



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 2NX9 / pdb_00002nx9
Title : Crystal structure of the carboxyltransferase domain of the oxaloacetate decarboxylase Na⁺ pump from *Vibrio cholerae*
Authors : Studer, R.; Dimroth, P.
Deposited on : 2006-11-17
Resolution : 1.70 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

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

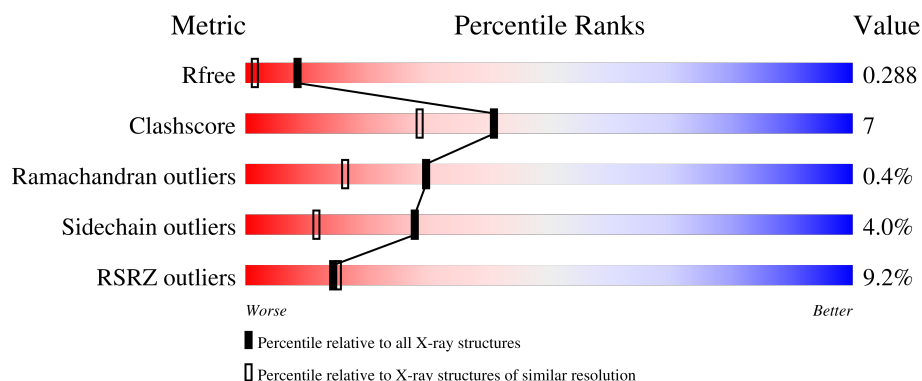
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 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	464	
1	B	464	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7541 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 Oxaloacetate decarboxylase 2, subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	1	0
			3492	2202	608	661	21			
1	B	453	Total	C	N	O	S	0	1	0
			3508	2211	611	665	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	cloning artifact	UNP Q6A1F6
A	458	GLU	-	cloning artifact	UNP Q6A1F6
A	459	HIS	-	expression tag	UNP Q6A1F6
A	460	HIS	-	expression tag	UNP Q6A1F6
A	461	HIS	-	expression tag	UNP Q6A1F6
A	462	HIS	-	expression tag	UNP Q6A1F6
A	463	HIS	-	expression tag	UNP Q6A1F6
A	464	HIS	-	expression tag	UNP Q6A1F6
B	457	LEU	-	cloning artifact	UNP Q6A1F6
B	458	GLU	-	cloning artifact	UNP Q6A1F6
B	459	HIS	-	expression tag	UNP Q6A1F6
B	460	HIS	-	expression tag	UNP Q6A1F6
B	461	HIS	-	expression tag	UNP Q6A1F6
B	462	HIS	-	expression tag	UNP Q6A1F6
B	463	HIS	-	expression tag	UNP Q6A1F6
B	464	HIS	-	expression tag	UNP Q6A1F6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	315	Total 315	O 315	0	0
3	B	224	Total 224	O 224	0	0

- Molecule 1: Oxaloacetate decarboxylase 2, subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.83Å 91.66Å 116.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.70 35.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.00-1.70) 98.5 (35.00-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.284 0.238 , 0.288	Depositor DCC
R_{free} test set	5272 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7541	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

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	0.87	1/3551 (0.0%)	1.12	12/4817 (0.2%)
1	B	0.69	1/3567 (0.0%)	0.98	7/4839 (0.1%)
All	All	0.78	2/7118 (0.0%)	1.05	19/9656 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	HIS	ND1-CE1	6.78	1.39	1.32
1	B	209	HIS	ND1-CE1	5.05	1.37	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	VAL	N-CA-C	6.71	117.50	108.11
1	A	77	MET	CA-C-N	5.89	125.51	119.56
1	A	77	MET	C-N-CA	5.89	125.51	119.56
1	B	207	HIS	CG-CD2-NE2	5.65	112.85	107.20
1	B	250	VAL	N-CA-C	5.65	116.29	110.36
1	A	209	HIS	CG-CD2-NE2	5.54	112.73	107.20
1	A	152	SER	CA-C-N	5.49	125.16	119.56
1	A	152	SER	C-N-CA	5.49	125.16	119.56
1	A	214	LEU	N-CA-C	-5.41	107.33	114.31
1	A	178	LYS	N-CA-CB	-5.41	102.22	110.65
1	A	173	ASP	N-CA-C	-5.39	105.84	112.90
1	B	209	HIS	CG-CD2-NE2	5.30	112.50	107.20
1	B	215	ALA	N-CA-C	5.28	117.03	111.28
1	A	328	ILE	CB-CA-C	-5.26	108.70	113.70
1	B	145	GLY	N-CA-C	-5.21	105.64	112.82
1	B	363	LYS	N-CA-C	-5.20	105.61	111.28
1	B	207	HIS	CE1-NE2-CD2	-5.13	103.87	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	THR	CA-C-N	5.09	124.70	119.05
1	A	185	THR	C-N-CA	5.09	124.70	119.05

There are no chirality outliers.

There are no planarity outliers.

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	A	3492	0	3533	51	0
1	B	3508	0	3548	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	315	0	0	0	0
3	B	224	0	0	0	0
All	All	7541	0	7081	92	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 7.

All (92) 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:316:ASN:HB2	1:B:317:ALA:HA	1.19	1.09
1:B:148:CYS:SG	1:B:178:LYS:NZ	2.41	0.94
1:A:246:THR:O	1:A:250:VAL:HG23	1.73	0.89
1:B:316:ASN:HB2	1:B:317:ALA:CA	2.03	0.88
1:B:394:ALA:H	1:B:395:GLY:HA2	1.43	0.84
1:A:425:GLN:HE21	1:A:425:GLN:HA	1.43	0.81
1:B:316:ASN:CB	1:B:317:ALA:HA	2.05	0.76
1:B:122:ALA:O	1:B:339:PRO:HG2	1.86	0.76
1:B:108:ARG:HD3	1:B:435:ASP:OD1	1.91	0.70
1:B:12:ASP:HB2	1:B:44:TYR:CE1	2.26	0.69
1:A:126:VAL:HA	1:A:129:MET:HE3	1.74	0.69
1:A:74:LYS:HE2	1:A:113:GLY:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ALA:N	1:B:395:GLY:HA2	2.08	0.68
1:A:175:ILE:HD12	1:A:202:VAL:HG21	1.75	0.67
1:B:330:ARG:HB3	1:B:361:ARG:HH22	1.60	0.67
1:A:107:GLU:O	1:A:111:LYS:HG2	1.95	0.67
1:A:288:MET:HE1	1:A:292:ASP:HB2	1.77	0.66
1:A:338:LEU:HD22	1:A:344:THR:CG2	2.25	0.66
1:A:308:MET:HE1	1:A:328:ILE:HD11	1.77	0.66
1:B:175:ILE:HD12	1:B:202:VAL:HG21	1.79	0.65
1:A:148:CYS:SG	1:A:178:LYS:NZ	2.70	0.64
1:B:108:ARG:HD2	1:B:434:ILE:HG23	1.80	0.63
1:A:215:ALA:O	1:A:219:LEU:HD13	1.97	0.63
1:A:288:MET:CE	1:A:292:ASP:HB2	2.30	0.61
1:B:29:ILE:HD13	1:B:69:ARG:HG3	1.84	0.60
1:B:157:LEU:O	1:B:161:VAL:HG23	2.02	0.59
1:A:132:ALA:O	1:A:136:VAL:HG23	2.04	0.58
1:A:123:MET:HE2	1:A:338:LEU:HD23	1.85	0.57
1:A:338:LEU:HD22	1:A:344:THR:HG23	1.86	0.57
1:B:104:THR:HG21	1:B:411:MET:HE2	1.87	0.56
1:A:288:MET:O	1:A:288:MET:HG3	2.06	0.56
1:B:97:TYR:OH	1:B:442:LEU:HA	2.06	0.55
1:A:200:VAL:HG12	1:A:202:VAL:HG22	1.88	0.55
1:A:15:LEU:O	1:A:19:HIS:HE1	1.90	0.55
1:B:328:ILE:HB	1:B:329:PRO:HD3	1.87	0.55
1:A:19:HIS:HD2	1:A:25:THR:HA	1.71	0.55
1:B:108:ARG:HD2	1:B:434:ILE:CG2	2.36	0.55
1:B:132:ALA:O	1:B:136:VAL:HG23	2.06	0.54
1:A:425:GLN:HA	1:A:425:GLN:NE2	2.19	0.54
1:A:10:VAL:O	1:A:45:TRP:N	2.36	0.52
1:A:349:GLY:O	1:A:353:VAL:HG23	2.10	0.52
1:B:156:ASN:OD1	1:B:158:GLN:HG2	2.10	0.52
1:A:304:MET:HG2	1:A:308:MET:HE2	1.91	0.52
1:B:276:ASP:O	1:B:279:LYS:HB2	2.10	0.51
1:A:336:GLY:O	1:A:381:PRO:HD2	2.10	0.51
1:A:35:ILE:O	1:A:35:ILE:HG13	2.11	0.51
1:A:87:ARG:O	1:A:87:ARG:CG	2.58	0.51
1:B:230:VAL:HG21	1:B:249:LEU:CD2	2.42	0.50
1:A:87:ARG:O	1:A:87:ARG:HG2	2.12	0.50
1:A:133:LEU:CD2	1:A:143:ALA:HB1	2.42	0.49
1:A:29:ILE:HD13	1:A:69:ARG:HG3	1.93	0.49
1:A:65:ASP:HB3	1:A:68:GLN:HB3	1.95	0.49
1:B:8:VAL:HG23	1:B:258:TYR:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD22	1:A:344:THR:HG21	1.94	0.48
1:A:133:LEU:HD23	1:A:143:ALA:HB1	1.96	0.48
1:B:163:VAL:HA	1:B:166:GLN:HE21	1.77	0.48
1:B:223:ILE:HA	1:B:227:VAL:HG12	1.96	0.47
1:A:219:LEU:HD22	1:A:244:PRO:HG2	1.97	0.47
1:B:223:ILE:HD13	1:B:253:LEU:HD11	1.96	0.47
1:B:258:TYR:O	1:B:259:ASP:C	2.59	0.46
1:B:393:LEU:HB3	1:B:396:ALA:H	1.80	0.46
1:A:11:THR:HA	1:A:46:SER:O	2.15	0.46
1:B:126:VAL:HA	1:B:129:MET:HE3	1.96	0.45
1:B:23:PHE:HB2	1:B:284:PHE:HB2	1.99	0.45
1:B:35:ILE:HD11	1:B:270:ILE:HA	1.97	0.45
1:B:386:THR:HA	1:B:387:GLU:HA	1.69	0.45
1:A:187:TYR:CD2	1:B:256:THR:HG21	2.52	0.45
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.78	0.45
1:B:315:GLN:HB3	1:B:316:ASN:C	2.41	0.45
1:A:316:ASN:CG	1:A:317:ALA:H	2.24	0.44
1:A:142:HIS:CD2	1:A:142:HIS:C	2.94	0.44
1:A:347:ILE:HG12	1:A:368:GLU:HB3	2.00	0.44
1:B:35:ILE:HD13	1:B:273:TYR:CG	2.53	0.44
1:B:387:GLU:HB2	1:B:390:ALA:HB3	1.98	0.44
1:A:311:GLN:HE22	1:A:350:THR:HA	1.83	0.44
1:A:37:GLN:O	1:A:41:GLN:HG2	2.18	0.42
1:A:137:LYS:HB3	1:A:137:LYS:HE3	1.83	0.42
1:A:18:ALA:O	1:A:22:LEU:HG	2.20	0.42
1:B:394:ALA:N	1:B:395:GLY:CA	2.80	0.42
1:A:18:ALA:O	1:A:22:LEU:HB2	2.20	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.87	0.42
1:A:23:PHE:HB2	1:A:284:PHE:HB2	2.02	0.41
1:A:223:ILE:HD13	1:A:253:LEU:HD11	2.01	0.41
1:A:411:MET:HE2	1:A:434:ILE:HD11	2.02	0.41
1:B:219:LEU:HD22	1:B:244:PRO:HG2	2.02	0.41
1:A:65:ASP:OD1	1:A:67:TRP:HB2	2.21	0.41
1:B:178:LYS:HE2	1:B:180:MET:HE3	2.02	0.41
1:B:347:ILE:HG12	1:B:368:GLU:HB3	2.02	0.41
1:A:258:TYR:O	1:A:259:ASP:C	2.64	0.41
1:B:312:LEU:O	1:B:316:ASN:HA	2.21	0.41
1:A:308:MET:CE	1:A:328:ILE:HD11	2.50	0.40
1:B:197:LYS:HA	1:B:197:LYS:HD2	1.89	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	450/464 (97%)	431 (96%)	16 (4%)	3 (1%)	18	7
1	B	452/464 (97%)	435 (96%)	16 (4%)	1 (0%)	43	28
All	All	902/928 (97%)	866 (96%)	32 (4%)	4 (0%)	30	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ALA
1	B	394	ALA
1	A	259	ASP
1	A	316	ASN

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	374/386 (97%)	357 (96%)	17 (4%)	24	9
1	B	376/386 (97%)	363 (96%)	13 (4%)	32	15
All	All	750/772 (97%)	720 (96%)	30 (4%)	28	12

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	50	TRP

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Mol	Chain	Res	Type
1	A	70	LEU
1	A	110	VAL
1	A	138	LYS
1	A	151	THR
1	A	178	LYS
1	A	202	VAL
1	A	227	VAL
1	A	288	MET
1	A	338	LEU
1	A	341	VAL
1	A	386	THR
1	A	413	THR
1	A	425	GLN
1	A	434	ILE
1	A	454	ARG
1	B	2	THR
1	B	25	THR
1	B	30	ASP
1	B	50	TRP
1	B	134	GLN
1	B	138	LYS
1	B	169	GLU
1	B	178	LYS
1	B	288	MET
1	B	315	GLN
1	B	338	LEU
1	B	391	ARG
1	B	397	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	90	ASN
1	A	134	GLN
1	A	307	ASN
1	A	311	GLN
1	A	425	GLN
1	B	19	HIS
1	B	90	ASN
1	B	112	ASN
1	B	158	GLN

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Mol	Chain	Res	Type
1	B	166	GLN
1	B	314	GLN
1	B	315	GLN
1	B	346	GLN
1	B	385	ASN
1	B	425	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, 2 are 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](#)

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	451/464 (97%)	0.45	30 (6%) 24 26	3, 16, 37, 57	1 (0%)
1	B	453/464 (97%)	0.70	53 (11%) 9 9	5, 19, 39, 49	1 (0%)
All	All	904/928 (97%)	0.58	83 (9%) 14 15	3, 17, 38, 57	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	ALA	8.4
1	B	430	ALA	4.8
1	B	394	ALA	4.5
1	B	386	THR	4.2
1	A	412	PRO	3.8
1	B	413	THR	3.8
1	A	317	ALA	3.8
1	B	419	LEU	3.6
1	B	435	ASP	3.5
1	B	454	ARG	3.5
1	B	439	THR	3.3
1	B	428	THR	3.3
1	B	412	PRO	3.3
1	B	438	LEU	3.3
1	B	420	GLN	3.2
1	B	433	ALA	3.2
1	B	429	LEU	3.1
1	B	453	ASN	3.1
1	A	419	LEU	3.0
1	A	312	LEU	2.9
1	A	357	VAL	2.9
1	A	428	THR	2.9
1	B	401	CYS	2.9
1	B	448	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	433	ALA	2.8
1	B	414	LEU	2.8
1	A	446	VAL	2.8
1	A	306	THR	2.8
1	A	452	ALA	2.7
1	A	430	ALA	2.7
1	B	98	ALA	2.7
1	B	316	ASN	2.7
1	B	384	VAL	2.7
1	B	416	ASP	2.7
1	A	409	ALA	2.7
1	B	452	ALA	2.7
1	A	395	GLY	2.6
1	B	436	ASP	2.6
1	A	434	ILE	2.6
1	B	396	ALA	2.6
1	B	450	PHE	2.5
1	A	440	ILE	2.5
1	A	413	THR	2.5
1	B	411	MET	2.5
1	A	318	LEU	2.5
1	A	321	LEU	2.5
1	B	317	ALA	2.5
1	B	404	ALA	2.5
1	A	418	VAL	2.5
1	B	431	GLU	2.5
1	B	2	THR	2.4
1	B	446	VAL	2.4
1	A	422	ALA	2.4
1	A	316	ASN	2.3
1	B	158	GLN	2.3
1	B	427	ILE	2.3
1	B	441	ALA	2.3
1	A	429	LEU	2.3
1	B	318	LEU	2.2
1	B	337	PHE	2.2
1	B	387	GLU	2.2
1	B	392	VAL	2.2
1	B	364	THR	2.2
1	A	432	ASN	2.2
1	B	432	ASN	2.2
1	B	365	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	440	ILE	2.2
1	A	390	ALA	2.2
1	B	97	TYR	2.2
1	B	415	GLN	2.1
1	B	390	ALA	2.1
1	B	423	LYS	2.1
1	A	407	ILE	2.1
1	B	418	VAL	2.1
1	B	383	PRO	2.1
1	B	434	ILE	2.1
1	B	251	ALA	2.0
1	A	356	VAL	2.0
1	A	416	ASP	2.0
1	A	393	LEU	2.0
1	A	426	HIS	2.0
1	B	367	LYS	2.0
1	B	362	TYR	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	ZN	A	601	1/1	0.99	0.19	34,34,34,34	0
2	ZN	B	602	1/1	0.99	0.18	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.