



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:22 PM GMT

PDB ID : 1TEL  
Title : Crystal structure of a RubisCO-like protein from *Chlorobium tepidum*  
Authors : Fedorov, A.A.; Fedorov, E.V.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2004-05-25  
Resolution : 2.70 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

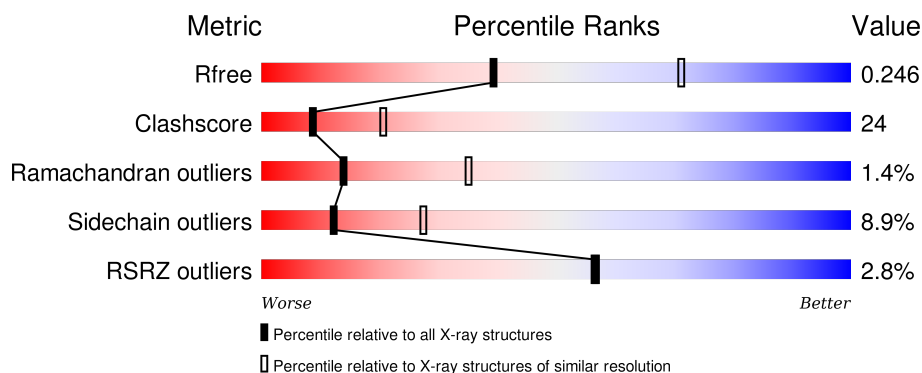
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	435	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>27%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	435	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>6%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6651 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 ribulose biphosphate carboxylase, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3286	2098	552	616	20			
1	B	428	Total	C	N	O	S	0	0	0
			3318	2116	558	624	20			

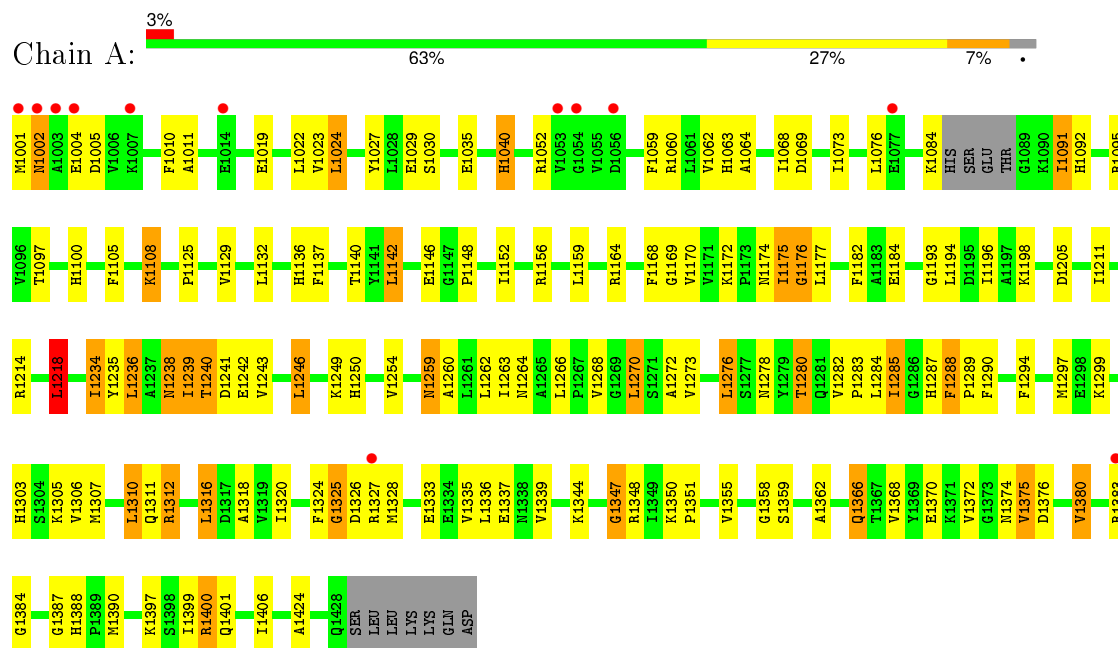
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total	O	0	0
			24	24		
2	B	23	Total	O	0	0
			23	23		

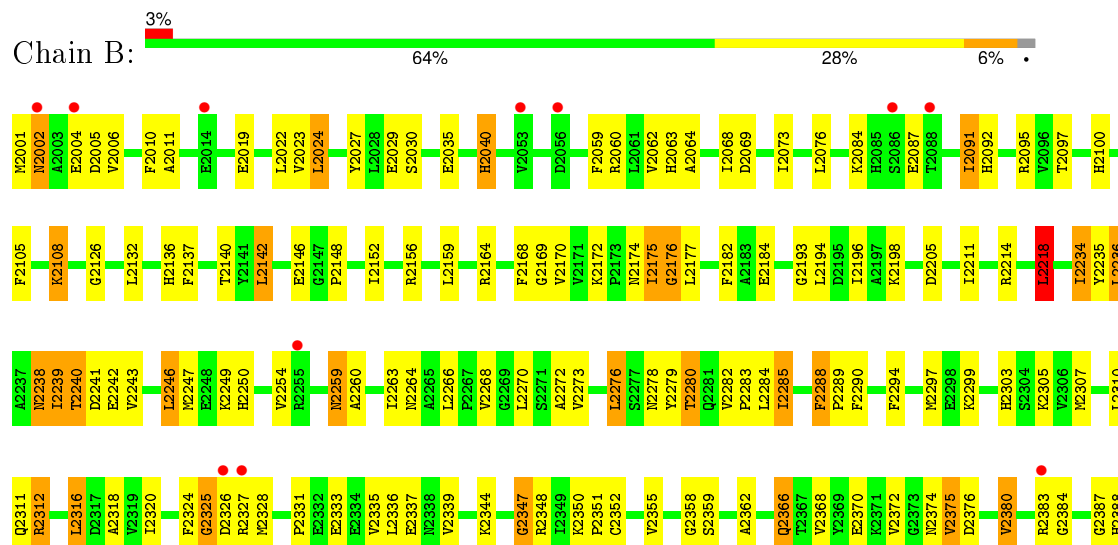
### 3 Residue-property plots [i](#)

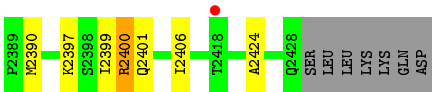
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ribulose biphosphate carboxylase, large subunit



- Molecule 1: ribulose biphosphate carboxylase, large subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.11Å 77.71Å 88.76Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 19.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.70) 99.6 (19.91-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.01 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.209 , 0.248 0.208 , 0.246	Depositor DCC
$R_{free}$ test set	1199 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 24732 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.43	0/3363	0.69	1/4559 (0.0%)
1	B	0.43	0/3397	0.69	1/4607 (0.0%)
All	All	0.43	0/6760	0.69	2/9166 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	2218	LEU	CA-CB-CG	-5.22	103.30	115.30
1	A	1218	LEU	CA-CB-CG	-5.10	103.58	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3286	0	3242	161	0
1	B	3318	0	3268	162	0
2	A	24	0	0	1	0
2	B	23	0	0	0	0
All	All	6651	0	6510	309	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 24.

All (309) 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:2238:ASN:HD21	1:B:2240:THR:HG23	1.10	1.08
1:A:1238:ASN:HD21	1:A:1240:THR:HG23	1.07	1.05
1:B:2238:ASN:HD21	1:B:2240:THR:CG2	1.72	1.01
1:A:1076:LEU:HD12	1:A:1091:ILE:HD11	1.45	0.99
1:A:1238:ASN:HD21	1:A:1240:THR:CG2	1.74	0.98
1:A:1159:LEU:HD21	1:A:1234:ILE:HG22	1.45	0.97
1:B:2374:ASN:HD22	1:B:2376:ASP:H	1.15	0.95
1:B:2259:ASN:HD22	1:B:2259:ASN:H	1.16	0.93
1:A:1259:ASN:HD22	1:A:1259:ASN:H	1.17	0.93
1:B:2159:LEU:HD21	1:B:2234:ILE:HG22	1.51	0.93
1:A:1374:ASN:HD22	1:A:1376:ASP:H	1.16	0.92
1:B:2235:TYR:H	1:B:2259:ASN:HD21	0.96	0.91
1:A:1235:TYR:H	1:A:1259:ASN:HD21	0.94	0.91
1:A:1235:TYR:N	1:A:1259:ASN:HD21	1.68	0.90
1:B:2235:TYR:N	1:B:2259:ASN:HD21	1.70	0.90
1:B:2280:THR:HG21	1:B:2284:LEU:HD13	1.54	0.89
1:A:1397:LYS:O	1:A:1401:GLN:HG3	1.73	0.88
1:A:1280:THR:HG21	1:A:1284:LEU:HD13	1.55	0.87
1:B:2383:ARG:NH1	1:B:2384:GLY:H	1.73	0.87
1:A:1383:ARG:NH1	1:A:1384:GLY:H	1.72	0.86
1:B:2152:ILE:O	1:B:2156:ARG:HG3	1.76	0.86
1:B:2196:ILE:HG12	1:B:2234:ILE:CG2	2.07	0.84
1:A:1152:ILE:O	1:A:1156:ARG:HG3	1.78	0.83
1:A:1196:ILE:HG12	1:A:1234:ILE:CG2	2.08	0.83
1:B:2235:TYR:H	1:B:2259:ASN:ND2	1.77	0.82
1:B:2196:ILE:HG12	1:B:2234:ILE:HG23	1.61	0.82
1:A:1196:ILE:HG12	1:A:1234:ILE:HG23	1.59	0.82
1:B:2397:LYS:O	1:B:2401:GLN:HG3	1.79	0.81
1:A:1235:TYR:H	1:A:1259:ASN:ND2	1.76	0.81
1:A:1238:ASN:ND2	1:A:1240:THR:HG23	1.92	0.80
1:B:2076:LEU:HD12	1:B:2091:ILE:HD11	1.66	0.77
1:A:1259:ASN:H	1:A:1259:ASN:ND2	1.82	0.77
1:B:2259:ASN:H	1:B:2259:ASN:ND2	1.83	0.77
1:B:2234:ILE:HD11	1:B:2260:ALA:HB3	1.66	0.76
1:B:2238:ASN:ND2	1:B:2240:THR:HG23	1.94	0.76
1:A:1084:LYS:NZ	1:B:2331:PRO:HA	2.00	0.76
1:A:1234:ILE:HD11	1:A:1260:ALA:HB3	1.66	0.76
1:B:2087:GLU:HG3	1:B:2126:GLY:HA2	1.66	0.76
1:B:2002:ASN:HD22	1:B:2002:ASN:N	1.84	0.75
1:A:1002:ASN:HD22	1:A:1002:ASN:N	1.83	0.75
1:A:1193:GLY:HA3	1:A:1400:ARG:HD2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1388:HIS:HD2	1:A:1390:MET:H	1.38	0.72
1:B:2239:ILE:HG13	1:B:2249:LYS:HB3	1.71	0.72
1:A:1239:ILE:HG13	1:A:1249:LYS:HB3	1.71	0.71
1:A:1266:LEU:HD11	1:A:1307:MET:HE2	1.70	0.71
1:B:2388:HIS:HD2	1:B:2390:MET:H	1.37	0.71
1:A:1001:MET:C	1:A:1002:ASN:HD22	1.95	0.70
1:B:2234:ILE:C	1:B:2234:ILE:HD13	2.11	0.70
1:A:1234:ILE:C	1:A:1234:ILE:HD13	2.12	0.70
1:B:2234:ILE:HG12	1:B:2259:ASN:ND2	2.06	0.70
1:B:2266:LEU:HD11	1:B:2307:MET:HE2	1.73	0.69
1:B:2193:GLY:HA3	1:B:2400:ARG:HD2	1.73	0.69
1:B:2001:MET:C	1:B:2002:ASN:HD22	1.95	0.69
1:A:1234:ILE:HG12	1:A:1259:ASN:ND2	2.08	0.68
1:B:2282:VAL:HG13	1:B:2283:PRO:HD2	1.75	0.68
1:A:1159:LEU:HD21	1:A:1234:ILE:CG2	2.24	0.67
1:B:2388:HIS:CD2	1:B:2390:MET:H	2.12	0.67
1:A:1388:HIS:CD2	1:A:1390:MET:H	2.12	0.66
1:A:1282:VAL:HG13	1:A:1283:PRO:HD2	1.75	0.66
1:B:2268:VAL:HG12	1:B:2272:ALA:HB3	1.77	0.66
1:A:1400:ARG:CG	1:A:1400:ARG:HH21	2.09	0.65
1:A:1156:ARG:NH2	1:A:1164:ARG:O	2.30	0.65
1:A:1170:VAL:O	1:A:1172:LYS:HD3	1.95	0.65
1:B:2170:VAL:O	1:B:2172:LYS:HD3	1.96	0.64
1:A:1268:VAL:HG12	1:A:1272:ALA:HB3	1.79	0.64
1:A:1374:ASN:ND2	1:A:1376:ASP:H	1.93	0.64
1:B:2238:ASN:ND2	1:B:2240:THR:CG2	2.56	0.64
1:A:1240:THR:HG21	1:A:1264:ASN:ND2	2.12	0.64
1:B:2169:GLY:HA3	1:B:2194:LEU:HD21	1.80	0.64
1:B:2400:ARG:HH21	1:B:2400:ARG:CG	2.09	0.64
1:A:1238:ASN:ND2	1:A:1240:THR:CG2	2.57	0.64
1:B:2374:ASN:ND2	1:B:2376:ASP:H	1.92	0.63
1:A:1260:ALA:HA	1:A:1282:VAL:CG1	2.29	0.63
1:B:2366:GLN:O	1:B:2370:GLU:HG3	1.99	0.63
1:B:2260:ALA:HA	1:B:2282:VAL:CG1	2.28	0.62
1:B:2156:ARG:NH2	1:B:2164:ARG:O	2.31	0.62
1:B:2240:THR:HG21	1:B:2264:ASN:ND2	2.15	0.62
1:A:1366:GLN:O	1:A:1370:GLU:HG3	1.98	0.61
1:A:1169:GLY:HA3	1:A:1194:LEU:HD21	1.81	0.61
1:A:1062:VAL:HG13	2:A:3046:HOH:O	2.00	0.61
1:A:1266:LEU:HD11	1:A:1307:MET:CE	2.30	0.61
1:A:1146:GLU:HG2	1:A:1278:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:LYS:HZ2	1:B:2331:PRO:HA	1.66	0.60
1:B:2333:GLU:O	1:B:2337:GLU:HG3	2.02	0.60
1:A:1148:PRO:HG2	1:A:1350:LYS:HB2	1.84	0.60
1:B:2366:GLN:HG2	1:B:2406:ILE:HG12	1.84	0.60
1:B:2148:PRO:HG2	1:B:2350:LYS:HB2	1.84	0.59
1:A:1333:GLU:O	1:A:1337:GLU:HG3	2.02	0.59
1:B:2146:GLU:HG2	1:B:2278:ASN:OD1	2.02	0.59
1:A:1240:THR:HG22	1:A:1263:ILE:HA	1.85	0.59
1:A:1366:GLN:HG2	1:A:1406:ILE:HG12	1.84	0.59
1:A:1002:ASN:N	1:A:1002:ASN:ND2	2.50	0.59
1:B:2073:ILE:HD11	1:B:2095:ARG:HG2	1.84	0.59
1:B:2266:LEU:HD11	1:B:2307:MET:CE	2.33	0.58
1:A:1259:ASN:N	1:A:1259:ASN:HD22	1.85	0.58
1:B:2002:ASN:ND2	1:B:2002:ASN:N	2.50	0.57
1:A:1059:PHE:CG	1:B:2176:GLY:HA3	2.39	0.57
1:B:2159:LEU:HD21	1:B:2234:ILE:CG2	2.29	0.57
1:A:1164:ARG:HA	1:A:1375:VAL:HG21	1.87	0.57
1:B:2164:ARG:HA	1:B:2375:VAL:HG21	1.85	0.57
1:A:1263:ILE:HD11	1:A:1273:VAL:HG13	1.87	0.57
1:B:2019:GLU:OE1	1:B:2140:THR:HG23	2.05	0.57
1:B:2027:TYR:CE2	1:B:2299:LYS:HB3	2.39	0.57
1:B:2175:ILE:O	1:B:2177:LEU:N	2.38	0.56
1:A:1400:ARG:CB	1:A:1400:ARG:HH21	2.18	0.56
1:A:1176:GLY:HA3	1:B:2059:PHE:CG	2.41	0.56
1:A:1243:VAL:HA	1:A:1246:LEU:HD22	1.87	0.56
1:B:2241:ASP:OD1	1:B:2249:LYS:HE3	2.05	0.56
1:A:1175:ILE:O	1:A:1177:LEU:N	2.38	0.56
1:B:2400:ARG:HH21	1:B:2400:ARG:CB	2.19	0.56
1:A:1211:ILE:HD13	1:A:1239:ILE:HD12	1.86	0.55
1:A:1238:ASN:HD22	1:A:1239:ILE:N	2.05	0.55
1:B:2240:THR:HG22	1:B:2263:ILE:HA	1.88	0.55
1:B:2312:ARG:HD3	1:B:2350:LYS:O	2.06	0.55
1:A:1239:ILE:HG13	1:A:1249:LYS:CB	2.36	0.55
1:B:2368:VAL:O	1:B:2372:VAL:HG23	2.07	0.55
1:A:1193:GLY:CA	1:A:1400:ARG:HD2	2.36	0.55
1:B:2327:ARG:HD2	1:B:2359:SER:HB2	1.89	0.55
1:B:2236:LEU:HD21	1:B:2285:ILE:CG2	2.37	0.55
1:A:1073:ILE:HD11	1:A:1095:ARG:HG2	1.89	0.55
1:A:1328:MET:HG3	1:A:1358:GLY:HA3	1.89	0.55
1:B:2022:LEU:HD22	1:B:2105:PHE:HZ	1.71	0.55
1:B:2091:ILE:HD12	1:B:2092:HIS:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:ARG:NH2	1:A:1400:ARG:HG2	2.22	0.55
1:B:2366:GLN:HG2	1:B:2406:ILE:CG1	2.37	0.55
1:B:2243:VAL:HA	1:B:2246:LEU:HD22	1.88	0.55
1:B:2001:MET:HB2	1:B:2040:HIS:ND1	2.22	0.54
1:B:2214:ARG:HG2	1:B:2218:LEU:HD13	1.89	0.54
1:B:2239:ILE:HG13	1:B:2249:LYS:CB	2.37	0.54
1:B:2400:ARG:NH2	1:B:2400:ARG:HG2	2.21	0.54
1:B:2205:ASP:HB2	1:B:2211:ILE:CD1	2.38	0.54
1:B:2263:ILE:HD12	1:B:2273:VAL:HG22	1.90	0.54
1:B:2211:ILE:HD13	1:B:2239:ILE:HD12	1.89	0.54
1:B:2193:GLY:O	1:B:2400:ARG:HD2	2.08	0.54
1:A:1366:GLN:HG2	1:A:1406:ILE:CG1	2.38	0.54
1:A:1027:TYR:CE2	1:A:1299:LYS:HB3	2.43	0.54
1:B:2211:ILE:HG21	1:B:2239:ILE:HD11	1.90	0.53
1:A:1211:ILE:HG21	1:A:1239:ILE:HD11	1.90	0.53
1:A:1091:ILE:HD12	1:A:1092:HIS:N	2.23	0.53
1:A:1214:ARG:HG2	1:A:1218:LEU:HD13	1.90	0.53
1:B:2238:ASN:C	1:B:2238:ASN:HD22	2.11	0.53
1:B:2263:ILE:HD11	1:B:2273:VAL:HG13	1.89	0.53
1:A:1241:ASP:OD1	1:A:1249:LYS:HE3	2.09	0.53
1:B:2238:ASN:HD22	1:B:2239:ILE:N	2.05	0.53
1:A:1400:ARG:HB3	1:A:1400:ARG:HH21	1.74	0.53
1:B:2400:ARG:HH21	1:B:2400:ARG:HG2	1.73	0.53
1:B:2030:SER:O	1:B:2091:ILE:HA	2.08	0.53
1:B:2087:GLU:HG3	1:B:2126:GLY:CA	2.37	0.53
1:A:1001:MET:HB2	1:A:1040:HIS:ND1	2.23	0.53
1:B:2282:VAL:HG13	1:B:2283:PRO:CD	2.38	0.53
1:B:2324:PHE:O	1:B:2325:GLY:O	2.27	0.53
1:A:1030:SER:O	1:A:1091:ILE:HA	2.10	0.52
1:A:1019:GLU:OE1	1:A:1140:THR:HG23	2.08	0.52
1:A:1205:ASP:HB2	1:A:1211:ILE:CD1	2.40	0.52
1:B:2193:GLY:CA	1:B:2400:ARG:HD2	2.39	0.52
1:A:1312:ARG:HD3	1:A:1350:LYS:O	2.09	0.52
1:A:1059:PHE:CD2	1:B:2176:GLY:HA3	2.45	0.52
1:B:2241:ASP:OD2	1:B:2242:GLU:N	2.39	0.52
1:A:1263:ILE:HD12	1:A:1273:VAL:HG22	1.90	0.52
1:A:1236:LEU:HD21	1:A:1285:ILE:CG2	2.39	0.52
1:A:1282:VAL:HG13	1:A:1283:PRO:CD	2.39	0.52
1:B:2182:PHE:HD1	1:B:2218:LEU:HD11	1.75	0.52
1:B:2347:GLY:O	1:B:2348:ARG:HB2	2.09	0.52
1:A:1238:ASN:C	1:A:1238:ASN:HD22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:GLY:O	1:A:1348:ARG:HB2	2.08	0.51
1:B:2307:MET:O	1:B:2311:GLN:HG3	2.10	0.51
1:A:1400:ARG:HG2	1:A:1400:ARG:HH21	1.76	0.51
1:A:1234:ILE:HA	1:A:1259:ASN:OD1	2.11	0.51
1:A:1383:ARG:HH11	1:A:1384:GLY:H	1.58	0.51
1:B:2276:LEU:HD13	1:B:2284:LEU:HD11	1.91	0.51
1:B:2091:ILE:HD12	1:B:2091:ILE:C	2.31	0.51
1:A:1327:ARG:HD2	1:A:1359:SER:HB2	1.92	0.51
1:B:2259:ASN:N	1:B:2259:ASN:ND2	2.49	0.50
1:A:1193:GLY:O	1:A:1400:ARG:HD2	2.11	0.50
1:A:1241:ASP:OD2	1:A:1242:GLU:N	2.39	0.50
1:A:1266:LEU:HD21	1:A:1307:MET:HE2	1.94	0.50
1:B:2328:MET:HG3	1:B:2358:GLY:HA3	1.93	0.50
1:A:1259:ASN:N	1:A:1259:ASN:ND2	2.48	0.50
1:A:1368:VAL:O	1:A:1372:VAL:HG23	2.10	0.50
1:A:1276:LEU:HD13	1:A:1284:LEU:HD11	1.92	0.50
1:A:1182:PHE:HD1	1:A:1218:LEU:HD11	1.76	0.50
1:A:1241:ASP:OD2	1:B:2108:LYS:HG2	2.12	0.50
1:A:1307:MET:O	1:A:1311:GLN:HG3	2.12	0.50
1:B:2250:HIS:CD2	1:B:2280:THR:HG22	2.48	0.49
1:B:2400:ARG:HB3	1:B:2400:ARG:HH21	1.77	0.49
1:B:2023:VAL:HB	1:B:2136:HIS:HB2	1.93	0.49
1:A:1022:LEU:HD22	1:A:1105:PHE:HZ	1.76	0.49
1:B:2238:ASN:ND2	1:B:2238:ASN:C	2.66	0.49
1:A:1175:ILE:HG21	1:B:2063:HIS:HB3	1.93	0.49
1:A:1076:LEU:HB2	1:A:1091:ILE:CG1	2.42	0.49
1:B:2182:PHE:CD1	1:B:2218:LEU:HD11	2.47	0.49
1:A:1250:HIS:CD2	1:A:1280:THR:HG22	2.48	0.49
1:B:2234:ILE:HA	1:B:2259:ASN:OD1	2.11	0.49
1:B:2250:HIS:HD2	1:B:2280:THR:HG22	1.78	0.49
1:A:1076:LEU:CD1	1:A:1091:ILE:HD11	2.30	0.49
1:A:1280:THR:CG2	1:A:1284:LEU:HD13	2.38	0.49
1:B:2335:VAL:O	1:B:2339:VAL:HG23	2.13	0.48
1:A:1335:VAL:O	1:A:1339:VAL:HG23	2.13	0.48
1:A:1312:ARG:NH1	1:A:1351:PRO:HA	2.28	0.48
1:A:1320:ILE:HA	1:A:1355:VAL:HB	1.95	0.48
1:A:1297:MET:HG3	1:B:2297:MET:HG3	1.93	0.48
1:B:2362:ALA:HB2	1:B:2399:ILE:HD13	1.95	0.48
1:A:1312:ARG:NH2	1:A:1344:LYS:O	2.39	0.48
1:A:1294:PHE:HB3	1:B:2294:PHE:HB3	1.95	0.48
1:A:1182:PHE:CD1	1:A:1218:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:GLU:HG3	1:A:1129:VAL:HB	1.95	0.48
1:A:1238:ASN:C	1:A:1238:ASN:ND2	2.66	0.48
1:B:2250:HIS:O	1:B:2254:VAL:HG23	2.14	0.48
1:B:2001:MET:N	1:B:2040:HIS:HE1	2.12	0.48
1:A:1023:VAL:HB	1:A:1136:HIS:HB2	1.96	0.48
1:B:2196:ILE:HG12	1:B:2234:ILE:HG21	1.93	0.47
1:A:1324:PHE:O	1:A:1325:GLY:O	2.31	0.47
1:B:2060:ARG:HA	1:B:2064:ALA:HB2	1.96	0.47
1:A:1091:ILE:C	1:A:1091:ILE:HD12	2.35	0.47
1:A:1211:ILE:HD13	1:A:1239:ILE:CD1	2.44	0.47
1:A:1250:HIS:HD2	1:A:1280:THR:HG22	1.79	0.47
1:A:1001:MET:N	1:A:1040:HIS:HE1	2.13	0.47
1:A:1236:LEU:HD21	1:A:1285:ILE:HG23	1.97	0.47
1:B:2168:PHE:HB2	1:B:2380:VAL:HG13	1.97	0.47
1:B:2312:ARG:NH1	1:B:2351:PRO:HA	2.30	0.47
1:A:1243:VAL:HG11	1:B:2243:VAL:HG11	1.97	0.47
1:B:2320:ILE:HA	1:B:2355:VAL:HB	1.96	0.47
1:A:1011:ALA:O	1:A:1068:ILE:HA	2.15	0.46
1:A:1234:ILE:HD13	1:A:1235:TYR:N	2.31	0.46
1:B:2236:LEU:HD21	1:B:2285:ILE:HG23	1.97	0.46
1:B:2234:ILE:HD13	1:B:2235:TYR:N	2.30	0.46
1:A:1303:HIS:ND1	1:A:1305:LYS:HG2	2.31	0.46
1:A:1168:PHE:HB2	1:A:1380:VAL:HG13	1.98	0.46
1:B:2238:ASN:ND2	1:B:2240:THR:H	2.14	0.46
1:B:2011:ALA:O	1:B:2068:ILE:HA	2.15	0.46
1:B:2288:PHE:N	1:B:2289:PRO:HD3	2.31	0.46
1:A:1238:ASN:ND2	1:A:1240:THR:H	2.13	0.46
1:A:1328:MET:CG	1:A:1358:GLY:HA3	2.46	0.46
1:A:1239:ILE:O	1:A:1239:ILE:HG23	2.16	0.45
1:A:1211:ILE:HD12	1:A:1249:LYS:HD2	1.97	0.45
1:B:2383:ARG:HH11	1:B:2384:GLY:H	1.58	0.45
1:B:2266:LEU:HD21	1:B:2307:MET:HE2	1.98	0.45
1:B:2214:ARG:HG2	1:B:2218:LEU:CD1	2.45	0.45
1:A:1214:ARG:HG2	1:A:1218:LEU:CD1	2.47	0.45
1:B:2239:ILE:O	1:B:2239:ILE:HG23	2.16	0.45
1:B:2328:MET:CG	1:B:2358:GLY:HA3	2.46	0.45
1:A:1060:ARG:HA	1:A:1064:ALA:HB2	1.97	0.45
1:B:2303:HIS:ND1	1:B:2305:LYS:HG2	2.30	0.45
1:A:1362:ALA:HB2	1:A:1399:ILE:HD13	1.97	0.45
1:B:2002:ASN:O	1:B:2005:ASP:N	2.50	0.45
1:B:2312:ARG:NH2	1:B:2344:LYS:O	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:PHE:N	1:A:1289:PRO:HD3	2.32	0.45
1:A:1250:HIS:O	1:A:1254:VAL:HG23	2.17	0.44
1:B:2156:ARG:NH1	1:B:2376:ASP:OD2	2.51	0.44
1:A:1234:ILE:HD11	1:A:1260:ALA:CB	2.43	0.44
1:A:1156:ARG:NH1	1:A:1376:ASP:OD2	2.51	0.44
1:B:2211:ILE:HD13	1:B:2239:ILE:CD1	2.47	0.44
1:A:1084:LYS:HZ1	1:B:2331:PRO:HA	1.78	0.44
1:A:1285:ILE:HB	1:A:1318:ALA:HB3	1.99	0.44
1:B:2168:PHE:CB	1:B:2380:VAL:HG13	2.47	0.44
1:B:2280:THR:HB	1:B:2282:VAL:O	2.17	0.44
1:B:2366:GLN:HA	1:B:2406:ILE:HD11	2.00	0.44
1:A:1108:LYS:HG2	1:B:2241:ASP:OD2	2.18	0.44
1:B:2289:PRO:O	1:B:2290:PHE:HB3	2.18	0.43
1:A:1259:ASN:O	1:A:1282:VAL:HG13	2.18	0.43
1:A:1289:PRO:O	1:A:1290:PHE:HB3	2.18	0.43
1:A:1306:VAL:O	1:A:1310:LEU:HD22	2.18	0.43
1:B:2010:PHE:CZ	1:B:2035:GLU:HG2	2.53	0.43
1:A:1010:PHE:CZ	1:A:1035:GLU:HG2	2.54	0.43
1:B:2211:ILE:HD12	1:B:2249:LYS:HD2	2.00	0.43
1:A:1390:MET:CE	1:A:1424:ALA:HB2	2.49	0.43
1:B:2285:ILE:HB	1:B:2318:ALA:HB3	2.00	0.43
1:A:1137:PHE:HB3	1:A:1142:LEU:HD13	2.01	0.43
1:B:2196:ILE:HG23	1:B:2234:ILE:HD12	2.01	0.43
1:B:2312:ARG:HG3	1:B:2352:CYS:SG	2.58	0.43
1:A:1280:THR:HB	1:A:1282:VAL:O	2.18	0.43
1:A:1002:ASN:O	1:A:1005:ASP:N	2.52	0.42
1:A:1168:PHE:CB	1:A:1380:VAL:HG13	2.48	0.42
1:B:2068:ILE:HD11	1:B:2097:THR:HG22	2.01	0.42
1:B:2024:LEU:HD21	1:B:2100:HIS:HB2	2.00	0.42
1:B:2029:GLU:HA	1:B:2092:HIS:O	2.19	0.42
1:A:1311:GLN:HB3	1:A:1316:LEU:HD23	2.01	0.42
1:B:2062:VAL:HG22	1:B:2063:HIS:CD2	2.55	0.42
1:B:2084:LYS:HE3	1:B:2084:LYS:HB2	1.81	0.42
1:A:1068:ILE:HD11	1:A:1097:THR:HG22	2.00	0.42
1:B:2205:ASP:HB2	1:B:2211:ILE:HD12	2.01	0.42
1:A:1196:ILE:HG23	1:A:1234:ILE:HD12	2.02	0.42
1:A:1196:ILE:HG12	1:A:1234:ILE:HG21	1.96	0.42
1:A:1062:VAL:HG22	1:A:1063:HIS:CD2	2.54	0.42
1:A:1052:ARG:HD3	1:B:2177:LEU:HD21	2.02	0.41
1:B:2280:THR:CG2	1:B:2284:LEU:HD13	2.37	0.41
1:B:2311:GLN:HB3	1:B:2316:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:ILE:O	1:A:1069:ASP:HB2	2.21	0.41
1:B:2238:ASN:HD21	1:B:2240:THR:HG22	1.75	0.41
1:B:2383:ARG:HH12	1:B:2387:GLY:HA3	1.85	0.41
1:B:2068:ILE:O	1:B:2069:ASP:HB2	2.21	0.41
1:B:2137:PHE:HB3	1:B:2142:LEU:HD13	2.02	0.41
1:A:1024:LEU:HD21	1:A:1100:HIS:HB2	2.02	0.41
1:B:2214:ARG:O	1:B:2218:LEU:HD12	2.21	0.41
1:A:1214:ARG:O	1:A:1218:LEU:HD12	2.21	0.41
1:A:1287:HIS:CD2	1:A:1289:PRO:HD3	2.56	0.41
1:A:1383:ARG:HH12	1:A:1387:GLY:HA3	1.85	0.41
1:A:1076:LEU:HB2	1:A:1091:ILE:HG13	2.03	0.41
1:B:2390:MET:CE	1:B:2424:ALA:HB2	2.50	0.41
1:A:1262:LEU:HD12	1:A:1285:ILE:O	2.21	0.41
1:A:1176:GLY:HA3	1:B:2059:PHE:CD2	2.56	0.41
1:B:2247:MET:HG2	1:B:2279:TYR:CD2	2.55	0.40
1:A:1146:GLU:CD	1:A:1146:GLU:H	2.24	0.40
1:B:2022:LEU:HD22	1:B:2105:PHE:CZ	2.54	0.40
1:B:2259:ASN:HD22	1:B:2259:ASN:N	1.86	0.40
1:B:2259:ASN:O	1:B:2282:VAL:HG13	2.21	0.40
1:B:2005:ASP:O	1:B:2006:VAL:C	2.60	0.40
1:B:2194:LEU:HD12	1:B:2194:LEU:HA	1.93	0.40
1:A:1270:LEU:HD21	1:A:1307:MET:CE	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	420/435 (97%)	383 (91%)	31 (7%)	6 (1%)	14	35
1	B	426/435 (98%)	388 (91%)	32 (8%)	6 (1%)	14	35
All	All	846/870 (97%)	771 (91%)	63 (7%)	12 (1%)	14	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1175	ILE
1	A	1176	GLY
1	A	1326	ASP
1	B	2175	ILE
1	B	2176	GLY
1	B	2326	ASP
1	A	1325	GLY
1	A	1347	GLY
1	B	2325	GLY
1	B	2347	GLY
1	A	1288	PHE
1	B	2288	PHE

### 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	350/361 (97%)	318 (91%)	32 (9%)	12	26
1	B	354/361 (98%)	323 (91%)	31 (9%)	12	28
All	All	704/722 (98%)	641 (91%)	63 (9%)	12	27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	ASN
1	A	1004	GLU
1	A	1024	LEU
1	A	1040	HIS
1	A	1091	ILE
1	A	1108	LYS
1	A	1125	PRO
1	A	1132	LEU
1	A	1142	LEU
1	A	1174	ASN
1	A	1184	GLU

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Mol	Chain	Res	Type
1	A	1198	LYS
1	A	1218	LEU
1	A	1234	ILE
1	A	1236	LEU
1	A	1238	ASN
1	A	1239	ILE
1	A	1240	THR
1	A	1246	LEU
1	A	1259	ASN
1	A	1270	LEU
1	A	1276	LEU
1	A	1280	THR
1	A	1285	ILE
1	A	1310	LEU
1	A	1312	ARG
1	A	1316	LEU
1	A	1336	LEU
1	A	1366	GLN
1	A	1375	VAL
1	A	1380	VAL
1	A	1400	ARG
1	B	2002	ASN
1	B	2004	GLU
1	B	2024	LEU
1	B	2040	HIS
1	B	2091	ILE
1	B	2108	LYS
1	B	2132	LEU
1	B	2142	LEU
1	B	2174	ASN
1	B	2184	GLU
1	B	2198	LYS
1	B	2218	LEU
1	B	2234	ILE
1	B	2236	LEU
1	B	2238	ASN
1	B	2239	ILE
1	B	2240	THR
1	B	2246	LEU
1	B	2259	ASN
1	B	2270	LEU
1	B	2276	LEU

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Mol	Chain	Res	Type
1	B	2280	THR
1	B	2285	ILE
1	B	2310	LEU
1	B	2312	ARG
1	B	2316	LEU
1	B	2336	LEU
1	B	2366	GLN
1	B	2375	VAL
1	B	2380	VAL
1	B	2400	ARG

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	1002	ASN
1	A	1049	GLN
1	A	1078	GLN
1	A	1160	ASN
1	A	1238	ASN
1	A	1259	ASN
1	A	1281	GLN
1	A	1287	HIS
1	A	1338	ASN
1	A	1366	GLN
1	A	1374	ASN
1	A	1388	HIS
1	B	2002	ASN
1	B	2049	GLN
1	B	2078	GLN
1	B	2160	ASN
1	B	2217	HIS
1	B	2238	ASN
1	B	2259	ASN
1	B	2281	GLN
1	B	2287	HIS
1	B	2338	ASN
1	B	2366	GLN
1	B	2374	ASN
1	B	2388	HIS

### 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	424/435 (97%)	-0.22	12 (2%) 56 57	5, 16, 34, 55	0
1	B	428/435 (98%)	-0.20	12 (2%) 56 57	4, 16, 35, 53	0
All	All	852/870 (97%)	-0.21	24 (2%) 56 57	4, 16, 35, 55	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2053	VAL	4.1
1	A	1002	ASN	3.9
1	A	1054	GLY	3.8
1	B	2327	ARG	3.6
1	B	2004	GLU	3.5
1	A	1056	ASP	3.4
1	B	2326	ASP	3.3
1	B	2014	GLU	3.2
1	A	1327	ARG	3.1
1	A	1053	VAL	3.0
1	A	1014	GLU	2.9
1	A	1004	GLU	2.8
1	B	2056	ASP	2.7
1	A	1383	ARG	2.6
1	B	2383	ARG	2.6
1	A	1007	LYS	2.5
1	B	2002	ASN	2.5
1	A	1001	MET	2.4
1	A	1003	ALA	2.3
1	B	2255	ARG	2.2
1	B	2088	THR	2.2
1	B	2086	SER	2.1
1	A	1077	GLU	2.1
1	B	2418	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 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.