



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:10 AM UTC

PDB ID : 4LOT / pdb_00004lot
Title : C1s CUB2-CCP1-CCP2
Authors : Wallis, R.; Venkatraman Girija, U.; Moody, P.C.E.; Marshall, J.E.
Deposited on : 2013-07-13
Resolution : 2.92 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

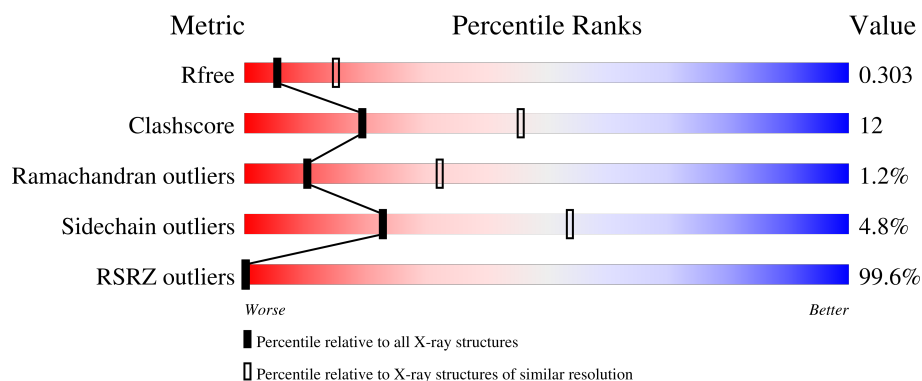
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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 $\leq 5\%$. 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	249	98% 68%29%..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1908 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.

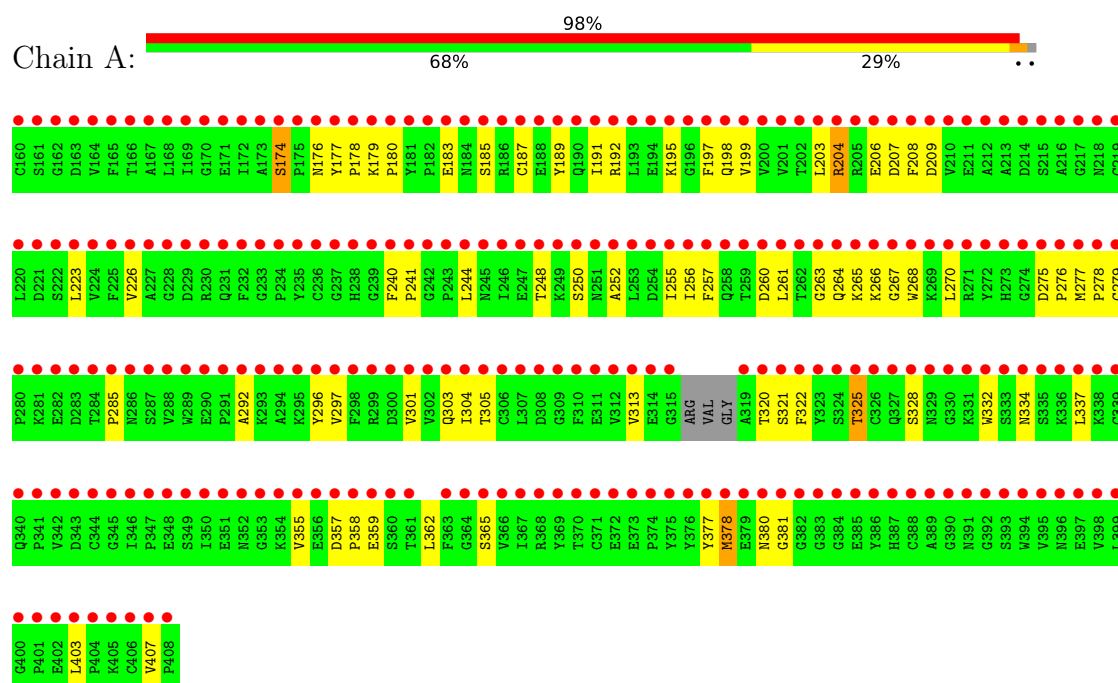
- Molecule 1 is a protein called Complement C1s subcomponent heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1908	1205	314	375	14	0	0	0

3 Residue-property plots

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: Complement C1s subcomponent heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.04Å 58.59Å 51.21Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	54.22 – 2.92 54.22 – 2.92	Depositor EDS
% Data completeness (in resolution range)	92.7 (54.22-2.92) 94.3 (54.22-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.266 , 0.292 0.283 , 0.303	Depositor DCC
R_{free} test set	450 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	1.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 128.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
Reported twinning fraction	0.050 for -h,-k,l	Depositor
Outliers	3 of 9463 reflections (0.032%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1908	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% 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	0.31	0/1959	0.86	3/2661 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	VAL	N-CA-C	6.40	116.89	110.23
1	A	174	SER	CA-C-N	6.22	127.61	119.84
1	A	174	SER	C-N-CA	6.22	127.61	119.84

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	1908	0	1791	43	0
All	All	1908	0	1791	43	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 12.

All (43) 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:176:ASN:HB3	1:A:179:LYS:HD2	1.69	0.74
1:A:278:PRO:HA	1:A:297:VAL:HA	1.71	0.73
1:A:203:LEU:HD12	1:A:270:LEU:HB3	1.74	0.70
1:A:203:LEU:HD21	1:A:208:PHE:HB2	1.75	0.69
1:A:263:GLY:O	1:A:265:LYS:N	2.27	0.68
1:A:204:ARG:HB3	1:A:207:ASP:HB2	1.81	0.63
1:A:189:TYR:HB2	1:A:255:ILE:HB	1.83	0.60
1:A:380:ASN:OD1	1:A:381:GLY:N	2.34	0.60
1:A:174:SER:HB3	1:A:268:TRP:H	1.69	0.58
1:A:195:LYS:HG2	1:A:328:SER:HB2	1.89	0.55
1:A:187:CYS:HB2	1:A:257:PHE:HB3	1.90	0.53
1:A:199:VAL:O	1:A:248:THR:OG1	2.21	0.53
1:A:359:GLU:OE1	1:A:359:GLU:N	2.41	0.52
1:A:362:LEU:O	1:A:365:SER:OG	2.26	0.51
1:A:197:PHE:HE1	1:A:276:PRO:HG3	1.76	0.51
1:A:378:MET:SD	1:A:380:ASN:ND2	2.84	0.51
1:A:183:GLU:HB2	1:A:260:ASP:O	2.11	0.50
1:A:301:VAL:HG22	1:A:325:THR:HG22	1.94	0.49
1:A:192:ARG:HH21	1:A:252:ALA:HB1	1.77	0.49
1:A:250:SER:OG	1:A:252:ALA:O	2.30	0.48
1:A:198:GLN:HB3	1:A:277:MET:SD	2.53	0.48
1:A:223:LEU:HB2	1:A:257:PHE:HD2	1.78	0.48
1:A:192:ARG:NH2	1:A:252:ALA:HB1	2.29	0.48
1:A:207:ASP:O	1:A:268:TRP:HA	2.15	0.46
1:A:209:ASP:HB3	1:A:267:GLY:H	1.80	0.46
1:A:279:CYS:HB3	1:A:332:TRP:CE2	2.52	0.45
1:A:303:GLN:OE1	1:A:305:THR:OG1	2.34	0.45
1:A:180:PRO:HA	1:A:265:LYS:O	2.17	0.45
1:A:275:ASP:HA	1:A:276:PRO:HD3	1.87	0.45
1:A:191:ILE:O	1:A:192:ARG:HD3	2.18	0.44
1:A:334:ASN:HB3	1:A:337:LEU:HG	2.00	0.44
1:A:223:LEU:HB2	1:A:257:PHE:CD2	2.53	0.43
1:A:177:TYR:CG	1:A:178:PRO:HA	2.53	0.43
1:A:174:SER:O	1:A:177:TYR:HB2	2.19	0.42
1:A:292:ALA:HA	1:A:296:TYR:OH	2.20	0.42
1:A:240:PHE:HA	1:A:241:PRO:HD3	1.68	0.41
1:A:266:LYS:HB3	1:A:266:LYS:HE2	1.79	0.41
1:A:357:ASP:HA	1:A:358:PRO:HD3	1.90	0.41
1:A:304:ILE:HD13	1:A:322:PHE:CE1	2.56	0.41
1:A:377:TYR:N	1:A:407:VAL:O	2.44	0.41
1:A:177:TYR:CD1	1:A:178:PRO:HA	2.56	0.40
1:A:187:CYS:O	1:A:256:ILE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASP:CG	1:A:261:LEU:H	2.26	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	242/249 (97%)	216 (89%)	23 (10%)	3 (1%)	10 32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	285	PRO
1	A	378	MET

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	210/212 (99%)	200 (95%)	10 (5%)	23 54

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	SER
1	A	204	ARG
1	A	206	GLU
1	A	226	VAL
1	A	244	LEU
1	A	320	THR
1	A	321	SER
1	A	325	THR
1	A	355	VAL
1	A	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	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	246/249 (98%)	4.63	245 (99%) 0 0	78, 128, 193, 263	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	SER	8.7
1	A	345	GLY	8.6
1	A	189	TYR	8.5
1	A	381	GLY	8.4
1	A	363	PHE	7.6
1	A	339	CYS	7.3
1	A	225	PHE	7.3
1	A	164	VAL	7.1
1	A	165	PHE	7.1
1	A	295	LYS	7.1
1	A	308	ASP	7.0
1	A	323	TYR	6.8
1	A	207	ASP	6.8
1	A	231	GLN	6.7
1	A	205	ARG	6.7
1	A	357	ASP	6.7
1	A	282	GLU	6.6
1	A	397	GLU	6.6
1	A	252	ALA	6.6
1	A	237	GLY	6.5
1	A	368	ARG	6.5
1	A	226	VAL	6.5
1	A	332	TRP	6.4
1	A	384	GLY	6.4
1	A	161	SER	6.4
1	A	356	GLU	6.3
1	A	235	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	THR	6.3
1	A	275	ASP	6.3
1	A	220	LEU	6.2
1	A	219	CYS	6.2
1	A	312	VAL	6.2
1	A	304	ILE	6.1
1	A	322	PHE	6.1
1	A	373	GLU	6.0
1	A	364	GLY	5.9
1	A	313	VAL	5.9
1	A	172	ILE	5.9
1	A	243	PRO	5.9
1	A	369	TYR	5.9
1	A	272	TYR	5.8
1	A	193	LEU	5.8
1	A	294	ALA	5.8
1	A	382	GLY	5.7
1	A	269	LYS	5.7
1	A	197	PHE	5.7
1	A	375	TYR	5.6
1	A	199	VAL	5.6
1	A	160	CYS	5.6
1	A	191	ILE	5.6
1	A	261	LEU	5.6
1	A	354	LYS	5.6
1	A	212	ALA	5.6
1	A	401	PRO	5.5
1	A	168	LEU	5.5
1	A	289	TRP	5.5
1	A	306	CYS	5.5
1	A	218	ASN	5.5
1	A	372	GLU	5.4
1	A	211	GLU	5.4
1	A	394	TRP	5.4
1	A	392	GLY	5.4
1	A	340	GLN	5.4
1	A	233	GLY	5.4
1	A	334	ASN	5.3
1	A	216	ALA	5.3
1	A	204	ARG	5.3
1	A	214	ASP	5.3
1	A	234	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	256	ILE	5.3
1	A	182	PRO	5.3
1	A	374	PRO	5.3
1	A	215	SER	5.3
1	A	406	CYS	5.3
1	A	346	ILE	5.2
1	A	264	GLN	5.2
1	A	169	ILE	5.2
1	A	187	CYS	5.2
1	A	377	TYR	5.2
1	A	398	VAL	5.2
1	A	162	GLY	5.2
1	A	387	HIS	5.2
1	A	399	LEU	5.2
1	A	296	TYR	5.2
1	A	298	PHE	5.1
1	A	404	PRO	5.1
1	A	229	ASP	5.1
1	A	390	GLY	5.0
1	A	163	ASP	5.0
1	A	376	TYR	5.0
1	A	249	LYS	5.0
1	A	200	VAL	5.0
1	A	355	VAL	5.0
1	A	251	ASN	5.0
1	A	202	THR	5.0
1	A	380	ASN	5.0
1	A	403	LEU	5.0
1	A	327	GLN	5.0
1	A	290	GLU	5.0
1	A	179	LYS	5.0
1	A	358	PRO	5.0
1	A	257	PHE	4.9
1	A	217	GLY	4.9
1	A	383	GLY	4.9
1	A	359	GLU	4.9
1	A	208	PHE	4.9
1	A	190	GLN	4.9
1	A	171	GLU	4.8
1	A	279	CYS	4.8
1	A	302	VAL	4.8
1	A	336	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	241	PRO	4.8
1	A	230	ARG	4.8
1	A	330	GLY	4.8
1	A	391	ASN	4.8
1	A	255	ILE	4.8
1	A	228	GLY	4.7
1	A	232	PHE	4.7
1	A	203	LEU	4.7
1	A	321	SER	4.7
1	A	178	PRO	4.7
1	A	263	GLY	4.7
1	A	305	THR	4.6
1	A	335	SER	4.6
1	A	288	VAL	4.6
1	A	396	ASN	4.6
1	A	239	GLY	4.6
1	A	284	THR	4.6
1	A	378	MET	4.6
1	A	326	CYS	4.6
1	A	371	CYS	4.5
1	A	314	GLU	4.5
1	A	238	HIS	4.4
1	A	223	LEU	4.4
1	A	310	PHE	4.4
1	A	188	GLU	4.3
1	A	286	ASN	4.3
1	A	320	THR	4.3
1	A	177	TYR	4.3
1	A	367	ILE	4.3
1	A	276	PRO	4.3
1	A	365	SER	4.3
1	A	210	VAL	4.3
1	A	405	LYS	4.3
1	A	347	PRO	4.2
1	A	366	VAL	4.2
1	A	324	SER	4.2
1	A	266	LYS	4.2
1	A	297	VAL	4.2
1	A	221	ASP	4.2
1	A	242	GLY	4.2
1	A	183	GLU	4.2
1	A	240	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	245	ASN	4.2
1	A	198	GLN	4.1
1	A	348	GLU	4.1
1	A	254	ASP	4.1
1	A	407	VAL	4.0
1	A	167	ALA	4.0
1	A	270	LEU	4.0
1	A	194	GLU	4.0
1	A	280	PRO	4.0
1	A	247	GLU	4.0
1	A	222	SER	4.0
1	A	342	VAL	4.0
1	A	343	ASP	3.9
1	A	192	ARG	3.9
1	A	395	VAL	3.9
1	A	175	PRO	3.9
1	A	224	VAL	3.9
1	A	166	THR	3.9
1	A	385	GLU	3.9
1	A	328	SER	3.9
1	A	244	LEU	3.9
1	A	285	PRO	3.9
1	A	206	GLU	3.8
1	A	176	ASN	3.8
1	A	352	ASN	3.8
1	A	319	ALA	3.8
1	A	301	VAL	3.8
1	A	331	LYS	3.8
1	A	386	TYR	3.8
1	A	307	LEU	3.8
1	A	361	THR	3.8
1	A	402	GLU	3.7
1	A	273	HIS	3.7
1	A	379	GLU	3.7
1	A	271	ARG	3.7
1	A	344	CYS	3.7
1	A	184	ASN	3.7
1	A	281	LYS	3.6
1	A	337	LEU	3.6
1	A	370	THR	3.6
1	A	253	LEU	3.6
1	A	236	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	309	GLY	3.5
1	A	246	ILE	3.5
1	A	291	PRO	3.5
1	A	274	GLY	3.5
1	A	350	ILE	3.4
1	A	338	LYS	3.4
1	A	170	GLY	3.4
1	A	349	SER	3.4
1	A	329	ASN	3.4
1	A	303	GLN	3.4
1	A	201	VAL	3.4
1	A	393	SER	3.4
1	A	180	PRO	3.3
1	A	173	ALA	3.3
1	A	333	SER	3.3
1	A	260	ASP	3.3
1	A	311	GLU	3.3
1	A	268	TRP	3.3
1	A	351	GLU	3.2
1	A	258	GLN	3.2
1	A	181	TYR	3.1
1	A	195	LYS	3.0
1	A	278	PRO	3.0
1	A	299	ARG	3.0
1	A	341	PRO	3.0
1	A	293	LYS	2.9
1	A	196	GLY	2.9
1	A	209	ASP	2.9
1	A	227	ALA	2.9
1	A	283	ASP	2.9
1	A	213	ALA	2.8
1	A	248	THR	2.8
1	A	400	GLY	2.8
1	A	277	MET	2.8
1	A	300	ASP	2.8
1	A	360	SER	2.7
1	A	186	ARG	2.7
1	A	292	ALA	2.7
1	A	265	LYS	2.6
1	A	389	ALA	2.6
1	A	408	PRO	2.6
1	A	388	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	325	THR	2.6
1	A	259	THR	2.3
1	A	353	GLY	2.3
1	A	174	SER	2.3
1	A	287	SER	2.3
1	A	267	GLY	2.2
1	A	185	SER	2.2
1	A	315	GLY	2.1

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.