



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4BD9 / pdb_00004bd9
Title : Structure of the complex between SmCI and human carboxypeptidase A4
Authors : Alonso-del-Ribero, M.; Reytor, M.L.; Trejo, S.A.; Chavez, M.A.; Aviles, F.X.;
Reverter, D.
Deposited on : 2012-10-05
Resolution : 2.20 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

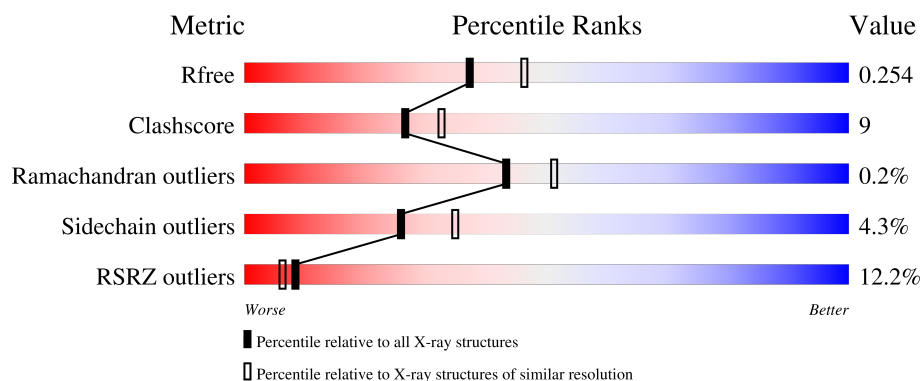
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	310	9% 80% 16% ••
2	B	165	17% 82% 13% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3829 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 CARBOXYPEPTIDASE A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2408	1533	418	449	8			

- Molecule 2 is a protein called CARBOXYPEPTIDASE INHIBITOR SMCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1297	802	218	258	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	ALA	ASN	engineered mutation	UNP P84875

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

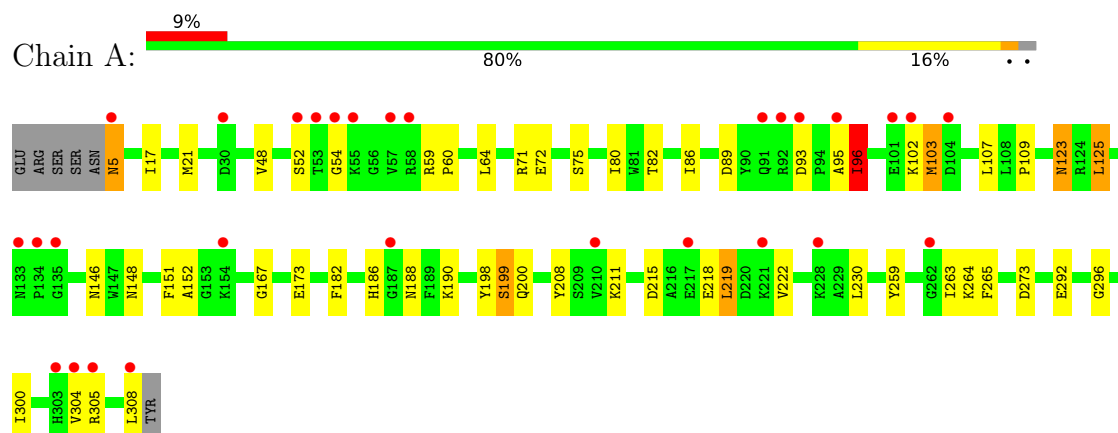
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	44	Total	O	0	0
			44	44		

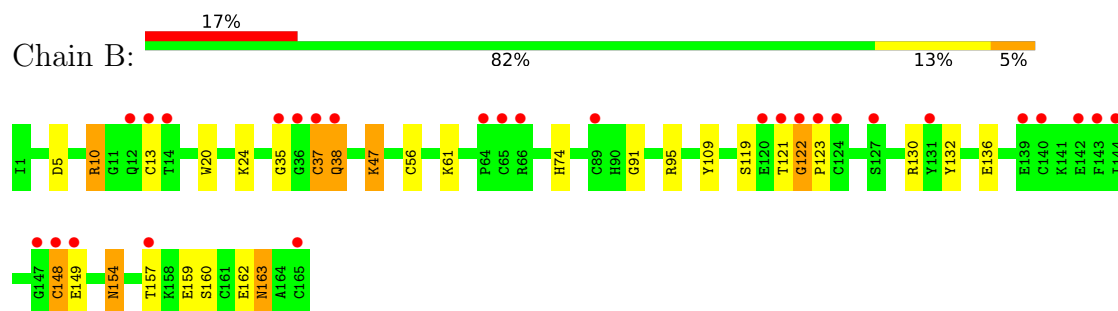
3 Residue-property plots [i](#)

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: CARBOXYPEPTIDASE A4



• Molecule 2: CARBOXYPEPTIDASE INHIBITOR SMCI



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.67Å 138.67Å 161.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.86 – 2.20 38.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.86-2.20) 99.4 (38.86-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.223 , 0.254 0.222 , 0.254	Depositor DCC
R_{free} test set	2369 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3829	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.55	0/2475	0.86	3/3365 (0.1%)
2	B	0.71	2/1332 (0.2%)	0.89	4/1798 (0.2%)
All	All	0.61	2/3807 (0.1%)	0.87	7/5163 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	148	CYS	C-N	-16.13	1.16	1.33
2	B	37	CYS	C-N	7.14	1.43	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	GLN	O-C-N	-8.38	110.77	121.33
2	B	122	GLY	CA-C-N	5.38	124.71	118.85
2	B	122	GLY	C-N-CA	5.38	124.71	118.85
1	A	96	ILE	CB-CA-C	-5.27	105.11	112.02
2	B	10	ARG	N-CA-C	-5.26	106.37	112.89
1	A	167	GLY	CA-C-N	5.11	124.90	119.28
1	A	167	GLY	C-N-CA	5.11	124.90	119.28

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	2408	0	2325	42	0
2	B	1297	0	1147	26	0
3	A	1	0	0	0	0
4	A	79	0	0	3	0
4	B	44	0	0	0	0
All	All	3829	0	3472	67	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 9.

All (67) 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:186:HIS:HD2	1:A:188:ASN:H	1.19	0.90
1:A:89:ASP:HB3	1:A:96:ILE:HD11	1.67	0.77
2:B:130:ARG:HH11	2:B:154:ASN:HD21	1.33	0.76
1:A:93:ASP:OD2	1:A:95:ALA:HB3	1.94	0.68
2:B:123:PRO:HG3	2:B:149:GLU:OE1	1.94	0.67
2:B:154:ASN:HD22	2:B:154:ASN:C	2.02	0.66
1:A:186:HIS:CD2	1:A:188:ASN:H	2.06	0.66
2:B:91:GLY:HA3	2:B:95:ARG:NH1	2.11	0.66
2:B:157:THR:HG23	2:B:160:SER:H	1.62	0.65
1:A:54:GLY:HA3	1:A:59:ARG:HD2	1.78	0.65
1:A:190:LYS:HG3	1:A:308:LEU:HD11	1.82	0.62
2:B:119:SER:HB3	2:B:132:TYR:CD2	2.34	0.61
1:A:146:ASN:HD21	1:A:173:GLU:H	1.48	0.60
1:A:59:ARG:HB3	1:A:60:PRO:HD2	1.83	0.60
1:A:264:LYS:HE2	1:A:265:PHE:CE1	2.37	0.60
1:A:218:GLU:O	1:A:222:VAL:HG23	2.02	0.59
1:A:123:ASN:C	1:A:123:ASN:HD22	2.11	0.58
2:B:130:ARG:HH11	2:B:154:ASN:ND2	2.01	0.57
2:B:13:CYS:HB2	2:B:35:GLY:O	2.06	0.56
2:B:20:TRP:CZ3	2:B:47:LYS:HD3	2.41	0.55
1:A:109:PRO:HD2	4:A:2026:HOH:O	2.07	0.55
1:A:102:LYS:HG3	1:A:305:ARG:HG3	1.89	0.55
1:A:125:LEU:HG	2:B:109:TYR:HB3	1.89	0.54
1:A:190:LYS:HE3	1:A:308:LEU:HD11	1.89	0.54
1:A:93:ASP:HB3	1:A:96:ILE:HD11	1.89	0.53
2:B:5:ASP:HA	2:B:24:LYS:HD2	1.89	0.53
1:A:198:TYR:O	1:A:199:SER:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:THR:HG22	2:B:160:SER:HB2	1.91	0.52
2:B:91:GLY:HA3	2:B:95:ARG:HH12	1.75	0.51
1:A:259:TYR:HA	1:A:263:ILE:O	2.11	0.51
1:A:230:LEU:HG	1:A:292:GLU:HG3	1.94	0.50
2:B:159:GLU:HA	2:B:162:GLU:HG2	1.95	0.49
1:A:5:ASN:HD22	1:A:5:ASN:N	2.11	0.49
1:A:107:LEU:O	1:A:109:PRO:HD3	2.13	0.49
1:A:148:ASN:ND2	4:A:2055:HOH:O	2.46	0.48
1:A:182:PHE:C	1:A:182:PHE:CD1	2.92	0.48
1:A:82:THR:O	1:A:86:ILE:HG13	2.14	0.47
1:A:198:TYR:O	1:A:199:SER:HB2	2.14	0.47
1:A:146:ASN:ND2	1:A:173:GLU:H	2.13	0.47
2:B:123:PRO:CG	2:B:149:GLU:OE1	2.61	0.47
1:A:89:ASP:CB	1:A:96:ILE:HD11	2.41	0.46
2:B:56:CYS:O	2:B:74:HIS:HD2	1.98	0.46
2:B:119:SER:HB3	2:B:132:TYR:CG	2.51	0.45
2:B:123:PRO:HG3	2:B:149:GLU:CD	2.40	0.45
1:A:151:PHE:O	1:A:152:ALA:HB3	2.17	0.45
1:A:17:ILE:O	1:A:21:MET:HG3	2.17	0.44
2:B:61:LYS:HD3	2:B:91:GLY:HA2	2.00	0.43
1:A:96:ILE:H	1:A:96:ILE:HG13	1.32	0.43
1:A:60:PRO:O	1:A:103:MET:HB2	2.18	0.43
2:B:121:THR:HG23	2:B:122:GLY:O	2.19	0.43
2:B:123:PRO:CD	2:B:149:GLU:OE1	2.67	0.43
1:A:93:ASP:HB3	1:A:96:ILE:CD1	2.48	0.43
1:A:200:GLN:HE21	1:A:273:ASP:HA	1.84	0.43
2:B:91:GLY:CA	2:B:95:ARG:HH12	2.32	0.43
1:A:300:ILE:O	1:A:304:VAL:HG23	2.18	0.43
1:A:230:LEU:C	1:A:230:LEU:HD23	2.45	0.42
2:B:159:GLU:O	2:B:163:ASN:HB2	2.19	0.42
1:A:208:TYR:CD1	1:A:208:TYR:C	2.97	0.42
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.81	0.42
1:A:215:ASP:OD1	1:A:264:LYS:HD2	2.20	0.42
2:B:157:THR:CG2	2:B:160:SER:HB2	2.51	0.41
1:A:52:SER:HA	4:A:2027:HOH:O	2.19	0.41
1:A:72:GLU:O	1:A:75:SER:HB3	2.20	0.41
1:A:296:GLY:O	1:A:300:ILE:HG13	2.20	0.41
2:B:148:CYS:O	2:B:149:GLU:HB2	2.21	0.40
2:B:38:GLN:OE1	2:B:38:GLN:HA	2.21	0.40
1:A:5:ASN:N	1:A:5:ASN:ND2	2.70	0.40

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	295/310 (95%)	273 (92%)	21 (7%)	1 (0%)	36	42
2	B	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
All	All	458/475 (96%)	429 (94%)	28 (6%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER

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	254/260 (98%)	243 (96%)	11 (4%)	26	35
2	B	139/139 (100%)	133 (96%)	6 (4%)	26	35
All	All	393/399 (98%)	376 (96%)	17 (4%)	26	35

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	48	VAL
1	A	64	LEU
1	A	71	ARG
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	96	ILE
1	A	103	MET
1	A	123	ASN
1	A	125	LEU
1	A	211	LYS
1	A	219	LEU
2	B	10	ARG
2	B	37	CYS
2	B	47	LYS
2	B	136	GLU
2	B	154	ASN
2	B	163	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	123	ASN
1	A	146	ASN
1	A	171	ASN
1	A	184	GLN
1	A	186	HIS
1	A	200	GLN
1	A	303	HIS
2	B	19	GLN
2	B	74	HIS
2	B	110	GLN
2	B	117	GLN
2	B	154	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	148:CYS	C	149:GLU	N	1.16

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	304/310 (98%)	0.57	29 (9%)	14 11	17, 36, 61, 73	0
2	B	165/165 (100%)	0.80	28 (16%)	4 3	21, 38, 58, 71	0
All	All	469/475 (98%)	0.65	57 (12%)	8 6	17, 36, 60, 73	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	37	CYS	4.8
1	A	308	LEU	4.4
2	B	148	CYS	4.3
2	B	12	GLN	4.1
1	A	95	ALA	4.0
1	A	54	GLY	3.7
2	B	36	GLY	3.7
2	B	65	CYS	3.7
2	B	131	TYR	3.6
2	B	66	ARG	3.6
1	A	92	ARG	3.5
1	A	30	ASP	3.4
1	A	210	VAL	3.4
1	A	101	GLU	3.3
2	B	147	GLY	3.3
1	A	304	VAL	3.3
2	B	149	GLU	3.2
2	B	123	PRO	3.2
1	A	133	ASN	3.2
2	B	14	THR	3.1
2	B	120	GLU	3.1
2	B	124	CYS	3.1
1	A	134	PRO	3.1
2	B	121	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	140	CYS	3.0
2	B	144	ILE	3.0
1	A	305	ARG	2.9
1	A	57	VAL	2.8
2	B	139	GLU	2.8
1	A	154	LYS	2.8
2	B	13	CYS	2.8
2	B	89	CYS	2.8
1	A	221	LYS	2.7
2	B	38	GLN	2.6
2	B	165	CYS	2.6
1	A	262	GLY	2.6
1	A	228	LYS	2.5
1	A	217	GLU	2.4
1	A	58	ARG	2.4
1	A	5	ASN	2.4
1	A	53	THR	2.4
2	B	35	GLY	2.3
1	A	135	GLY	2.3
2	B	157	THR	2.3
1	A	187	GLY	2.3
1	A	52	SER	2.2
2	B	64	PRO	2.2
1	A	303	HIS	2.2
2	B	122	GLY	2.2
2	B	127	SER	2.1
1	A	93	ASP	2.1
2	B	143	PHE	2.1
2	B	142	GLU	2.1
1	A	104	ASP	2.1
1	A	55	LYS	2.0
1	A	102	LYS	2.0
1	A	91	GLN	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	500	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.