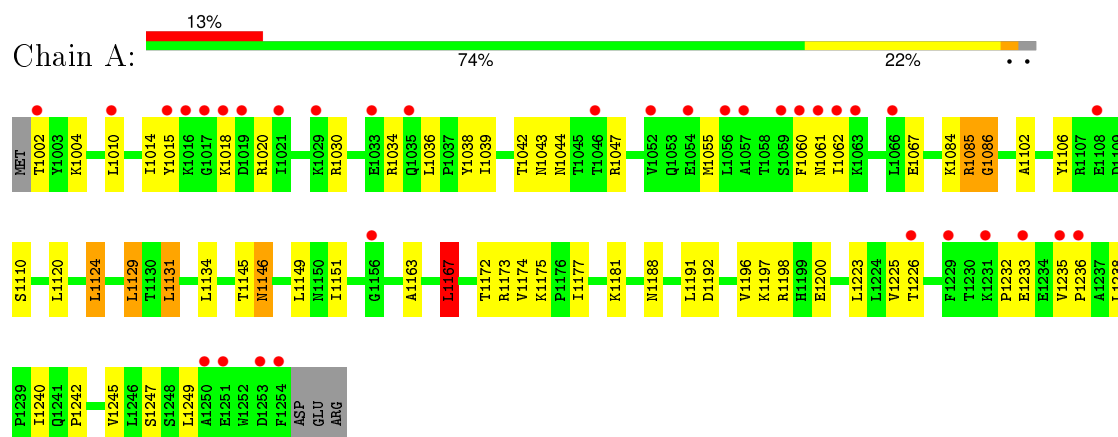
- Molecule 1 is a protein called putative phosphatases involved in N-acetyl-glucosamine catabolism.

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			

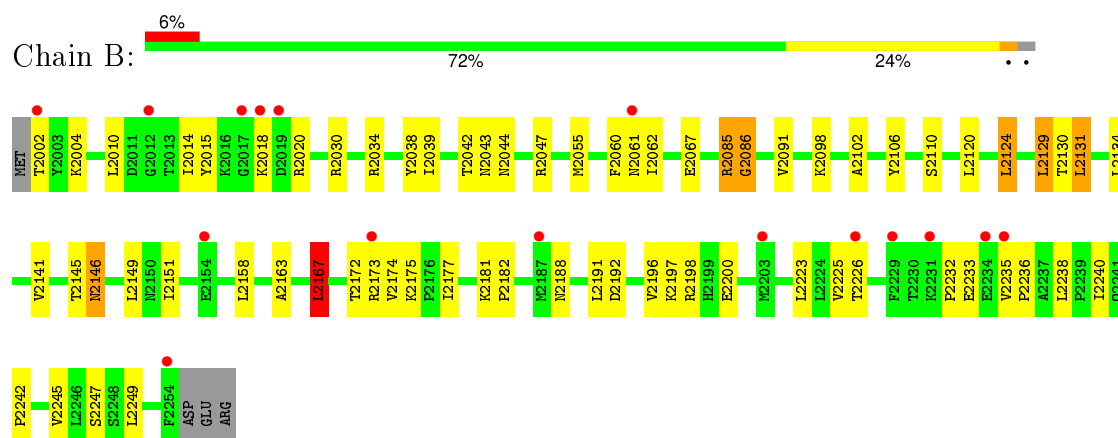
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

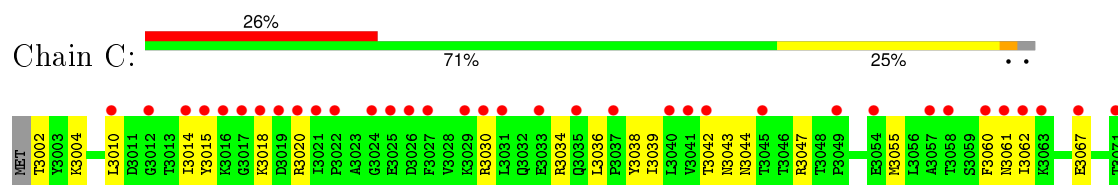
- Molecule 1: putative phosphatases involved in N-acetyl-glucosamine catabolism

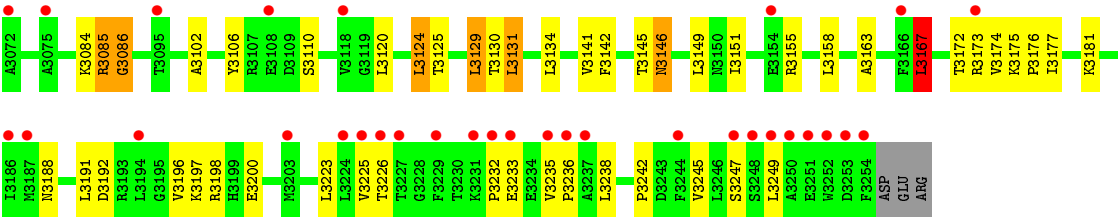


- Molecule 1: putative phosphatases involved in N-acetyl-glucosamine catabolism

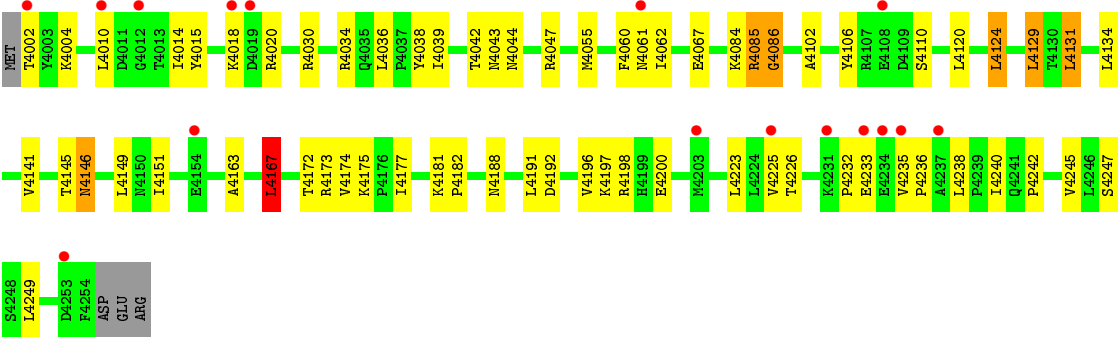


- Molecule 1: putative phosphatases involved in N-acetyl-glucosamine catabolism





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	2394 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 47812 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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:D:4235:VAL:CG2	1:D:4236:PRO:HD3	2.28	0.63
1:B:2235:VAL:CG2	1:B:2236: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

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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:C:3018:LYS:N	1:C:3018:LYS:HD2	2.27	0.49
1:B:2067:GLU:H	1:B:2067:GLU:CD	2.16	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:D:4124:LEU:HD21	1:D:4129:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2151:ILE:HG23	1:B:2151:ILE:O	2.13	0.48
1:C:3047:ARG:NH1	1:C:3055:MET:SD	2.86	0.48
1:C:3232:PRO:O	1:C:3235:VAL:HG22	2.13	0.48
1:A:1014:ILE:HG13	1:A:1015:TYR:HD1	1.79	0.48
1:C:3151:ILE:HG23	1:C:3151:ILE:O	2.12	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:2232:PRO:O	1:B:2235:VAL:HG22	2.14	0.48
1:B:2014:ILE:HG13	1:B:2015:TYR:HD1	1.79	0.48
1:B:2235:VAL:HA	1:B:2238:LEU:HG	1.96	0.47
1:A:1020:ARG:HB3	1:A:1060:PHE:HD1	1.79	0.47
1:D:4043:ASN:HD21	1:D:4181:LYS:N	2.05	0.47
1:A:1232:PRO:O	1:A:1235:VAL:HG22	2.14	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:D:4020:ARG:HB3	1:D:4060:PHE:HD1	1.80	0.47
1:B:2242:PRO:HG2	1:B:2245:VAL:HG22	1.96	0.47
1:A:1124:LEU:HD21	1:A:1129:LEU:HD13	1.96	0.47
1:D:4110:SER:HB2	1:D:4131:LEU:HG	1.97	0.47
1:A:1151:ILE:HG23	1:A:1151:ILE:O	2.15	0.47
1:D:4235:VAL:HA	1:D:4238:LEU:HG	1.96	0.47
1:C:3242:PRO:HG2	1:C:3245:VAL:HG22	1.96	0.47
1:B:2020:ARG:HB3	1:B:2060:PHE:HD1	1.79	0.47
1:C:3020:ARG:HB3	1:C:3060:PHE:HD1	1.80	0.47
1:A:1018:LYS:N	1:A:1018:LYS:HD2	2.29	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:B:2233:GLU:O	1:B:2236:PRO:HD2	2.16	0.46
1:B:2149:LEU:HD22	1:B:2149:LEU:H	1.81	0.46
1:C:3110:SER:HB2	1:C:3131:LEU:HG	1.97	0.46
1:A:1110:SER:HB2	1:A:1131: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

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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:D:4038:TYR:C	1:D:4039:ILE:HD12	2.37	0.44
1:C:3124:LEU:HD21	1:C:3129:LEU:HD13	1.99	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:B:2196:VAL:HG12	1:B:2197:LYS:O	2.18	0.43
1:A:1167:LEU:HB2	1:D:4167:LEU:HB2	2.00	0.43
1:D:4196:VAL:HG12	1:D:4197:LYS:O	2.17	0.43
1:B:2110:SER:HB2	1:B:2131:LEU:HG	2.00	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: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:A:1085:ARG:O	1:A:1086:GLY:O	2.37	0.43
1:D:4020:ARG:NH1	1:D:4061:ASN:HD22	2.17	0.43
1:D:4010:LEU:HD23	1:D:4014:ILE:HD11	2.01	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:D:4167:LEU:C	1:D:4167:LEU:CD1	2.87	0.42
1:C:3085:ARG:O	1:C:3086:GLY:C	2.57	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

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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:D:4010:LEU:CD2	1:D:4014:ILE:HD11	2.50	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:B:2085:ARG:O	1:B:2086:GLY:O	2.38	0.42
1:A:1038:TYR:C	1:A:1039:ILE:HD12	2.40	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: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:2124:LEU:O	1:C:3125:THR:HA	2.20	0.42
1:C:3167:LEU:C	1:C:3167:LEU:HD12	2.41	0.42
1:B:2172:THR:O	1:B:2173:ARG:HB2	2.20	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:B:2167:LEU:HD12	1:B:2167:LEU:C	2.39	0.41
1:A:1225:VAL:HG11	1:A:1249:LEU:CD2	2.50	0.41
1:D:4034:ARG:HB2	1:D:4036:LEU:HG	2.02	0.41
1:B:2146:ASN:N	1:B:2146:ASN:HD22	2.19	0.41
1:C:3223:LEU:C	1:C:3223:LEU:HD23	2.41	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:A:1146:ASN:HD22	1:A:1146:ASN:N	2.19	0.41
1:A:1084:LYS:HG3	1:A:1084:LYS:O	2.20	0.41
1:D:4181:LYS:HE3	1:D:4181:LYS:HB2	1.89	0.41
1:D:4084:LYS:HG3	1:D:4084:LYS:O	2.20	0.41
1:C:3102:ALA:HA	1:C:3106:TYR:O	2.21	0.41
1:D:4223:LEU:HD23	1:D:4223:LEU:C	2.41	0.41
1:B:2102:ALA:HA	1:B:2106:TYR:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3181:LYS:HB2	1:C:3181:LYS:HE3	1.91	0.40
1:B:2225:VAL:HG11	1:B:2249:LEU:CD2	2.51	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%)	39	48
1	B	251/257 (98%)	243 (97%)	7 (3%)	1 (0%)	39	48
1	C	251/257 (98%)	243 (97%)	7 (3%)	1 (0%)	39	48
1	D	251/257 (98%)	243 (97%)	7 (3%)	1 (0%)	39	48
All	All	1004/1028 (98%)	972 (97%)	28 (3%)	4 (0%)	39	48

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%)	23	30
1	B	212/216 (98%)	198 (93%)	14 (7%)	21	27
1	C	212/216 (98%)	199 (94%)	13 (6%)	23	30
1	D	212/216 (98%)	198 (93%)	14 (7%)	21	27
All	All	848/864 (98%)	794 (94%)	54 (6%)	22	28

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

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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

Some 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

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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 [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.

## 5.8 Polymer linkage issues [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	253/257 (98%)	0.87	34 (13%) 4 7	16, 37, 59, 70	0
1	B	253/257 (98%)	0.48	16 (6%) 23 31	12, 26, 55, 63	0
1	C	253/257 (98%)	1.42	67 (26%) 1 1	16, 41, 62, 70	0
1	D	253/257 (98%)	0.42	16 (6%) 23 31	12, 26, 54, 62	0
All	All	1012/1028 (98%)	0.80	133 (13%) 5 7	12, 34, 58, 70	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3250	ALA	6.9
1	C	3022	PRO	6.9
1	C	3029	LYS	6.7
1	C	3254	PHE	6.5
1	C	3016	LYS	5.8
1	C	3057	ALA	5.7
1	C	3063	LYS	5.2
1	A	1017	GLY	5.2
1	C	3017	GLY	5.1
1	C	3061	ASN	5.1
1	C	3014	ILE	4.9
1	C	3235	VAL	4.8
1	C	3253	ASP	4.7
1	C	3019	ASP	4.6
1	C	3018	LYS	4.5
1	A	1019	ASP	4.4
1	B	2235	VAL	4.3
1	C	3021	ILE	4.3
1	A	1236	PRO	4.2
1	D	4154	GLU	4.2
1	C	3035	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	3249	LEU	3.9
1	A	1033	GLU	3.8
1	C	3058	THR	3.8
1	A	1062	ILE	3.7
1	C	3248	SER	3.6
1	C	3027	PHE	3.6
1	A	1054	GLU	3.6
1	A	1233	GLU	3.6
1	C	3247	SER	3.5
1	C	3033	GLU	3.5
1	A	1253	ASP	3.4
1	C	3010	LEU	3.4
1	C	3024	GLY	3.4
1	A	1059	SER	3.4
1	C	3020	ARG	3.4
1	A	1029	LYS	3.4
1	B	2154	GLU	3.3
1	D	4002	THR	3.3
1	C	3067	GLU	3.3
1	C	3251	GLU	3.3
1	A	1015	TYR	3.3
1	A	1063	LYS	3.2
1	C	3031	LEU	3.2
1	B	2187	MET	3.2
1	A	1229	PHE	3.2
1	C	3236	PRO	3.2
1	B	2061	ASN	3.2
1	C	3012	GLY	3.1
1	A	1010	LEU	3.1
1	D	4018	LYS	3.1
1	D	4061	ASN	3.1
1	C	3026	ASP	3.1
1	C	3252	TRP	3.1
1	A	1061	ASN	3.1
1	C	3229	PHE	3.0
1	C	3225	VAL	3.0
1	A	1254	PHE	3.0
1	C	3233	GLU	3.0
1	C	3062	ILE	3.0
1	C	3231	LYS	3.0
1	B	2203	MET	2.9
1	C	3030	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1060	PHE	2.9
1	B	2229	PHE	2.9
1	A	1231	LYS	2.9
1	D	4019	ASP	2.9
1	C	3042	THR	2.9
1	C	3226	THR	2.9
1	C	3015	TYR	2.9
1	C	3224	LEU	2.9
1	C	3227	THR	2.8
1	B	2231	LYS	2.8
1	A	1021	ILE	2.8
1	C	3060	PHE	2.8
1	A	1251	GLU	2.8
1	A	1018	LYS	2.8
1	A	1057	ALA	2.8
1	A	1056	LEU	2.8
1	A	1250	ALA	2.8
1	C	3054	GLU	2.8
1	D	4108	GLU	2.7
1	A	1016	LYS	2.7
1	D	4225	VAL	2.7
1	B	2018	LYS	2.6
1	C	3108	GLU	2.6
1	C	3244	PHE	2.6
1	C	3071	THR	2.6
1	C	3045	THR	2.6
1	A	1035	GLN	2.6
1	C	3037	PRO	2.6
1	D	4235	VAL	2.6
1	B	2012	GLY	2.6
1	B	2002	THR	2.6
1	B	2234	GLU	2.5
1	C	3232	PRO	2.5
1	D	4012	GLY	2.5
1	D	4010	LEU	2.5
1	A	1235	VAL	2.5
1	B	2019	ASP	2.4
1	A	1108	GLU	2.4
1	B	2017	GLY	2.4
1	C	3237	ALA	2.4
1	D	4233	GLU	2.4
1	A	1002	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2226	THR	2.3
1	D	4203	MET	2.3
1	D	4231	LYS	2.3
1	C	3187	MET	2.3
1	A	1226	THR	2.3
1	C	3118	VAL	2.3
1	C	3186	ILE	2.3
1	C	3075	ALA	2.2
1	C	3166	PHE	2.2
1	C	3173	ARG	2.2
1	A	1156	GLY	2.2
1	C	3049	PRO	2.2
1	C	3194	LEU	2.2
1	B	2173	ARG	2.2
1	A	1046	THR	2.2
1	C	3095	THR	2.2
1	C	3025	GLU	2.2
1	B	2254	PHE	2.1
1	C	3154	GLU	2.1
1	A	1066	LEU	2.1
1	C	3203	MET	2.1
1	C	3072	ALA	2.1
1	A	1052	VAL	2.1
1	C	3041	VAL	2.1
1	C	3040	LEU	2.0
1	D	4237	ALA	2.0
1	D	4253	ASP	2.0
1	D	4234	GLU	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.