Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:09 PM GMT

PDB ID	:	1IY9
Title	:	Crystal structure of spermidine synthase
Authors	:	Tan, A.Y.; Smith, P.C.; Shen, J.; Xiao, R.; Acton, T.; Rost, B.; Montelione, G.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2002-07-26
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

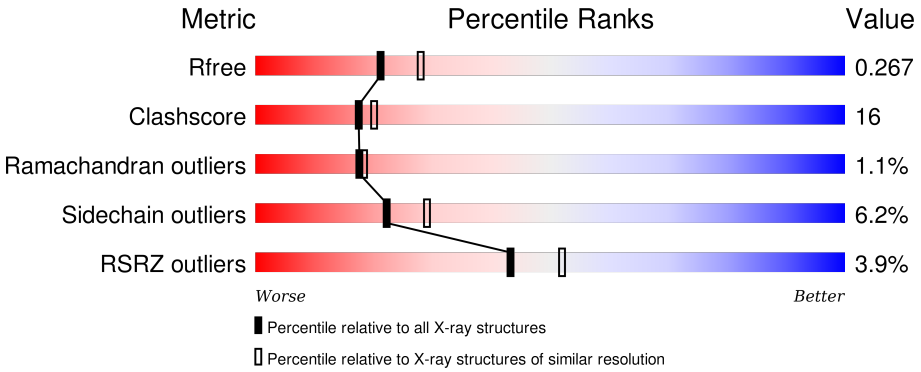
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 >=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 <=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	275	3% 73% 23% ·
1	B	275	4% 71% 24% ·
1	C	275	4% 75% 20% ·
1	D	275	4% 73% 22% ·

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9099 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 Spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			
1	B	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			
1	C	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			
1	D	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			

- Molecule 2 is water.

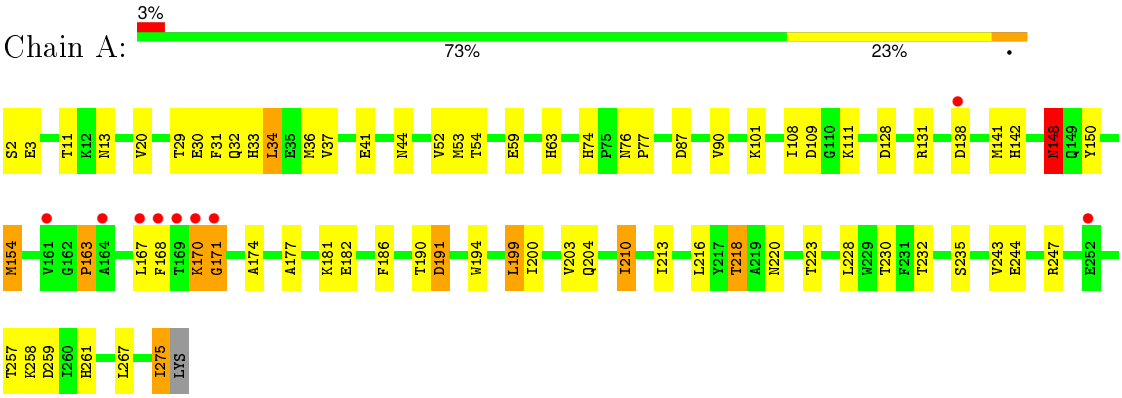
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total	O	0	0
			92	92		
2	B	79	Total	O	0	0
			79	79		
2	C	66	Total	O	0	0
			66	66		
2	D	86	Total	O	0	0
			86	86		

3 Residue-property plots (i)

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.

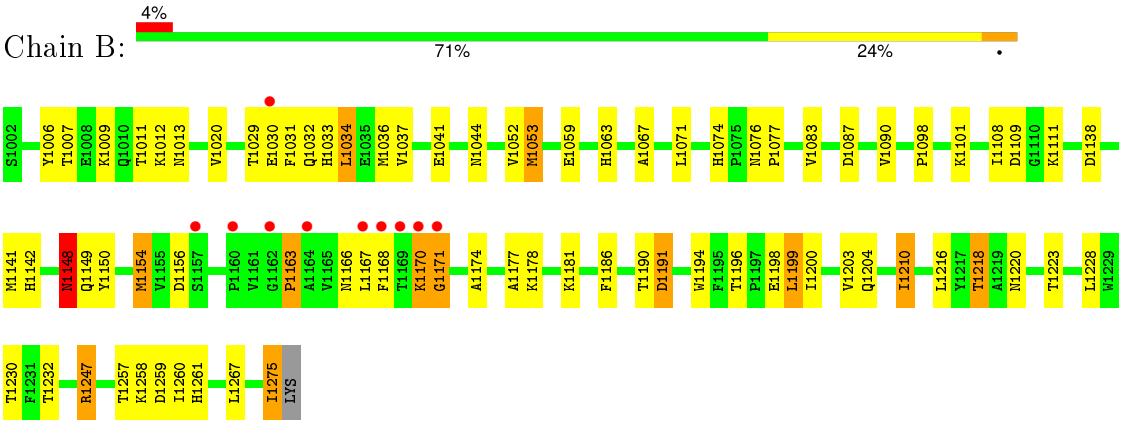
- Molecule 1: Spermidine synthase

Chain A:



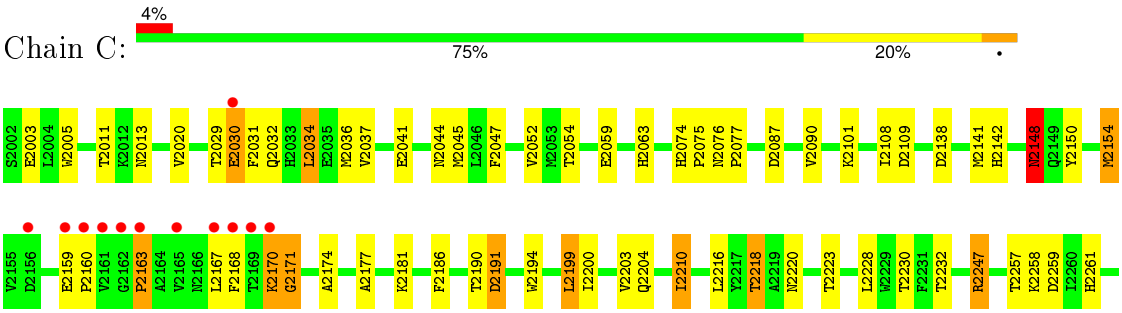
- Molecule 1: Spermidine synthase

Chain B:

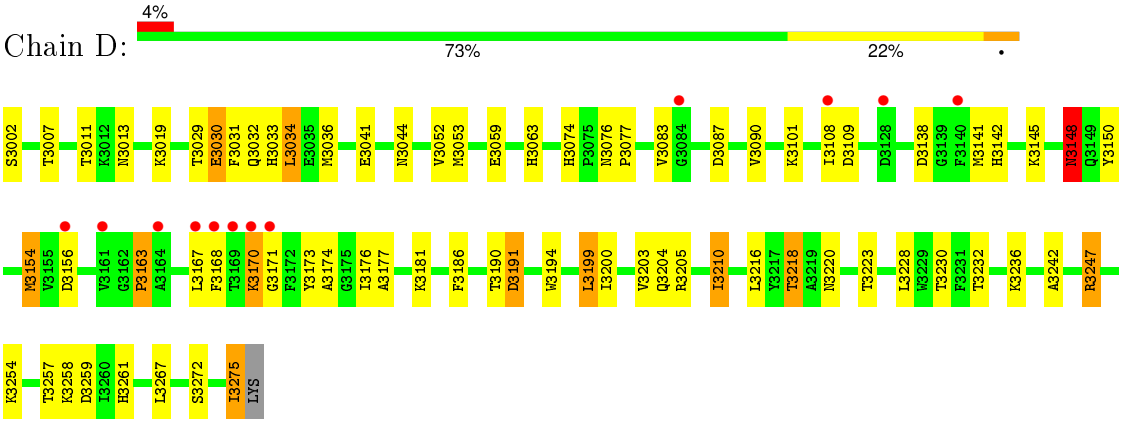


- Molecule 1: Spermidine synthase

Chain C:



• Molecule 1: Spermidine synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.10Å 105.80Å 121.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 48.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.8 (100.00-2.30) 86.8 (48.52-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.79 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.208 , 0.254 0.226 , 0.267	Depositor DCC
R_{free} test set	2446 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 51692 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9099	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, 0.375 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	0.62	0/2251	0.78	1/3055 (0.0%)
1	B	0.60	1/2251 (0.0%)	0.78	1/3055 (0.0%)
1	C	0.61	0/2251	0.77	1/3055 (0.0%)
1	D	0.62	0/2251	0.77	1/3055 (0.0%)
All	All	0.61	1/9004 (0.0%)	0.78	4/12220 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1053	MET	SD-CE	5.18	2.06	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3034	LEU	CA-CB-CG	6.11	129.35	115.30
1	C	2034	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	34	LEU	CA-CB-CG	5.90	128.87	115.30
1	B	1034	LEU	CA-CB-CG	5.59	128.16	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	2194	0	2167	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2194	0	2167	80	0
1	C	2194	0	2167	67	0
1	D	2194	0	2167	74	0
2	A	92	0	0	13	0
2	B	79	0	0	16	0
2	C	66	0	0	9	0
2	D	86	0	0	16	0
All	All	9099	0	8668	279	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 16.

All (279) 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:D:3053:MET:SD	1:D:3053:MET:CE	2.05	1.45
1:B:1053:MET:SD	1:B:1053:MET:CE	2.06	1.42
1:A:53:MET:SD	1:A:53:MET:CE	2.05	1.41
1:B:1190:THR:HG23	1:B:1230:THR:HG22	1.42	1.02
1:D:3190:THR:HG23	1:D:3230:THR:HG22	1.43	1.00
1:A:190:THR:HG23	1:A:230:THR:HG22	1.42	1.00
1:C:2190:THR:HG23	1:C:2230:THR:HG22	1.41	1.00
1:A:11:THR:HG22	1:A:13:ASN:H	1.27	1.00
1:C:2011:THR:HG22	1:C:2013:ASN:H	1.28	0.97
1:D:3011:THR:HG22	1:D:3013:ASN:H	1.26	0.96
1:B:1011:THR:HG22	1:B:1013:ASN:H	1.28	0.95
1:D:3216:LEU:HD11	1:D:3230:THR:HG23	1.50	0.93
1:D:3029:THR:HG22	1:D:3031:PHE:H	1.34	0.93
1:C:2029:THR:HG22	1:C:2031:PHE:H	1.34	0.92
1:A:29:THR:HG22	1:A:31:PHE:H	1.34	0.91
1:C:2037:VAL:HB	2:C:4034:HOH:O	1.70	0.90
1:B:1029:THR:HG22	1:B:1031:PHE:H	1.36	0.90
1:B:1216:LEU:HD11	1:B:1230:THR:HG23	1.53	0.89
1:A:216:LEU:HD11	1:A:230:THR:HG23	1.54	0.88
1:B:1257:THR:HG22	1:B:1259:ASP:H	1.38	0.88
1:C:2216:LEU:HD11	1:C:2230:THR:HG23	1.59	0.85
1:A:257:THR:HG22	1:A:259:ASP:H	1.43	0.83
1:B:1011:THR:HG21	1:C:2041:GLU:OE1	1.80	0.81
1:D:3257:THR:HG22	1:D:3259:ASP:H	1.47	0.80
1:A:190:THR:HG23	1:A:230:THR:CG2	2.13	0.79
1:D:3190:THR:HG23	1:D:3230:THR:CG2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3029:THR:HG21	1:D:3109:ASP:OD2	1.82	0.79
1:C:2257:THR:HG22	1:C:2259:ASP:H	1.48	0.79
1:B:1052:VAL:HG11	1:B:1223:THR:CG2	2.14	0.78
1:D:3191:ASP:O	1:D:3230:THR:HB	1.84	0.78
1:C:2190:THR:HG23	1:C:2230:THR:CG2	2.14	0.78
1:A:191:ASP:O	1:A:230:THR:HB	1.85	0.77
1:D:3052:VAL:HG11	1:D:3223:THR:CG2	2.15	0.77
1:A:128:ASP:HB3	2:A:4189:HOH:O	1.84	0.76
1:B:1216:LEU:HD11	1:B:1230:THR:CG2	2.15	0.76
1:B:1177:ALA:HB2	1:B:1210:ILE:HD11	1.66	0.76
1:B:1190:THR:HG23	1:B:1230:THR:CG2	2.15	0.76
1:A:29:THR:HG21	1:A:109:ASP:OD2	1.85	0.76
1:A:111:LYS:HD3	2:A:4027:HOH:O	1.84	0.76
1:B:1041:GLU:OE1	1:C:2011:THR:HG21	1.86	0.75
1:D:3216:LEU:HD11	1:D:3230:THR:CG2	2.15	0.75
1:C:2191:ASP:O	1:C:2230:THR:HB	1.85	0.75
1:B:1191:ASP:O	1:B:1230:THR:HB	1.87	0.74
1:A:11:THR:HG21	1:D:3041:GLU:OE1	1.88	0.74
1:D:3272:SER:HB2	2:D:4074:HOH:O	1.87	0.74
1:D:3177:ALA:HB2	1:D:3210:ILE:HD11	1.70	0.74
1:A:216:LEU:HD11	1:A:230:THR:CG2	2.18	0.74
1:A:52:VAL:HG11	1:A:223:THR:CG2	2.17	0.74
1:C:2029:THR:HG21	1:C:2109:ASP:OD2	1.87	0.74
1:B:1029:THR:HG21	1:B:1109:ASP:OD2	1.88	0.73
1:C:2052:VAL:HG11	1:C:2223:THR:CG2	2.19	0.73
1:C:2177:ALA:HB2	1:C:2210:ILE:HD11	1.71	0.72
1:C:2216:LEU:HD11	1:C:2230:THR:CG2	2.18	0.72
1:C:2138:ASP:HB3	1:C:2141:MET:HB2	1.71	0.72
2:B:4051:HOH:O	1:C:2257:THR:HG21	1.90	0.72
1:D:3170:LYS:HA	1:D:3170:LYS:HE2	1.72	0.71
1:A:177:ALA:HB2	1:A:210:ILE:HD11	1.73	0.70
1:D:3002:SER:HB3	2:D:4018:HOH:O	1.90	0.70
1:A:41:GLU:OE1	1:D:3011:THR:HG21	1.91	0.70
1:B:1052:VAL:HG11	1:B:1223:THR:HG22	1.73	0.70
1:C:2190:THR:CG2	1:C:2230:THR:HG22	2.20	0.69
1:A:170:LYS:HE2	1:A:170:LYS:HA	1.74	0.69
1:C:2174:ALA:HA	1:C:2210:ILE:HD13	1.75	0.69
1:A:33:HIS:HD2	2:B:4276:HOH:O	1.76	0.68
1:B:1257:THR:HG22	1:B:1259:ASP:N	2.07	0.68
1:D:3052:VAL:HG11	1:D:3223:THR:HG22	1.76	0.68
1:B:1190:THR:CG2	1:B:1230:THR:HG22	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3204:GLN:HG2	1:D:3275:ILE:HB	1.77	0.67
1:C:2170:LYS:HA	1:C:2170:LYS:HE2	1.74	0.67
1:B:1170:LYS:HA	1:B:1170:LYS:HE2	1.74	0.67
1:D:3254:LYS:HE2	2:D:4238:HOH:O	1.95	0.67
1:A:36:MET:HE1	1:A:44:ASN:HB3	1.77	0.67
1:A:54:THR:HG22	2:A:4036:HOH:O	1.95	0.67
1:B:1142:HIS:HD2	2:B:4247:HOH:O	1.77	0.67
1:D:3190:THR:CG2	1:D:3230:THR:HG22	2.23	0.66
1:B:1138:ASP:HB3	1:B:1141:MET:HB2	1.76	0.66
1:C:2148:ASN:HB2	1:C:2181:LYS:HA	1.76	0.66
1:D:3141:MET:SD	1:D:3163:PRO:HB2	2.35	0.66
1:A:174:ALA:HA	1:A:210:ILE:HD13	1.76	0.66
1:A:74:HIS:HD2	1:A:76:ASN:H	1.43	0.66
1:D:3148:ASN:HB2	1:D:3181:LYS:HA	1.78	0.66
1:A:138:ASP:HB3	1:A:141:MET:HB2	1.78	0.65
1:B:1148:ASN:HB2	1:B:1181:LYS:HA	1.77	0.65
1:B:1204:GLN:HG2	1:B:1275:ILE:HB	1.77	0.65
1:B:1074:HIS:HD2	1:B:1076:ASN:H	1.45	0.65
1:D:3142:HIS:HD2	2:D:4075:HOH:O	1.78	0.64
1:D:3138:ASP:HB3	1:D:3141:MET:HB2	1.79	0.64
1:D:3074:HIS:HD2	1:D:3076:ASN:H	1.46	0.64
1:A:190:THR:CG2	1:A:230:THR:HG22	2.23	0.64
1:D:3052:VAL:HG11	1:D:3223:THR:HG21	1.79	0.64
1:D:3174:ALA:HA	1:D:3210:ILE:HD13	1.79	0.64
1:C:2052:VAL:HG11	1:C:2223:THR:HG22	1.80	0.64
1:C:2074:HIS:HD2	1:C:2076:ASN:H	1.45	0.64
1:A:182:GLU:HG2	2:A:4008:HOH:O	1.96	0.64
1:C:2074:HIS:HB3	1:C:2077:PRO:HG3	1.80	0.63
1:B:1196:THR:HA	2:B:4305:HOH:O	1.97	0.63
1:A:148:ASN:HB2	1:A:181:LYS:HA	1.80	0.63
1:A:257:THR:HG22	1:A:259:ASP:N	2.12	0.63
1:A:52:VAL:HG11	1:A:223:THR:HG21	1.79	0.63
1:A:257:THR:HG21	2:D:4142:HOH:O	1.97	0.63
1:D:3257:THR:HG22	1:D:3259:ASP:N	2.12	0.63
1:A:52:VAL:HG11	1:A:223:THR:HG22	1.80	0.62
1:A:204:GLN:HG2	1:A:275:ILE:HB	1.81	0.62
1:B:1098:PRO:HD2	2:B:4132:HOH:O	1.98	0.62
1:B:1052:VAL:HG11	1:B:1223:THR:HG21	1.81	0.62
1:B:1174:ALA:HA	1:B:1210:ILE:HD13	1.81	0.61
1:C:2052:VAL:HG11	1:C:2223:THR:HG21	1.82	0.61
1:C:2036:MET:HE1	1:C:2044:ASN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:MET:SD	1:B:1163:PRO:HB2	2.41	0.60
1:D:3074:HIS:HB3	1:D:3077:PRO:HG3	1.83	0.60
1:C:2204:GLN:HG2	1:C:2275:ILE:HB	1.83	0.60
1:D:3053:MET:SD	2:D:4213:HOH:O	2.56	0.60
1:D:3036:MET:HE1	1:D:3044:ASN:HB3	1.82	0.60
1:A:194:TRP:HE1	1:D:3220:ASN:HD21	1.49	0.60
1:D:3218:THR:HG23	1:D:3228:LEU:HD11	1.83	0.60
1:C:2258:LYS:O	1:C:2261:HIS:HB3	2.02	0.60
1:B:1220:ASN:HD21	1:C:2194:TRP:HE1	1.49	0.59
1:C:2257:THR:HG22	1:C:2259:ASP:N	2.17	0.59
1:B:1036:MET:HE1	1:B:1044:ASN:HB3	1.85	0.59
1:B:1059:GLU:OE1	1:B:1063:HIS:HD2	1.86	0.59
1:B:1177:ALA:HB2	1:B:1210:ILE:CD1	2.33	0.58
1:B:1071:LEU:HD12	2:B:4067:HOH:O	2.04	0.58
1:B:1074:HIS:HB3	1:B:1077:PRO:HG3	1.85	0.58
1:D:3205:ARG:HD3	2:D:4094:HOH:O	2.01	0.58
1:A:74:HIS:HB3	1:A:77:PRO:HG3	1.85	0.58
1:A:247:ARG:HG3	2:A:4177:HOH:O	2.02	0.57
1:A:2:SER:HA	1:B:1006:TYR:OH	2.04	0.57
1:C:2045:MET:HB3	2:C:4034:HOH:O	2.05	0.57
1:B:1111:LYS:HD3	2:B:4215:HOH:O	2.03	0.57
1:C:2011:THR:HG22	1:C:2013:ASN:N	2.11	0.57
1:D:3108:ILE:HG23	1:D:3138:ASP:HA	1.86	0.57
1:D:3030:GLU:CD	1:D:3030:GLU:H	2.06	0.56
1:B:1220:ASN:ND2	1:C:2194:TRP:HE1	2.04	0.56
1:A:220:ASN:HD21	1:D:3194:TRP:HE1	1.53	0.56
1:D:3247:ARG:O	1:D:3247:ARG:HD3	2.06	0.56
1:B:1149:GLN:HG2	2:B:4234:HOH:O	2.05	0.56
1:C:2030:GLU:H	1:C:2030:GLU:CD	2.09	0.56
1:D:3258:LYS:HG2	2:D:4029:HOH:O	2.06	0.56
1:B:1108:ILE:HG23	1:B:1138:ASP:HA	1.88	0.56
1:B:1198:GLU:HG2	2:B:4305:HOH:O	2.05	0.56
1:C:2142:HIS:HE1	1:C:2150:TYR:OH	1.89	0.56
1:A:194:TRP:HE1	1:D:3220:ASN:ND2	2.03	0.56
1:C:2108:ILE:HG23	1:C:2138:ASP:HA	1.87	0.55
1:D:3059:GLU:OE1	1:D:3063:HIS:HD2	1.89	0.55
1:A:29:THR:HG21	1:A:109:ASP:CG	2.27	0.55
1:C:2218:THR:HG23	1:C:2228:LEU:HD11	1.87	0.55
1:C:2059:GLU:OE1	1:C:2063:HIS:HD2	1.90	0.55
1:B:1011:THR:HG22	1:B:1013:ASN:N	2.11	0.55
1:A:108:ILE:HG23	1:A:138:ASP:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:GLU:H	1:B:1030:GLU:CD	2.10	0.54
1:C:2141:MET:SD	1:C:2163:PRO:HB2	2.48	0.54
1:A:131:ARG:HG3	2:A:4244:HOH:O	2.07	0.54
1:A:59:GLU:OE1	1:A:63:HIS:HD2	1.90	0.54
1:A:11:THR:HG22	1:A:13:ASN:N	2.10	0.54
1:D:3029:THR:HG21	1:D:3109:ASP:CG	2.28	0.54
1:C:2029:THR:HG21	1:C:2109:ASP:CG	2.28	0.54
1:B:1218:THR:HG23	1:B:1228:LEU:HD11	1.88	0.54
1:B:1247:ARG:O	1:B:1247:ARG:HD3	2.07	0.54
1:A:142:HIS:HE1	1:A:150:TYR:OH	1.91	0.54
1:A:30:GLU:CD	1:A:30:GLU:H	2.10	0.54
1:A:74:HIS:HE1	2:A:4230:HOH:O	1.90	0.53
1:D:3258:LYS:O	1:D:3261:HIS:HB3	2.07	0.53
1:B:1029:THR:HG21	1:B:1109:ASP:CG	2.28	0.53
1:A:29:THR:HG22	1:A:30:GLU:N	2.23	0.53
1:B:1142:HIS:HE1	1:B:1150:TYR:OH	1.92	0.53
1:B:1257:THR:HG21	2:C:4033:HOH:O	2.08	0.53
1:B:1258:LYS:HE2	2:B:4212:HOH:O	2.08	0.53
1:B:1011:THR:HG23	2:C:4147:HOH:O	2.07	0.53
1:C:2177:ALA:HB2	1:C:2210:ILE:CD1	2.39	0.53
1:D:3199:LEU:HD22	1:D:3203:VAL:HG23	1.91	0.52
1:C:2247:ARG:O	1:C:2247:ARG:HD3	2.10	0.52
1:B:1190:THR:HG21	1:B:1232:THR:OG1	2.10	0.52
1:D:3142:HIS:HE1	1:D:3150:TYR:OH	1.93	0.52
1:A:220:ASN:ND2	1:D:3194:TRP:HE1	2.07	0.52
1:C:2054:THR:HG22	2:C:4120:HOH:O	2.10	0.51
1:A:3:GLU:HB2	1:B:1007:THR:O	2.10	0.51
1:A:247:ARG:HD3	1:A:247:ARG:O	2.10	0.51
2:C:4254:HOH:O	1:D:3033:HIS:HD2	1.93	0.51
1:C:2223:THR:O	1:C:2223:THR:HG22	2.11	0.51
1:A:199:LEU:HD22	1:A:203:VAL:HG23	1.91	0.51
1:B:1194:TRP:HE1	1:C:2220:ASN:HD21	1.59	0.51
1:C:2047:PHE:HE1	2:C:4034:HOH:O	1.92	0.51
1:D:3223:THR:HG22	1:D:3223:THR:O	2.11	0.51
1:A:29:THR:CG2	1:A:30:GLU:N	2.73	0.51
1:B:1200:ILE:O	1:B:1204:GLN:HB2	2.11	0.51
1:B:1199:LEU:HD22	1:B:1203:VAL:HG23	1.92	0.51
1:D:3242:ALA:HB3	2:D:4068:HOH:O	2.11	0.51
1:D:3029:THR:HG22	1:D:3030:GLU:N	2.26	0.50
1:D:3218:THR:CG2	1:D:3228:LEU:HD11	2.41	0.50
1:A:142:HIS:HD2	2:A:4013:HOH:O	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2199:LEU:HD22	1:C:2203:VAL:HG23	1.93	0.50
1:A:218:THR:HG23	1:A:228:LEU:HD11	1.92	0.50
1:C:2029:THR:HG22	1:C:2030:GLU:N	2.26	0.50
1:D:3029:THR:CG2	1:D:3030:GLU:N	2.75	0.49
1:C:2029:THR:CG2	1:C:2030:GLU:N	2.76	0.49
1:A:29:THR:HB	1:A:32:GLN:O	2.13	0.49
1:A:223:THR:O	1:A:223:THR:HG22	2.13	0.49
1:C:2003:GLU:HB2	1:D:3007:THR:O	2.12	0.49
1:B:1067:ALA:HB1	2:B:4067:HOH:O	2.13	0.49
1:D:3011:THR:HG22	1:D:3013:ASN:N	2.09	0.49
1:D:3177:ALA:HB2	1:D:3210:ILE:CD1	2.38	0.49
1:D:3200:ILE:O	1:D:3204:GLN:HB2	2.14	0.48
1:A:190:THR:HG21	1:A:232:THR:OG1	2.13	0.48
1:C:2190:THR:HG21	1:C:2232:THR:OG1	2.13	0.48
1:A:177:ALA:HB2	1:A:210:ILE:CD1	2.41	0.48
1:D:3190:THR:HG21	1:D:3232:THR:OG1	2.14	0.48
1:C:2029:THR:HB	1:C:2032:GLN:O	2.14	0.48
1:A:258:LYS:O	1:A:261:HIS:HB3	2.13	0.48
1:B:1194:TRP:HE1	1:C:2220:ASN:ND2	2.12	0.48
1:D:3029:THR:HB	1:D:3032:GLN:O	2.14	0.48
1:D:3257:THR:HG23	2:D:4029:HOH:O	2.13	0.48
1:B:1170:LYS:HB3	2:B:4301:HOH:O	2.13	0.48
2:A:4293:HOH:O	1:B:1033:HIS:HD2	1.97	0.48
1:B:1029:THR:HG22	1:B:1030:GLU:N	2.29	0.47
1:A:204:GLN:HE21	1:A:275:ILE:HD12	1.79	0.47
1:D:3145:LYS:HB2	2:D:4082:HOH:O	2.15	0.47
1:B:1258:LYS:O	1:B:1261:HIS:HB3	2.14	0.47
1:B:1029:THR:HB	1:B:1032:GLN:O	2.14	0.47
1:B:1223:THR:HG22	1:B:1223:THR:O	2.15	0.47
1:C:2074:HIS:HE1	2:C:4107:HOH:O	1.97	0.47
1:D:3168:PHE:HB2	1:D:3174:ALA:HB3	1.97	0.47
1:D:3176:ILE:HB	2:D:4083:HOH:O	2.14	0.47
1:A:244:GLU:HG2	2:A:4146:HOH:O	2.15	0.46
1:D:3019:LYS:HE3	2:D:4113:HOH:O	2.14	0.46
1:B:1178:LYS:HE3	2:B:4144:HOH:O	2.14	0.46
1:D:3216:LEU:CD1	1:D:3230:THR:HG23	2.35	0.45
1:C:2168:PHE:O	1:C:2171:GLY:N	2.50	0.45
1:B:1029:THR:CG2	1:B:1030:GLU:N	2.78	0.45
1:B:1218:THR:CG2	1:B:1228:LEU:HD11	2.46	0.45
1:D:3168:PHE:CB	1:D:3174:ALA:HB3	2.46	0.45
1:A:200:ILE:O	1:A:204:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2168:PHE:HB2	1:C:2174:ALA:HB3	1.99	0.45
1:C:2090:VAL:HG11	1:C:2154:MET:HG3	1.97	0.45
1:C:2218:THR:CG2	1:C:2228:LEU:HD11	2.47	0.45
1:A:258:LYS:HG2	2:A:4311:HOH:O	2.17	0.45
1:B:1260:ILE:HA	1:B:1260:ILE:HD13	1.83	0.45
1:D:3173:TYR:HA	2:D:4083:HOH:O	2.16	0.44
1:C:2168:PHE:CB	1:C:2174:ALA:HB3	2.47	0.44
1:B:1020:VAL:HG13	1:B:1037:VAL:HG13	2.00	0.44
1:C:2200:ILE:O	1:C:2204:GLN:HB2	2.18	0.44
1:C:2020:VAL:HG13	1:C:2037:VAL:HG13	2.00	0.44
1:B:1168:PHE:CB	1:B:1174:ALA:HB3	2.47	0.44
1:D:3142:HIS:CD2	2:D:4075:HOH:O	2.62	0.44
1:B:1168:PHE:HB2	1:B:1174:ALA:HB3	1.99	0.44
1:C:2075:PRO:HB3	2:C:4133:HOH:O	2.18	0.43
1:B:1216:LEU:CD1	1:B:1230:THR:HG23	2.36	0.43
1:A:168:PHE:CB	1:A:174:ALA:HB3	2.48	0.43
1:D:3077:PRO:HD3	1:D:3247:ARG:NH2	2.33	0.43
1:A:218:THR:CG2	1:A:228:LEU:HD11	2.49	0.43
1:D:3090:VAL:HG11	1:D:3154:MET:HG3	2.01	0.43
1:B:1036:MET:HB3	1:B:1036:MET:HE2	1.82	0.43
1:D:3236:LYS:HG2	2:D:4078:HOH:O	2.18	0.43
1:D:3204:GLN:HE21	1:D:3275:ILE:HD12	1.84	0.42
1:B:1168:PHE:O	1:B:1171:GLY:N	2.51	0.42
1:A:168:PHE:HB2	1:A:174:ALA:HB3	2.00	0.42
1:A:216:LEU:CD1	1:A:230:THR:HG23	2.39	0.42
1:D:3218:THR:HG23	1:D:3228:LEU:CD1	2.49	0.42
1:B:1009:LYS:HD2	1:C:2005:TRP:CH2	2.55	0.42
1:B:1142:HIS:CD2	2:B:4247:HOH:O	2.60	0.42
1:A:141:MET:SD	1:A:163:PRO:HB2	2.59	0.42
1:B:1083:VAL:O	1:B:1156:ASP:HB2	2.19	0.42
1:B:1166:ASN:O	1:B:1171:GLY:HA3	2.19	0.42
1:C:2216:LEU:CD1	1:C:2230:THR:HG23	2.41	0.42
1:A:77:PRO:HD3	1:A:247:ARG:NH2	2.35	0.42
1:B:1077:PRO:HD3	1:B:1247:ARG:NH2	2.35	0.42
1:B:1218:THR:HG21	2:B:4052:HOH:O	2.20	0.42
1:B:1012:LYS:HG3	2:B:4208:HOH:O	2.19	0.42
1:A:90:VAL:HG11	1:A:154:MET:HG3	2.02	0.42
1:C:2045:MET:HB2	1:C:2045:MET:HE3	1.93	0.41
1:D:3083:VAL:O	1:D:3156:ASP:HB2	2.21	0.41
1:A:168:PHE:O	1:A:171:GLY:N	2.52	0.41
1:A:20:VAL:HG13	1:A:37:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2170:LYS:HE2	1:C:2170:LYS:CA	2.48	0.41
1:A:54:THR:CG2	2:A:4036:HOH:O	2.63	0.41
1:C:2159:GLU:HA	1:C:2160:PRO:HD2	1.96	0.41
1:A:213:ILE:HB	1:A:235:SER:HB3	2.02	0.40
1:A:243:VAL:HB	2:A:4035:HOH:O	2.21	0.40
1:B:1090:VAL:HG11	1:B:1154:MET:HG3	2.02	0.40
1:C:2204:GLN:HE21	1:C:2275:ILE:HD12	1.87	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	272/275 (99%)	256 (94%)	13 (5%)	3 (1%)	17	18
1	B	272/275 (99%)	255 (94%)	14 (5%)	3 (1%)	17	18
1	C	272/275 (99%)	257 (94%)	12 (4%)	3 (1%)	17	18
1	D	272/275 (99%)	255 (94%)	14 (5%)	3 (1%)	17	18
All	All	1088/1100 (99%)	1023 (94%)	53 (5%)	12 (1%)	17	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	1171	GLY
1	C	2171	GLY
1	D	3171	GLY
1	A	148	ASN
1	B	1148	ASN
1	C	2148	ASN
1	D	3148	ASN

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Mol	Chain	Res	Type
1	D	3163	PRO
1	A	163	PRO
1	B	1163	PRO
1	C	2163	PRO

5.3.2 Protein sidechains

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	244/245 (100%)	230 (94%)	14 (6%)	25	34
1	B	244/245 (100%)	229 (94%)	15 (6%)	23	30
1	C	244/245 (100%)	228 (93%)	16 (7%)	21	27
1	D	244/245 (100%)	228 (93%)	16 (7%)	21	27
All	All	976/980 (100%)	915 (94%)	61 (6%)	22	29

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	87	ASP
1	A	101	LYS
1	A	148	ASN
1	A	154	MET
1	A	167	LEU
1	A	170	LYS
1	A	186	PHE
1	A	191	ASP
1	A	199	LEU
1	A	210	ILE
1	A	218	THR
1	A	267	LEU
1	A	275	ILE
1	B	1034	LEU
1	B	1087	ASP
1	B	1101	LYS

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Mol	Chain	Res	Type
1	B	1148	ASN
1	B	1154	MET
1	B	1167	LEU
1	B	1170	LYS
1	B	1186	PHE
1	B	1191	ASP
1	B	1199	LEU
1	B	1210	ILE
1	B	1218	THR
1	B	1247	ARG
1	B	1267	LEU
1	B	1275	ILE
1	C	2030	GLU
1	C	2034	LEU
1	C	2087	ASP
1	C	2101	LYS
1	C	2148	ASN
1	C	2154	MET
1	C	2167	LEU
1	C	2170	LYS
1	C	2186	PHE
1	C	2191	ASP
1	C	2199	LEU
1	C	2210	ILE
1	C	2218	THR
1	C	2247	ARG
1	C	2267	LEU
1	C	2275	ILE
1	D	3030	GLU
1	D	3034	LEU
1	D	3087	ASP
1	D	3101	LYS
1	D	3148	ASN
1	D	3154	MET
1	D	3167	LEU
1	D	3170	LYS
1	D	3186	PHE
1	D	3191	ASP
1	D	3199	LEU
1	D	3210	ILE
1	D	3218	THR
1	D	3247	ARG

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Mol	Chain	Res	Type
1	D	3267	LEU
1	D	3275	ILE

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

Mol	Chain	Res	Type
1	A	63	HIS
1	A	74	HIS
1	A	135	GLN
1	A	142	HIS
1	A	204	GLN
1	A	220	ASN
1	B	1063	HIS
1	B	1074	HIS
1	B	1135	GLN
1	B	1142	HIS
1	B	1204	GLN
1	B	1220	ASN
1	C	2063	HIS
1	C	2074	HIS
1	C	2135	GLN
1	C	2142	HIS
1	C	2204	GLN
1	C	2220	ASN
1	D	3033	HIS
1	D	3063	HIS
1	D	3074	HIS
1	D	3135	GLN
1	D	3142	HIS
1	D	3204	GLN
1	D	3220	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

There are no carbohydrates 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	274/275 (99%)	0.32	9 (3%) 50 59	19, 31, 57, 101	0
1	B	274/275 (99%)	0.17	10 (3%) 46 55	18, 32, 56, 101	0
1	C	274/275 (99%)	0.21	12 (4%) 38 47	18, 32, 56, 101	0
1	D	274/275 (99%)	0.30	12 (4%) 38 47	19, 32, 56, 100	0
All	All	1096/1100 (99%)	0.25	43 (3%) 43 52	18, 32, 59, 101	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	LYS	17.6
1	B	1169	THR	14.6
1	A	169	THR	14.1
1	C	2169	THR	13.4
1	C	2170	LYS	9.2
1	D	3170	LYS	8.1
1	D	3169	THR	7.6
1	D	3168	PHE	7.0
1	A	168	PHE	6.8
1	C	2168	PHE	6.2
1	B	1170	LYS	5.8
1	A	167	LEU	4.8
1	C	2161	VAL	4.5
1	A	171	GLY	4.3
1	B	1168	PHE	4.0
1	C	2167	LEU	4.0
1	C	2160	PRO	3.8
1	B	1167	LEU	3.7
1	C	2163	PRO	3.5
1	D	3167	LEU	3.4
1	C	2162	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	3128	ASP	3.3
1	D	3156	ASP	3.2
1	D	3171	GLY	3.0
1	B	1171	GLY	2.9
1	C	2159	GLU	2.9
1	A	164	ALA	2.9
1	D	3161	VAL	2.7
1	B	1162	GLY	2.6
1	D	3108	ILE	2.5
1	D	3140	PHE	2.5
1	A	252	GLU	2.4
1	B	1157	SER	2.3
1	C	2165	VAL	2.3
1	D	3084	GLY	2.2
1	B	1030	GLU	2.2
1	D	3164	ALA	2.2
1	B	1160	PRO	2.2
1	C	2156	ASP	2.1
1	B	1164	ALA	2.1
1	C	2030	GLU	2.1
1	A	161	VAL	2.1
1	A	138	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.