



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 AM UTC

PDB ID : 3PB6 / pdb_00003pb6
Title : Crystal structure of the catalytic domain of human Golgi-resident glutaminyl cyclase at pH 6.5
Authors : Huang, K.F.; Liaw, S.S.; Huang, W.L.; Chia, C.Y.; Lo, Y.C.; Chen, Y.L.; Wang, A.H.J.
Deposited on : 2010-10-20
Resolution : 1.05 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
Mogul : 2022.3.0, CSD as543be (2022)
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

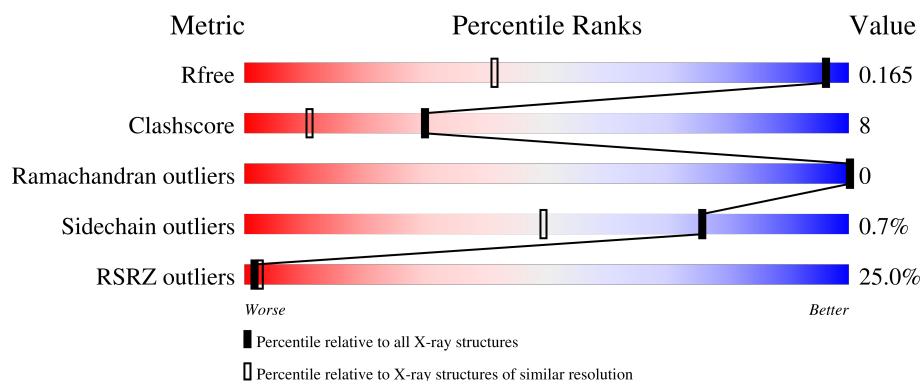
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1182 (1.08-1.04)
Clashscore	190562	1204 (1.08-1.04)
Ramachandran outliers	187476	1175 (1.08-1.04)
Sidechain outliers	187428	1176 (1.08-1.04)
RSRZ outliers	180081	1181 (1.08-1.04)

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	X	330	24% 81% 10% 5%

2 Entry composition [i](#)

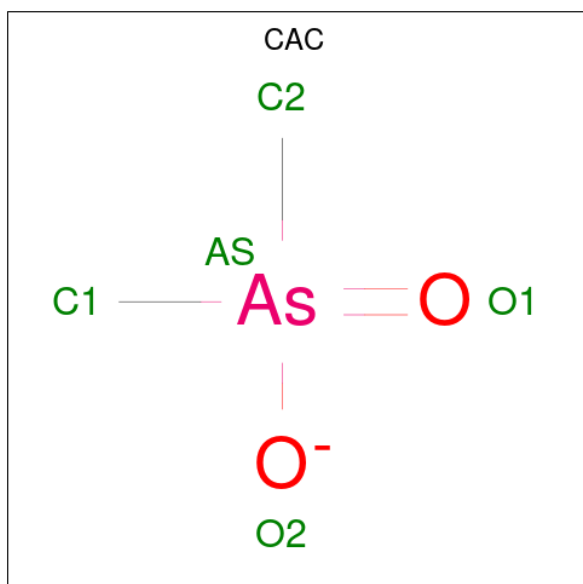
There are 4 unique types of molecules in this entry. The entry contains 2836 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutaminyl-peptide cyclotransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			

- Molecule 2 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	X	1	Total	As	C	O	0	0
			5	1	2	2		

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

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

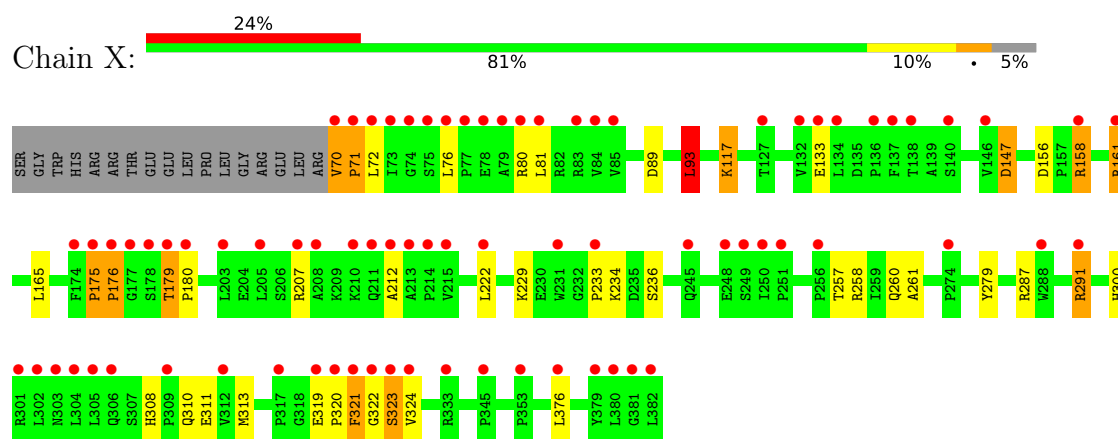
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	356	Total 356	O 356	0	0

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: Glutaminyl-peptide cyclotransferase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.10Å 68.53Å 77.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.05 30.00 – 1.05	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-1.05) 90.4 (30.00-1.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.138 , 0.158 0.167 , 0.165	Depositor DCC
R_{free} test set	6399 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	8.4	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 63.8	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	0.96	EDS
Total number of atoms	2836	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% 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

5.1 Standard geometry

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

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	X	1.47	21/2550 (0.8%)	1.20	14/3488 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	323	SER	C-N	-10.34	1.19	1.33
1	X	322	GLY	C-O	10.01	1.33	1.23
1	X	179	THR	CA-C	9.38	1.65	1.52
1	X	323	SER	CB-OG	-8.58	1.25	1.42
1	X	133	GLU	CB-CG	-7.19	1.30	1.52
1	X	324	VAL	N-CA	-6.90	1.38	1.46
1	X	147	ASP	CB-CG	-6.85	1.34	1.52
1	X	179	THR	C-O	-6.62	1.15	1.24
1	X	323	SER	C-O	-6.58	1.15	1.23
1	X	89	ASP	CG-OD1	-6.21	1.13	1.25
1	X	93	LEU	CG-CD2	-6.15	1.32	1.52
1	X	236	SER	CB-OG	-5.84	1.30	1.42
1	X	222	LEU	CG-CD1	-5.75	1.33	1.52
1	X	321	PHE	CD2-CE2	5.60	1.55	1.38
1	X	117	LYS	CG-CD	-5.59	1.35	1.52
1	X	311	GLU	CG-CD	5.47	1.65	1.52
1	X	71	PRO	N-CA	5.27	1.54	1.47
1	X	319	GLU	CA-CB	5.23	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	321	PHE	C-O	5.21	1.30	1.24
1	X	212	ALA	CA-CB	5.21	1.61	1.53
1	X	176	PRO	C-O	5.13	1.29	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	161	ARG	CD-NE-CZ	12.33	141.66	124.40
1	X	175	PRO	O-C-N	8.68	125.30	121.31
1	X	322	GLY	O-C-N	8.66	130.26	122.81
1	X	323	SER	CA-CB-OG	-6.66	97.79	111.10
1	X	161	ARG	CG-CD-NE	-6.32	98.09	112.00
1	X	158	ARG	CD-NE-CZ	5.87	132.61	124.40
1	X	158	ARG	CG-CD-NE	-5.86	99.10	112.00
1	X	93	LEU	CD1-CG-CD2	-5.51	98.67	110.80
1	X	311	GLU	CB-CG-CD	5.23	121.49	112.60
1	X	291	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	X	319	GLU	CB-CA-C	5.22	117.62	111.15
1	X	179	THR	CA-CB-CG2	5.05	119.08	110.50
1	X	323	SER	CA-C-N	5.03	130.87	122.57
1	X	323	SER	C-N-CA	5.03	130.87	122.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	323	SER	Mainchain

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	X	2474	0	2498	42	2
2	X	5	0	0	0	0
3	X	1	0	0	0	0
4	X	356	0	0	15	5
All	All	2836	0	2498	42	5

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 8.

All (42) 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:X:321:PHE:HA	4:X:732:HOH:O	1.09	1.23
1:X:300:HIS:HE1	4:X:724:HOH:O	1.49	0.94
1:X:287:ARG:NH2	4:X:738:HOH:O	2.02	0.93
1:X:70:VAL:HB	1:X:71:PRO:CD	2.06	0.85
1:X:321:PHE:CD1	4:X:732:HOH:O	2.32	0.81
1:X:70:VAL:HB	1:X:71:PRO:HD3	1.66	0.77
1:X:279:TYR:CD2	1:X:320:PRO:HD2	2.25	0.71
1:X:279:TYR:CE2	1:X:320:PRO:HD2	2.26	0.70
1:X:321:PHE:CA	4:X:732:HOH:O	1.91	0.69
1:X:165:LEU:HD11	1:X:376:LEU:HD21	1.79	0.63
1:X:72:LEU:HD12	1:X:291:ARG:NH1	2.17	0.60
1:X:72:LEU:HD12	1:X:291:ARG:HH12	1.67	0.59
1:X:300:HIS:HD2	1:X:308:HIS:ND1	2.03	0.57
1:X:233:PRO:HG2	4:X:684:HOH:O	2.03	0.57
1:X:234:LYS:NZ	4:X:675:HOH:O	2.38	0.56
1:X:207:ARG:HG3	1:X:207:ARG:NH1	2.20	0.55
1:X:321:PHE:CG	4:X:732:HOH:O	2.50	0.54
1:X:76:LEU:HD22	1:X:80:ARG:HD2	1.90	0.53
1:X:207:ARG:HG3	1:X:207:ARG:HH11	1.72	0.53
1:X:279:TYR:CE2	1:X:320:PRO:CD	2.91	0.53
1:X:161:ARG:HD2	1:X:261:ALA:HA	1.91	0.53
1:X:229:LYS:HZ3	1:X:229:LYS:HB3	1.71	0.53
1:X:229:LYS:HZ3	1:X:229:LYS:CB	2.22	0.53
1:X:258:ARG:HG2	4:X:514:HOH:O	2.08	0.52
1:X:161:ARG:HD2	1:X:261:ALA:C	2.34	0.52
1:X:161:ARG:CD	1:X:261:ALA:HA	2.41	0.50
1:X:257:THR:H	1:X:260:GLN:HE21	1.59	0.50
1:X:81:LEU:C	1:X:81:LEU:HD23	2.36	0.49
1:X:179:THR:HG22	4:X:631:HOH:O	2.12	0.49
1:X:180:PRO:HA	4:X:686:HOH:O	2.13	0.48
1:X:229:LYS:HZ2	1:X:229:LYS:HG3	1.17	0.47
1:X:156:ASP:OD2	1:X:158:ARG:HG2	2.15	0.47
1:X:310:GLN:HE21	1:X:313:MET:HE3	1.82	0.45
1:X:300:HIS:CE1	4:X:724:HOH:O	2.38	0.44
1:X:175:PRO:HA	1:X:176:PRO:HD3	1.91	0.43
1:X:229:LYS:HE3	4:X:638:HOH:O	2.19	0.42
1:X:257:THR:H	1:X:260:GLN:NE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:161:ARG:HD2	1:X:261:ALA:CA	2.50	0.41
1:X:117:LYS:HA	1:X:117:LYS:HD2	1.85	0.41
1:X:93:LEU:C	1:X:93:LEU:HD13	2.45	0.41
1:X:291:ARG:HD3	4:X:694:HOH:O	2.21	0.40
1:X:321:PHE:CB	4:X:732:HOH:O	2.50	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:754:HOH:O	4:X:755:HOH:O[3_555]	1.79	0.41
4:X:548:HOH:O	4:X:672:HOH:O[3_545]	1.82	0.38
4:X:600:HOH:O	4:X:618:HOH:O[4_456]	1.95	0.25
1:X:147:ASP:OD2	4:X:631:HOH:O[4_566]	2.00	0.20
1:X:71:PRO:CG	4:X:726:HOH:O[3_545]	2.18	0.02

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	X	311/330 (94%)	302 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	X	271/286 (95%)	269 (99%)	2 (1%)	76 49

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	70	VAL
1	X	93	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	131	HIS
1	X	260	GLN
1	X	300	HIS
1	X	303	ASN
1	X	310	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CAC	X	390	3	2,4,4	1.05	0	4,6,6	2.30	1 (25%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	390	CAC	O1-AS-C2	-4.02	106.50	111.50

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
1	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	323:SER	C	324:VAL	N	1.19

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	X	312/330 (94%)	1.45	78 (25%) 2 2	6, 11, 23, 32	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	321	PHE	11.1
1	X	70	VAL	7.6
1	X	79	ALA	6.6
1	X	322	GLY	6.0
1	X	320	PRO	5.9
1	X	323	SER	5.5
1	X	180	PRO	5.0
1	X	74	GLY	4.7
1	X	72	LEU	4.4
1	X	179	THR	4.3
1	X	176	PRO	4.2
1	X	71	PRO	4.1
1	X	174	PHE	4.0
1	X	77	PRO	4.0
1	X	178	SER	3.9
1	X	76	LEU	3.9
1	X	134	LEU	3.9
1	X	73	ILE	3.8
1	X	175	PRO	3.7
1	X	214	PRO	3.5
1	X	177	GLY	3.5
1	X	381	GLY	3.5
1	X	208	ALA	3.5
1	X	317	PRO	3.5
1	X	312	VAL	3.4
1	X	382	LEU	3.4
1	X	251	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	X	205	LEU	3.4
1	X	233	PRO	3.4
1	X	203	LEU	3.4
1	X	81	LEU	3.1
1	X	83	ARG	3.1
1	X	319	GLU	3.1
1	X	84	VAL	3.0
1	X	213	ALA	3.0
1	X	231	TRP	3.0
1	X	250	ILE	2.9
1	X	380	LEU	2.9
1	X	288	TRP	2.9
1	X	127	THR	2.9
1	X	309	PRO	2.9
1	X	306	GLN	2.8
1	X	85	VAL	2.8
1	X	158	ARG	2.8
1	X	215	VAL	2.7
1	X	324	VAL	2.7
1	X	303	ASN	2.6
1	X	80	ARG	2.6
1	X	245	GLN	2.6
1	X	133	GLU	2.6
1	X	161	ARG	2.6
1	X	212	ALA	2.6
1	X	379	TYR	2.5
1	X	207	ARG	2.5
1	X	291	ARG	2.4
1	X	211	GLN	2.4
1	X	249	SER	2.4
1	X	301	ARG	2.3
1	X	136	PRO	2.3
1	X	302	LEU	2.3
1	X	146	VAL	2.2
1	X	75	SER	2.2
1	X	248	GLU	2.2
1	X	132	VAL	2.2
1	X	222	LEU	2.1
1	X	333	ARG	2.1
1	X	345	PRO	2.1
1	X	138	THR	2.1
1	X	305	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	376	LEU	2.1
1	X	140	SER	2.1
1	X	353	PRO	2.1
1	X	210	LYS	2.1
1	X	304	LEU	2.0
1	X	78	GLU	2.0
1	X	256	PRO	2.0
1	X	274	PRO	2.0
1	X	137	PHE	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](#)

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($\text{\AA}^2$)	Q<0.9
2	CAC	X	390	5/5	1.00	0.06	8,8,10,10	0
3	ZN	X	400	1/1	1.00	0.02	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.