



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:45 PM UTC

PDB ID : 1YKW / pdb_00001ykw
Title : Crystal Structure of a Novel RuBisCO-Like Protein from the Green Sulfur Bacterium *Chlorobium tepidum*
Authors : Li, H.; Sawaya, M.R.; Tabita, F.R.; Eisenberg, D.
Deposited on : 2005-01-18
Resolution : 2.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

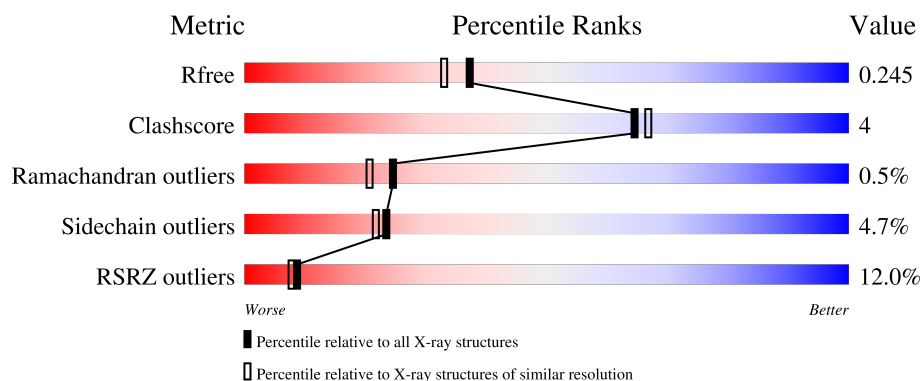
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	10% 84% 10% • 5%
1	B	435	12% 82% 12% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6736 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 RuBisCO-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3205	2048	537	602	18			
1	B	412	Total	C	N	O	S	0	2	0
			3214	2052	542	602	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	VAL	MET	engineered mutation	UNP Q8KBL4
B	328	VAL	MET	engineered mutation	UNP Q8KBL4

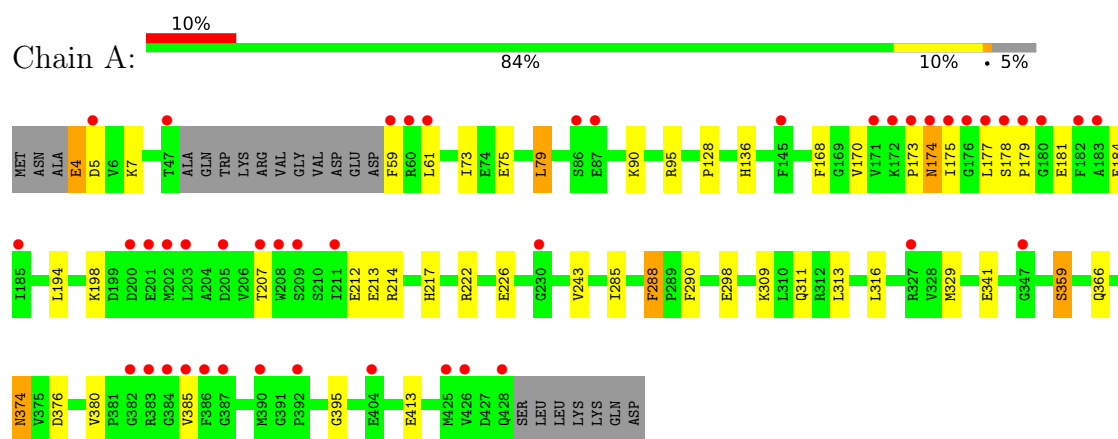
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	156	Total	O	0	0
			156	156		
2	B	161	Total	O	0	0
			161	161		

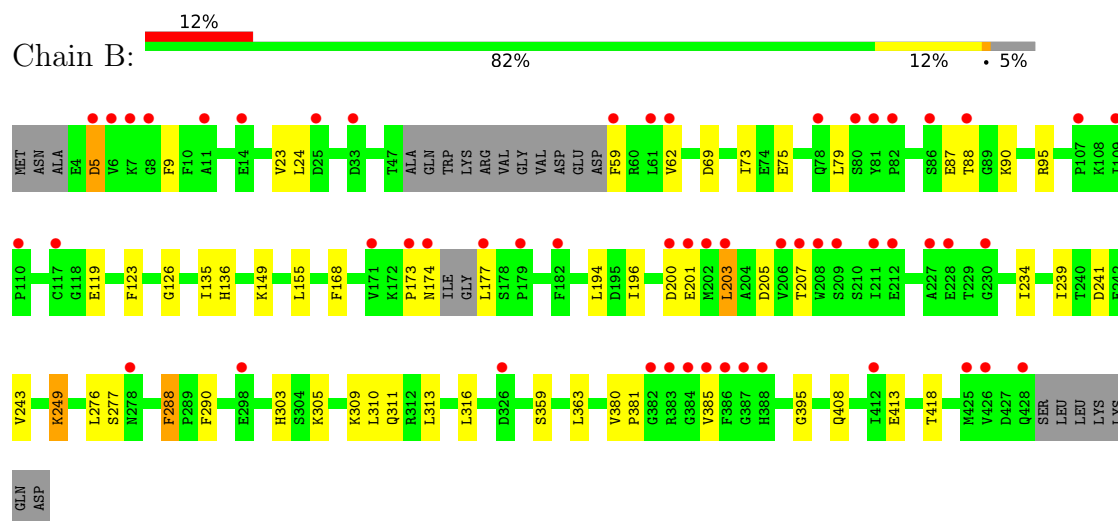
3 Residue-property plots [i](#)

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: RuBisCO-like protein



• Molecule 1: RuBisCO-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.35Å 78.45Å 90.37Å 90.00° 99.95° 90.00°	Depositor
Resolution (Å)	87.71 – 2.00 87.71 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.9 (87.71-2.00) 97.4 (87.71-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.201 , 0.245 0.201 , 0.245	Depositor DCC
R_{free} test set	2956 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.911	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6736	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.75	0/3281	1.04	3/4450 (0.1%)
1	B	0.74	0/3290	1.02	3/4460 (0.1%)
All	All	0.75	0/6571	1.03	6/8910 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	THR	N-CA-C	6.71	118.67	111.36
1	B	288	PHE	N-CA-C	6.47	124.10	109.81
1	B	310	LEU	N-CA-C	6.32	118.17	111.28
1	B	5	ASP	N-CA-C	6.01	119.81	107.37
1	A	288	PHE	N-CA-C	5.88	122.80	109.81
1	A	174	ASN	N-CA-C	5.32	117.51	111.02

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	3205	0	3163	27	0
1	B	3214	0	3166	26	0
2	A	156	0	0	5	0
2	B	161	0	0	1	0
All	All	6736	0	6329	50	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 4.

All (50) 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:205:ASP:HB2	1:B:249:LYS:HE3	1.62	0.81
1:B:303:HIS:HD2	1:B:305:LYS:H	1.29	0.80
1:B:311:GLN:HB3	1:B:316:LEU:HD12	1.66	0.78
1:A:73:ILE:HD11	1:A:95:ARG:HG3	1.73	0.71
1:A:243:VAL:HG11	1:B:243:VAL:HG11	1.73	0.70
1:A:136:HIS:ND1	2:A:490:HOH:O	2.24	0.70
1:B:75:GLU:OE2	1:B:90:LYS:HD2	1.95	0.67
1:B:203:LEU:O	1:B:203:LEU:HG	1.97	0.65
1:B:73:ILE:HD11	1:B:95:ARG:HG3	1.80	0.64
1:A:309:LYS:HE2	1:A:341:GLU:OE1	1.99	0.63
1:B:173:PRO:HD2	1:B:177:LEU:HD11	1.82	0.60
1:A:217:HIS:ND1	2:A:533:HOH:O	2.31	0.59
1:A:359:SER:HA	2:A:517:HOH:O	2.01	0.59
1:A:79:LEU:HD21	1:A:128:PRO:HG2	1.85	0.59
1:B:174:ASN:ND2	1:B:200:ASP:OD1	2.36	0.57
1:A:222:ARG:O	1:A:226:GLU:HG3	2.04	0.57
1:B:149:LYS:HD2	1:B:277:SER:O	2.05	0.56
1:A:170:VAL:HG22	1:A:198:LYS:HD3	1.88	0.56
1:A:173:PRO:HG2	1:A:177:LEU:HD11	1.87	0.55
1:A:385:VAL:HA	1:A:395:GLY:HA3	1.88	0.54
1:A:311:GLN:HB3	1:A:316:LEU:HD12	1.89	0.54
1:A:179:PRO:HG2	1:A:213:GLU:HG3	1.89	0.53
1:A:5:ASP:HB3	1:A:59:PHE:CE2	2.43	0.53
1:B:205:ASP:HB2	1:B:249:LYS:CE	2.34	0.53
1:B:87:GLU:HG3	1:B:126:GLY:HA2	1.90	0.52
1:B:196:ILE:HG12	1:B:234:ILE:HB	1.91	0.52
1:B:9:PHE:CZ	1:B:59:PHE:HB3	2.46	0.51
1:A:374:ASN:HD22	1:A:376:ASP:H	1.60	0.49
1:A:5:ASP:HB3	1:A:59:PHE:HE2	1.79	0.47
1:A:4:GLU:HA	1:A:4:GLU:OE1	2.14	0.47
1:A:168:PHE:HB2	1:A:380:VAL:HG22	1.96	0.47
1:B:385:VAL:HA	1:B:395:GLY:HA3	1.96	0.47
1:B:309:LYS:HG3	2:B:484:HOH:O	2.15	0.47
1:A:329:MET:CE	1:B:123:PHE:HA	2.45	0.46
1:A:174:ASN:HD22	1:A:175:ILE:HG12	1.81	0.46
1:B:241:ASP:OD2	1:B:249:LYS:HD2	2.16	0.46
1:A:178:SER:HB2	1:A:181:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASN:ND2	1:A:175:ILE:HG12	2.32	0.44
1:A:366:GLN:NE2	2:A:521:HOH:O	2.49	0.44
1:B:168:PHE:O	1:B:381:PRO:HD2	2.17	0.44
1:A:136:HIS:CE1	2:A:490:HOH:O	2.66	0.43
1:B:205:ASP:CB	1:B:249:LYS:HE3	2.39	0.43
1:A:329:MET:HE3	1:B:123:PHE:HA	2.01	0.42
1:A:179:PRO:HB3	1:A:214:ARG:HA	2.02	0.42
1:A:75:GLU:OE2	1:A:90:LYS:HD3	2.20	0.42
1:B:24:LEU:HD23	1:B:135:ILE:HG23	2.02	0.41
1:B:309:LYS:HB2	1:B:309:LYS:HE2	1.93	0.41
1:B:381:PRO:HG2	1:B:385:VAL:HG21	2.01	0.41
1:B:23:VAL:HB	1:B:136[B]:HIS:HB3	2.02	0.41
1:B:239:ILE:HD11	1:B:276:LEU:HD21	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	410/435 (94%)	396 (97%)	12 (3%)	2 (0%)	24	21
1	B	408/435 (94%)	393 (96%)	13 (3%)	2 (0%)	24	21
All	All	818/870 (94%)	789 (96%)	25 (3%)	4 (0%)	24	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	PHE
1	B	290	PHE
1	A	288	PHE
1	B	288	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	343/361 (95%)	330 (96%)	13 (4%)	29	29
1	B	344/361 (95%)	325 (94%)	19 (6%)	19	17
All	All	687/722 (95%)	655 (95%)	32 (5%)	23	22

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	7	LYS
1	A	61	LEU
1	A	79	LEU
1	A	184	GLU
1	A	194	LEU
1	A	212	GLU
1	A	285	ILE
1	A	298	GLU
1	A	313	LEU
1	A	359	SER
1	A	374	ASN
1	A	413	GLU
1	B	5	ASP
1	B	62	VAL
1	B	69	ASP
1	B	79	LEU
1	B	88	THR
1	B	119	GLU
1	B	155	LEU
1	B	194	LEU
1	B	201	GLU
1	B	203	LEU
1	B	207	THR
1	B	249	LYS
1	B	313	LEU
1	B	359	SER

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Mol	Chain	Res	Type
1	B	363	LEU
1	B	380	VAL
1	B	408	GLN
1	B	413	GLU
1	B	418	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	104	ASN
1	A	162	HIS
1	A	188	GLN
1	A	264	ASN
1	A	311	GLN
1	A	338	ASN
1	A	366	GLN
1	A	374	ASN
1	A	428	GLN
1	B	63	HIS
1	B	92	HIS
1	B	104	ASN
1	B	160	ASN
1	B	303	HIS
1	B	311	GLN
1	B	408	GLN

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 oligosaccharides 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, 95th 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	414/435 (95%)	0.92	45 (10%) 10 9	16, 25, 50, 62	0
1	B	412/435 (94%)	0.93	54 (13%) 7 6	11, 25, 50, 58	3 (0%)
All	All	826/870 (94%)	0.92	99 (11%) 9 8	11, 25, 50, 62	3 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	TRP	6.7
1	B	209	SER	6.2
1	B	207	THR	6.1
1	A	182	PHE	6.0
1	A	209	SER	5.8
1	A	174	ASN	5.8
1	A	384	GLY	5.6
1	A	179	PRO	5.3
1	A	175	ILE	5.1
1	A	173	PRO	5.1
1	B	179	PRO	5.0
1	B	182	PHE	4.7
1	B	171	VAL	4.7
1	B	208	TRP	4.5
1	B	200	ASP	4.5
1	B	387	GLY	4.5
1	B	386	PHE	4.4
1	A	61	LEU	4.4
1	B	384	GLY	4.3
1	A	171	VAL	4.3
1	B	201	GLU	4.2
1	A	386	PHE	4.1
1	B	5	ASP	4.1
1	B	174	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	59	PHE	4.0
1	A	177	LEU	3.9
1	A	207	THR	3.9
1	B	385	VAL	3.8
1	A	201	GLU	3.8
1	A	203	LEU	3.8
1	B	61	LEU	3.7
1	A	59	PHE	3.7
1	A	211	ILE	3.6
1	B	206	VAL	3.5
1	B	88	THR	3.5
1	B	82	PRO	3.4
1	A	178	SER	3.2
1	A	202	MET	3.2
1	B	382	GLY	3.2
1	B	211	ILE	3.1
1	B	81	TYR	3.1
1	A	205	ASP	3.0
1	B	202	MET	3.0
1	B	203	LEU	3.0
1	A	387	GLY	3.0
1	B	8	GLY	3.0
1	B	110	PRO	3.0
1	B	228	GLU	2.9
1	A	200	ASP	2.8
1	B	25	ASP	2.8
1	A	230	GLY	2.7
1	A	385	VAL	2.7
1	A	382	GLY	2.7
1	B	177	LEU	2.7
1	B	425	MET	2.7
1	B	173	PRO	2.6
1	B	62	VAL	2.6
1	B	212	GLU	2.5
1	A	5	ASP	2.5
1	B	107	PRO	2.5
1	B	6	VAL	2.5
1	B	426	VAL	2.5
1	A	404	GLU	2.5
1	B	326	ASP	2.4
1	B	388	HIS	2.4
1	B	383	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	109	ILE	2.4
1	A	425	MET	2.4
1	B	80	SER	2.4
1	A	60	ARG	2.4
1	A	176	GLY	2.4
1	A	87	GLU	2.3
1	B	227	ALA	2.3
1	A	145	PHE	2.3
1	A	426	VAL	2.3
1	B	86	SER	2.3
1	A	428	GLN	2.3
1	B	428	GLN	2.3
1	B	298	GLU	2.3
1	B	117	CYS	2.3
1	B	78	GLN	2.2
1	B	412	ILE	2.2
1	A	172	LYS	2.2
1	B	278	ASN	2.2
1	A	86	SER	2.2
1	A	327	ARG	2.2
1	A	392	PRO	2.1
1	A	383	ARG	2.1
1	A	183	ALA	2.1
1	B	7	LYS	2.1
1	A	47	THR	2.1
1	A	180	GLY	2.1
1	B	230	GLY	2.1
1	B	33	ASP	2.0
1	A	347	GLY	2.0
1	A	185	ILE	2.0
1	B	14	GLU	2.0
1	A	390	MET	2.0
1	B	11	ALA	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 oligosaccharides 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.