Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2021 – 12:04 PM EST

PDB ID	:	1WV2
Title	:	Crystal structure of thiamine biosynthesis protein from Pseudomonas Aeruginosa
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-12-10
Resolution	:	2.90 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:

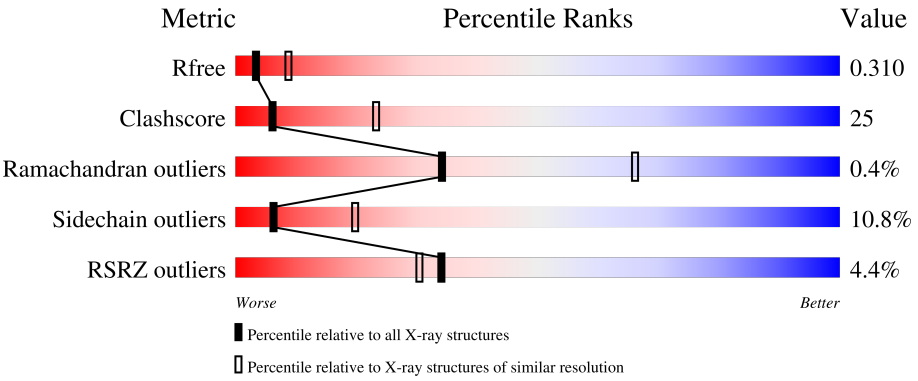
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	265	3% 51% 31% 5% 13%
1	B	265	5% 49% 31% · 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3384 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 Thiazole biosynthesis protein thiG.

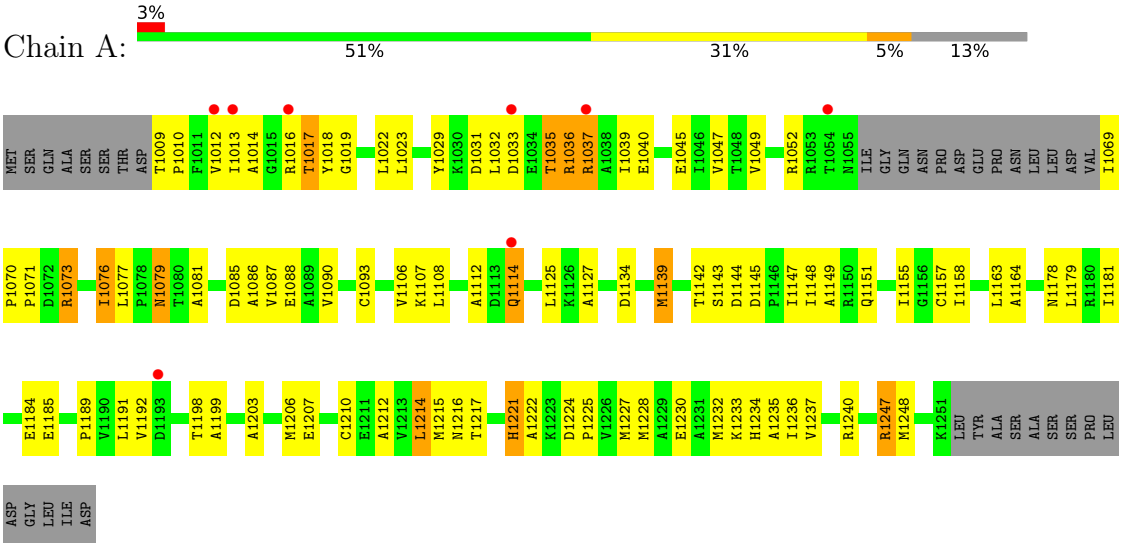
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1720	1086	301	320	13			
1	B	223	Total	C	N	O	S	0	0	0
			1664	1052	290	309	13			

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.

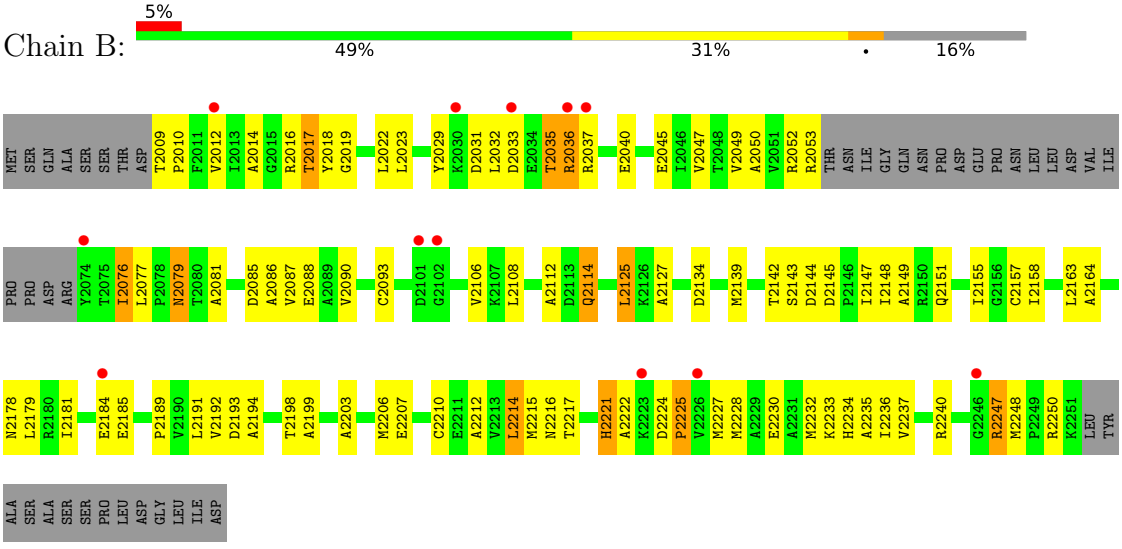
• Molecule 1: Thiazole biosynthesis protein thiG

Chain A:



• Molecule 1: Thiazole biosynthesis protein thiG

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	74.11Å 74.11Å 164.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.90 29.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.90) 98.1 (29.91-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.304 0.262 , 0.310	Depositor DCC
R_{free} test set	626 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3384	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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	0.41	0/1742	0.66	1/2363 (0.0%)
1	B	0.39	0/1684	0.65	1/2282 (0.0%)
All	All	0.40	0/3426	0.65	2/4645 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2139	MET	N-CA-C	-5.55	96.00	111.00
1	A	1139	MET	N-CA-C	-5.55	96.03	111.00

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	1720	0	1785	88	0
1	B	1664	0	1730	85	0
All	All	3384	0	3515	170	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 25.

All (170) 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:B:2049:VAL:HG12	1:B:2076:ILE:HD11	1.29	1.10
1:A:1049:VAL:HG12	1:A:1076:ILE:HD11	1.43	1.01
1:A:1016:ARG:HB3	1:A:1016:ARG:HH11	1.24	1.00
1:B:2016:ARG:HB3	1:B:2016:ARG:HH11	1.21	0.99
1:B:2079:ASN:HD21	1:B:2081:ALA:HB2	1.29	0.97
1:B:2036:ARG:HB3	1:B:2036:ARG:HH11	1.31	0.95
1:A:1079:ASN:HD21	1:A:1081:ALA:HB2	1.32	0.95
1:A:1036:ARG:HB3	1:A:1036:ARG:HH11	1.32	0.93
1:B:2093:CYS:SG	1:B:2106:VAL:HG11	2.12	0.89
1:A:1009:THR:HB	1:A:1010:PRO:HD2	1.56	0.86
1:B:2029:TYR:HB2	1:B:2035:THR:HG22	1.58	0.86
1:B:2031:ASP:O	1:B:2035:THR:HG23	1.75	0.85
1:A:1031:ASP:O	1:A:1035:THR:HG23	1.77	0.85
1:A:1029:TYR:HB2	1:A:1035:THR:HG22	1.60	0.84
1:B:2016:ARG:NH1	1:B:2016:ARG:HB3	1.91	0.84
1:A:1016:ARG:HB3	1:A:1016:ARG:NH1	1.93	0.83
1:A:1093:CYS:SG	1:A:1106:VAL:HG11	2.18	0.83
1:A:1148:ILE:HD12	1:A:1149:ALA:N	1.95	0.82
1:B:2012:VAL:HG12	1:B:2017:THR:HB	1.60	0.82
1:A:1052:ARG:NH1	1:A:1052:ARG:HB3	1.95	0.82
1:B:2052:ARG:HB3	1:B:2052:ARG:NH1	1.94	0.81
1:A:1039:ILE:HD11	1:A:1069:ILE:HG13	1.63	0.81
1:B:2148:ILE:HD12	1:B:2149:ALA:N	1.96	0.80
1:A:1012:VAL:HG12	1:A:1017:THR:HB	1.64	0.78
1:B:2049:VAL:CG1	1:B:2076:ILE:HD11	2.14	0.76
1:A:1148:ILE:HD12	1:A:1148:ILE:C	2.10	0.72
1:B:2181:ILE:O	1:B:2185:GLU:HG2	1.90	0.71
1:B:2012:VAL:CG1	1:B:2017:THR:HB	2.23	0.69
1:A:1145:ASP:OD1	1:A:1147:ILE:HG13	1.92	0.68
1:B:2145:ASP:OD1	1:B:2147:ILE:HG13	1.93	0.68
1:B:2029:TYR:CB	1:B:2035:THR:HG22	2.24	0.68
1:B:2009:THR:HB	1:B:2010:PRO:HD2	1.76	0.67
1:A:1247:ARG:HD3	1:A:1248:MET:O	1.94	0.67
1:A:1151:GLN:O	1:A:1155:ILE:HG23	1.96	0.66
1:A:1181:ILE:O	1:A:1185:GLU:HG2	1.94	0.66
1:A:1029:TYR:CB	1:A:1035:THR:HG22	2.25	0.66
1:A:1070:PRO:HB2	1:A:1073:ARG:HG3	1.78	0.66
1:A:1012:VAL:CG1	1:A:1017:THR:HB	2.26	0.65
1:B:2148:ILE:C	1:B:2148:ILE:HD12	2.17	0.64
1:B:2247:ARG:HD3	1:B:2248:MET:O	1.97	0.64
1:B:2022:LEU:HG	1:B:2022:LEU:O	1.98	0.63
1:B:2036:ARG:O	1:B:2040:GLU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2192:VAL:HG23	1:B:2210:CYS:SG	2.39	0.62
1:A:1036:ARG:O	1:A:1040:GLU:HB2	2.00	0.62
1:A:1112:ALA:CB	1:B:2147:ILE:HG21	2.31	0.61
1:B:2151:GLN:O	1:B:2155:ILE:HG23	2.01	0.60
1:B:2036:ARG:C	1:B:2036:ARG:HD2	2.22	0.60
1:A:1036:ARG:HD2	1:A:1036:ARG:C	2.23	0.60
1:B:2076:ILE:HD12	1:B:2077:LEU:N	2.17	0.59
1:A:1076:ILE:HD12	1:A:1077:LEU:N	2.18	0.59
1:B:2164:ALA:HB2	1:B:2192:VAL:CG1	2.32	0.58
1:A:1192:VAL:HG23	1:A:1210:CYS:SG	2.42	0.58
1:B:2217:THR:O	1:B:2221:HIS:HB2	2.03	0.58
1:A:1009:THR:HB	1:A:1010:PRO:CD	2.31	0.57
1:B:2022:LEU:HB2	1:B:2236:ILE:HG12	1.86	0.57
1:B:2086:ALA:HA	1:B:2127:ALA:HB2	1.86	0.57
1:B:2052:ARG:HB3	1:B:2052:ARG:HH11	1.68	0.57
1:A:1052:ARG:HH11	1:A:1052:ARG:HB3	1.67	0.57
1:B:2086:ALA:O	1:B:2090:VAL:HG23	2.06	0.56
1:B:2191:LEU:HG	1:B:2212:ALA:HB3	1.87	0.56
1:A:1158:ILE:O	1:A:1189:PRO:HD2	2.06	0.56
1:A:1191:LEU:HG	1:A:1212:ALA:HB3	1.88	0.56
1:A:1022:LEU:O	1:A:1022:LEU:HG	2.04	0.56
1:A:1206:MET:HE2	1:A:1240:ARG:HB2	1.87	0.56
1:B:2247:ARG:NH2	1:B:2250:ARG:HH12	2.03	0.56
1:A:1032:LEU:HD12	1:A:1032:LEU:N	2.21	0.56
1:B:2158:ILE:O	1:B:2189:PRO:HD2	2.04	0.56
1:B:2032:LEU:N	1:B:2032:LEU:HD12	2.21	0.56
1:A:1036:ARG:HB3	1:A:1036:ARG:NH1	2.14	0.55
1:A:1164:ALA:HB2	1:A:1192:VAL:CG1	2.35	0.55
1:B:2203:ALA:O	1:B:2207:GLU:HG3	2.05	0.55
1:A:1086:ALA:O	1:A:1090:VAL:HG23	2.06	0.55
1:B:2145:ASP:HB3	1:B:2148:ILE:HG13	1.88	0.55
1:B:2079:ASN:HD21	1:B:2081:ALA:CB	2.11	0.55
1:A:1039:ILE:CD1	1:A:1069:ILE:HG13	2.33	0.55
1:B:2036:ARG:HB3	1:B:2036:ARG:NH1	2.13	0.55
1:A:1086:ALA:HA	1:A:1127:ALA:HB2	1.89	0.55
1:A:1217:THR:O	1:A:1221:HIS:HB2	2.08	0.54
1:B:2036:ARG:HD3	1:B:2040:GLU:OE1	2.07	0.54
1:B:2076:ILE:HD12	1:B:2077:LEU:H	1.73	0.54
1:A:1203:ALA:O	1:A:1207:GLU:HG3	2.09	0.53
1:B:2164:ALA:HB2	1:B:2192:VAL:HG13	1.90	0.53
1:A:1036:ARG:HD3	1:A:1040:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2206:MET:HE2	1:B:2240:ARG:HB2	1.91	0.52
1:A:1164:ALA:HB2	1:A:1192:VAL:HG13	1.91	0.52
1:B:2142:THR:OG1	1:B:2143:SER:N	2.43	0.52
1:B:2016:ARG:CB	1:B:2016:ARG:HH11	2.08	0.52
1:B:2228:MET:O	1:B:2232:MET:HG2	2.10	0.52
1:A:1018:TYR:HB3	1:A:1045:GLU:OE1	2.10	0.52
1:A:1145:ASP:HB3	1:A:1148:ILE:HG13	1.92	0.52
1:A:1029:TYR:CG	1:A:1035:THR:HG22	2.46	0.51
1:B:2232:MET:HA	1:B:2235:ALA:HB3	1.92	0.51
1:A:1076:ILE:HD12	1:A:1077:LEU:H	1.75	0.51
1:A:1014:ALA:HB2	1:A:1158:ILE:HG21	1.92	0.51
1:B:2052:ARG:HB3	1:B:2052:ARG:CZ	2.40	0.51
1:A:1016:ARG:CB	1:A:1016:ARG:HH11	2.10	0.51
1:B:2029:TYR:CG	1:B:2035:THR:HG22	2.45	0.50
1:B:2163:LEU:HD12	1:B:2163:LEU:C	2.31	0.50
1:A:1019:GLY:H	1:A:1045:GLU:CD	2.15	0.50
1:A:1142:THR:OG1	1:A:1143:SER:N	2.43	0.50
1:A:1228:MET:O	1:A:1232:MET:HG2	2.12	0.50
1:B:2019:GLY:H	1:B:2045:GLU:CD	2.16	0.50
1:A:1049:VAL:CG1	1:A:1076:ILE:HD11	2.29	0.49
1:B:2145:ASP:HB3	1:B:2148:ILE:CG1	2.42	0.49
1:B:2009:THR:HB	1:B:2010:PRO:CD	2.42	0.49
1:B:2052:ARG:HH11	1:B:2052:ARG:CB	2.26	0.49
1:A:1052:ARG:CZ	1:A:1052:ARG:HB3	2.42	0.49
1:B:2050:ALA:CB	1:B:2053:ARG:HG2	2.43	0.49
1:A:1023:LEU:HD12	1:A:1023:LEU:N	2.27	0.49
1:A:1232:MET:HA	1:A:1235:ALA:HB3	1.95	0.48
1:B:2018:TYR:HB3	1:B:2045:GLU:OE1	2.14	0.48
1:B:2247:ARG:NH2	1:B:2250:ARG:NH1	2.60	0.48
1:A:1234:HIS:HA	1:A:1237:VAL:HG12	1.96	0.48
1:B:2222:ALA:O	1:B:2225:PRO:HD3	2.13	0.48
1:A:1052:ARG:HH11	1:A:1052:ARG:CB	2.26	0.48
1:B:2234:HIS:HA	1:B:2237:VAL:CG1	2.43	0.48
1:A:1163:LEU:HD12	1:A:1163:LEU:C	2.34	0.48
1:B:2023:LEU:HD12	1:B:2023:LEU:N	2.28	0.48
1:A:1222:ALA:O	1:A:1225:PRO:HD3	2.13	0.47
1:B:2079:ASN:ND2	1:B:2081:ALA:H	2.12	0.47
1:A:1079:ASN:HD21	1:A:1081:ALA:CB	2.15	0.47
1:B:2224:ASP:OD2	1:B:2227:MET:HB2	2.15	0.47
1:A:1148:ILE:CD1	1:A:1148:ILE:C	2.81	0.47
1:A:1234:HIS:HA	1:A:1237:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:LEU:HB2	1:A:1236:ILE:HG12	1.97	0.47
1:A:1224:ASP:OD2	1:A:1227:MET:HB2	2.16	0.46
1:A:1112:ALA:HB2	1:B:2147:ILE:HG21	1.96	0.46
1:B:2125:LEU:HA	1:B:2125:LEU:HD12	1.84	0.46
1:B:2234:HIS:HA	1:B:2237:VAL:HG12	1.97	0.46
1:A:1031:ASP:OD2	1:A:1033:ASP:HB2	2.16	0.45
1:A:1013:ILE:HG21	1:A:1139:MET:CE	2.47	0.45
1:B:2214:LEU:HD23	1:B:2215:MET:N	2.30	0.45
1:A:1232:MET:HE2	1:A:1232:MET:HB3	1.82	0.45
1:A:1145:ASP:HB3	1:A:1148:ILE:CG1	2.47	0.45
1:A:1079:ASN:ND2	1:A:1081:ALA:H	2.14	0.45
1:B:2085:ASP:HB2	1:B:2088:GLU:HG3	1.99	0.45
1:A:1085:ASP:HB2	1:A:1087:VAL:HG12	1.99	0.44
1:A:1214:LEU:HD23	1:A:1215:MET:N	2.31	0.44
1:A:1147:ILE:HG21	1:B:2112:ALA:CB	2.48	0.44
1:A:1023:LEU:CB	1:A:1214:LEU:HG	2.48	0.43
1:B:2031:ASP:OD2	1:B:2033:ASP:HB2	2.17	0.43
1:A:1230:GLU:O	1:A:1233:LYS:HB3	2.18	0.43
1:A:1013:ILE:HG21	1:A:1139:MET:HE1	2.01	0.42
1:A:1032:LEU:N	1:A:1032:LEU:CD1	2.82	0.42
1:A:1070:PRO:HA	1:A:1071:PRO:HD2	1.98	0.42
1:A:1114:GLN:CD	1:A:1114:GLN:N	2.73	0.42
1:B:2032:LEU:CD1	1:B:2032:LEU:N	2.82	0.42
1:A:1085:ASP:CB	1:A:1087:VAL:HG12	2.49	0.42
1:A:1199:ALA:HA	1:A:1232:MET:HE3	2.01	0.42
1:B:2085:ASP:HB2	1:B:2087:VAL:HG12	2.01	0.42
1:B:2050:ALA:HB3	1:B:2053:ARG:HG2	2.01	0.42
1:B:2230:GLU:O	1:B:2233:LYS:HB3	2.19	0.42
1:A:1085:ASP:HB2	1:A:1088:GLU:HG3	2.01	0.42
1:B:2085:ASP:CB	1:B:2087:VAL:HG12	2.50	0.42
1:A:1070:PRO:HB2	1:A:1073:ARG:CG	2.49	0.42
1:A:1069:ILE:HA	1:A:1070:PRO:HD3	1.79	0.42
1:B:2052:ARG:CB	1:B:2052:ARG:NH1	2.75	0.41
1:A:1052:ARG:NH1	1:A:1052:ARG:CB	2.76	0.41
1:B:2232:MET:HB3	1:B:2232:MET:HE2	1.84	0.41
1:B:2247:ARG:CZ	1:B:2250:ARG:NH1	2.83	0.41
1:B:2193:ASP:O	1:B:2194:ALA:HB3	2.20	0.41
1:B:2199:ALA:HA	1:B:2232:MET:HE3	2.02	0.41
1:B:2114:GLN:N	1:B:2114:GLN:CD	2.74	0.41
1:B:2144:ASP:O	1:B:2178:ASN:HB3	2.22	0.40
1:A:1037:ARG:HD3	1:A:1037:ARG:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2014:ALA:HB2	1:B:2158:ILE:HG21	2.04	0.40
1:A:1107:LYS:HA	1:A:1139:MET:O	2.22	0.40
1:A:1144:ASP:O	1:A:1178:ASN:HB3	2.22	0.40
1:B:2029:TYR:CD1	1:B:2035:THR:HG22	2.57	0.40
1:B:2012:VAL:HG12	1:B:2017:THR:CB	2.41	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	226/265 (85%)	206 (91%)	19 (8%)	1 (0%)	34	66
1	B	219/265 (83%)	198 (90%)	20 (9%)	1 (0%)	29	61
All	All	445/530 (84%)	404 (91%)	39 (9%)	2 (0%)	34	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1157	CYS
1	B	2157	CYS

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	180/210 (86%)	161 (89%)	19 (11%)	6 20
1	B	173/210 (82%)	154 (89%)	19 (11%)	6 19
All	All	353/420 (84%)	315 (89%)	38 (11%)	6 20

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1017	THR
1	A	1035	THR
1	A	1036	ARG
1	A	1037	ARG
1	A	1047	VAL
1	A	1073	ARG
1	A	1076	ILE
1	A	1079	ASN
1	A	1108	LEU
1	A	1114	GLN
1	A	1125	LEU
1	A	1134	ASP
1	A	1179	LEU
1	A	1184	GLU
1	A	1198	THR
1	A	1214	LEU
1	A	1216	ASN
1	A	1221	HIS
1	A	1247	ARG
1	B	2017	THR
1	B	2035	THR
1	B	2036	ARG
1	B	2037	ARG
1	B	2047	VAL
1	B	2076	ILE
1	B	2079	ASN
1	B	2108	LEU
1	B	2114	GLN
1	B	2125	LEU
1	B	2134	ASP
1	B	2179	LEU
1	B	2184	GLU
1	B	2198	THR
1	B	2214	LEU
1	B	2216	ASN

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Mol	Chain	Res	Type
1	B	2221	HIS
1	B	2225	PRO
1	B	2247	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1079	ASN
1	A	1130	GLN
1	A	1216	ASN
1	B	2079	ASN
1	B	2130	GLN
1	B	2216	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	230/265 (86%)	0.14	8 (3%)	44	38	24, 41, 77, 92	0
1	B	223/265 (84%)	0.35	12 (5%)	25	22	26, 53, 78, 96	0
All	All	453/530 (85%)	0.24	20 (4%)	34	30	24, 47, 78, 96	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2101	ASP	4.6
1	B	2102	GLY	3.6
1	A	1012	VAL	3.1
1	A	1037	ARG	3.1
1	B	2033	ASP	2.9
1	B	2226	VAL	2.9
1	A	1016	ARG	2.6
1	B	2246	GLY	2.5
1	B	2074	TYR	2.5
1	B	2037	ARG	2.5
1	B	2030	LYS	2.4
1	A	1193	ASP	2.3
1	B	2184	GLU	2.2
1	B	2012	VAL	2.2
1	B	2223	LYS	2.2
1	A	1114	GLN	2.2
1	A	1013	ILE	2.1
1	A	1033	ASP	2.1
1	B	2036	ARG	2.0
1	A	1054	THR	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.