



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 7N6H / pdb_00007n6h
Title : The crystal structure of the GH30 subfamily 10 enzyme, AcXbh30A from *Acetivibrio clariflavus*
Authors : Tan, K.; St John, F.J.
Deposited on : 2021-06-08
Resolution : 1.28 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

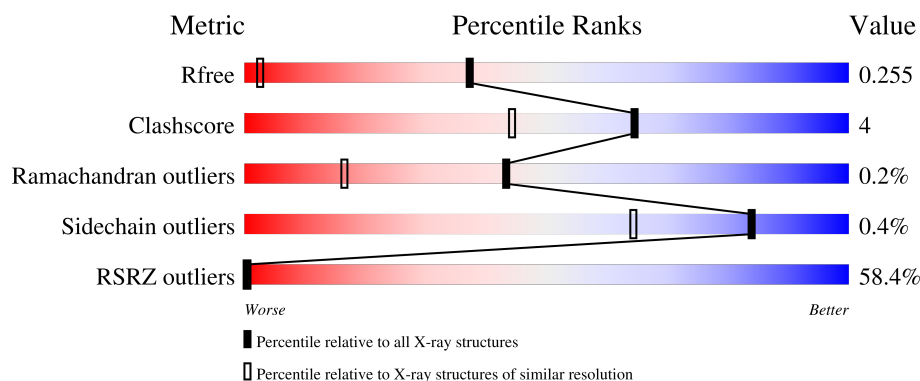
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.28 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	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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	444	61% 89% 8%
1	B	444	53% 88% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	508	-	-	X	-
2	CL	A	515	-	-	X	-
2	CL	B	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7649 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 AcXbh30A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	3	0
			3454	2194	570	679	11			
1	B	433	Total	C	N	O	S	0	1	0
			3443	2187	569	676	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP G8LU16
A	464	LEU	-	expression tag	UNP G8LU16
A	465	GLU	-	expression tag	UNP G8LU16
A	466	HIS	-	expression tag	UNP G8LU16
A	467	HIS	-	expression tag	UNP G8LU16
A	468	HIS	-	expression tag	UNP G8LU16
A	469	HIS	-	expression tag	UNP G8LU16
A	470	HIS	-	expression tag	UNP G8LU16
A	471	HIS	-	expression tag	UNP G8LU16
B	28	MET	-	initiating methionine	UNP G8LU16
B	464	LEU	-	expression tag	UNP G8LU16
B	465	GLU	-	expression tag	UNP G8LU16
B	466	HIS	-	expression tag	UNP G8LU16
B	467	HIS	-	expression tag	UNP G8LU16
B	468	HIS	-	expression tag	UNP G8LU16
B	469	HIS	-	expression tag	UNP G8LU16
B	470	HIS	-	expression tag	UNP G8LU16
B	471	HIS	-	expression tag	UNP G8LU16

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

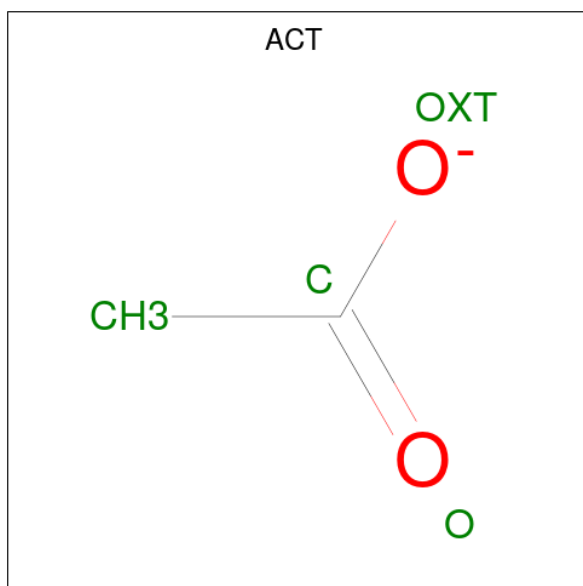
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	Cl	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total	Cl	0	0
			8	8		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

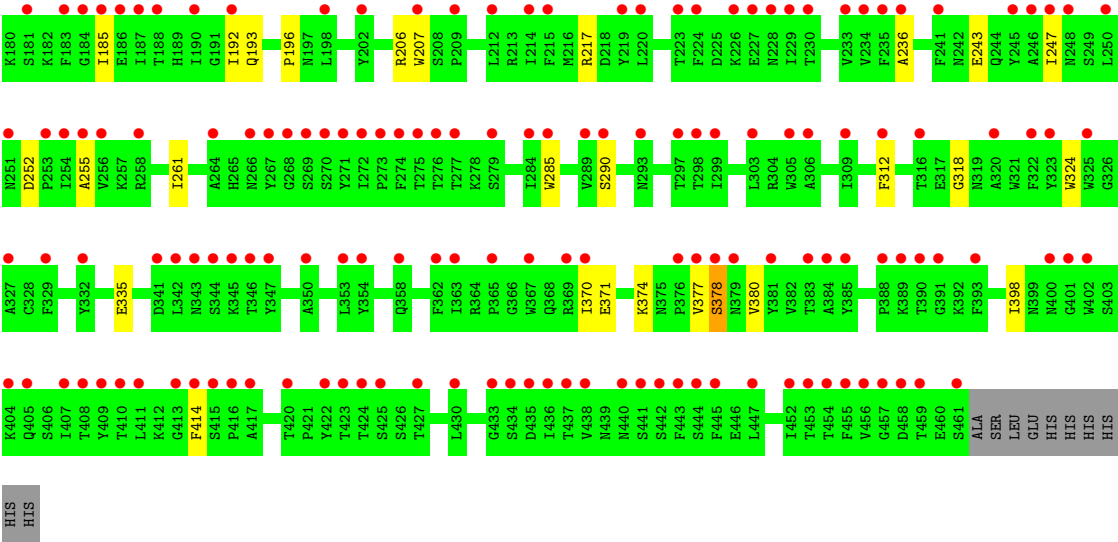


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	388	Total	O	0	0
			388	388		
4	B	329	Total	O	0	0
			329	329		





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.87Å 108.02Å 66.84Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	41.18 – 1.28 41.18 – 1.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (41.18-1.28) 96.3 (41.18-1.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.51 (at 1.28Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.202 , 0.254 0.202 , 0.255	Depositor DCC
R_{free} test set	10529 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.387 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: ACT, CL

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	0.07	0/3544	0.22	0/4821
1	B	0.07	0/3533	0.21	0/4806
All	All	0.07	0/7077	0.22	0/9627

There are no bond length outliers.

There are no bond angle outliers.

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	3454	0	3292	24	0
1	B	3443	0	3281	24	0
2	A	15	0	0	8	0
2	B	8	0	0	5	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	388	0	0	4	0
4	B	329	0	0	3	0
All	All	7649	0	6582	53	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 (53) 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)
2:A:510:CL:CL	4:A:896:HOH:O	2.38	0.78
1:A:213:ARG:NE	2:A:503:CL:CL	2.50	0.73
2:A:515:CL:CL	4:A:860:HOH:O	2.43	0.73
2:A:514:CL:CL	4:A:952:HOH:O	2.53	0.61
1:A:404:LYS:HG3	1:A:449:PRO:HD3	1.85	0.59
1:A:196:PRO:HG3	1:A:236:ALA:HB1	1.86	0.58
1:B:196:PRO:HG3	1:B:236:ALA:HB1	1.88	0.56
1:A:399:ASN:ND2	2:A:515:CL:CL	2.69	0.56
1:B:123:ILE:HG23	1:B:185:ILE:HD11	1.91	0.53
1:A:48:VAL:HG12	1:A:323:TYR:HB3	1.91	0.53
1:B:217:ARG:HA	4:B:728:HOH:O	2.09	0.53
1:A:171:TYR:O	1:A:175:HIS:ND1	2.39	0.52
1:B:98:ALA:N	2:B:508:CL:CL	2.80	0.52
2:B:503:CL:CL	4:B:902:HOH:O	2.56	0.51
1:A:249:SER:OG	2:A:508:CL:CL	2.61	0.51
1:A:36:TRP:HB2	1:A:414:PHE:CD1	2.46	0.51
1:B:36:TRP:HB2	1:B:414:PHE:CD1	2.46	0.51
1:B:290:SER:HB2	1:B:335:GLU:HA	1.94	0.49
1:B:252:ASP:HB3	1:B:255:ALA:HB3	1.95	0.49
1:A:290:SER:HB2	1:A:335:GLU:HA	1.94	0.48
1:A:123:ILE:HG23	1:A:185:ILE:HD11	1.95	0.48
1:B:104:LYS:HG2	2:B:505:CL:CL	2.52	0.46
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.68	0.46
1:B:374:LYS:HE2	1:B:374:LYS:HB2	1.81	0.46
1:A:40:TYR:OH	1:A:371:GLU:OE2	2.34	0.46
1:A:130:GLN:HG2	1:A:135:VAL:O	2.16	0.45
1:B:312:PHE:CZ	1:B:318:GLY:HA3	2.51	0.45
1:B:206:ARG:O	2:B:507:CL:CL	2.72	0.45
1:B:149:MET:HE1	1:B:171:TYR:HB2	1.99	0.45
1:A:248:ASN:HB2	2:A:508:CL:CL	2.54	0.45
1:A:243:GLU:O	1:A:247:ILE:HG13	2.17	0.44
1:A:312:PHE:CZ	1:A:318:GLY:HA3	2.52	0.44
1:A:271:TYR:OH	1:A:308:GLU:OE1	2.22	0.44
1:A:377:VAL:HG22	1:A:378:SER:H	1.83	0.44
1:A:412:LYS:NZ	4:A:628:HOH:O	2.49	0.44
1:B:243:GLU:O	1:B:247:ILE:HG13	2.17	0.43
1:A:249:SER:N	2:A:508:CL:CL	2.89	0.43
1:B:39:THR:HG22	1:B:370:ILE:HG22	2.00	0.43
1:B:171:TYR:O	1:B:175:HIS:ND1	2.49	0.43
1:A:107:GLN:HB2	1:A:113:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASP:HB3	1:B:371:GLU:HB3	2.00	0.42
2:B:503:CL:CL	4:B:642:HOH:O	2.59	0.42
1:B:78:ASP:N	1:B:78:ASP:OD1	2.51	0.41
1:A:196:PRO:HB2	1:A:207:TRP:HB2	2.01	0.41
1:B:130:GLN:HG2	1:B:135:VAL:O	2.19	0.41
1:B:168:TYR:OH	1:B:192:ILE:O	2.31	0.41
1:B:193:GLN:HG2	1:B:207:TRP:CD1	2.56	0.41
1:B:377:VAL:HG22	1:B:378:SER:H	1.85	0.41
1:A:193:GLN:HG2	1:A:207:TRP:CD1	2.56	0.41
1:B:380:VAL:HA	1:B:398:ILE:O	2.21	0.41
1:B:110:GLU:HB3	1:B:148:TRP:CZ3	2.56	0.40
1:A:404:LYS:H	1:A:404:LYS:HD2	1.84	0.40
1:B:261:ILE:HD13	1:B:285:TRP:CE2	2.56	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	433/444 (98%)	418 (96%)	14 (3%)	1 (0%)	43	16
1	B	432/444 (97%)	418 (97%)	13 (3%)	1 (0%)	43	16
All	All	865/888 (97%)	836 (97%)	27 (3%)	2 (0%)	43	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	TRP
1	B	324	TRP

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	376/384 (98%)	374 (100%)	2 (0%)	81	59
1	B	374/384 (97%)	373 (100%)	1 (0%)	86	66
All	All	750/768 (98%)	747 (100%)	3 (0%)	84	64

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	TRP
1	A	430	LEU
1	B	378	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	166	GLN
1	A	295	ASN
1	A	339	GLN
1	A	375	ASN
1	A	379	ASN
1	A	399	ASN
1	B	116	ASN
1	B	166	GLN
1	B	339	GLN
1	B	358	GLN

5.3.3 RNA

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 26 ligands modelled in this entry, 23 are monoatomic - leaving 3 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	$\# Z > 2$
3	ACT	A	517	-	3,3,3	1.33	0	3,3,3	1.30	0
3	ACT	A	516	-	3,3,3	1.35	0	3,3,3	1.39	0
3	ACT	B	509	-	3,3,3	1.36	0	3,3,3	1.26	0

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	433/444 (97%)	2.56	270 (62%) 0 0	7, 15, 21, 38	2 (0%)
1	B	433/444 (97%)	2.41	236 (54%) 0 0	8, 14, 21, 34	1 (0%)
All	All	866/888 (97%)	2.49	506 (58%) 0 0	7, 14, 21, 38	3 (0%)

All (506) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	ALA	8.1
1	B	123	ILE	8.0
1	A	456[A]	VAL	7.6
1	B	108	PRO	7.4
1	A	329	PHE	7.3
1	A	32	VAL	7.0
1	A	394	ALA	6.8
1	A	274	PHE	6.4
1	A	259	VAL	6.4
1	A	138	ILE	6.3
1	A	129	ILE	6.3
1	A	113	TRP	6.2
1	B	402	TRP	6.1
1	B	250	LEU	6.1
1	A	338	ILE	6.0
1	A	30	SER	6.0
1	B	31	THR	6.0
1	A	349	VAL	5.9
1	A	417	ALA	5.9
1	B	409	TYR	5.7
1	B	461	SER	5.6
1	B	272	ILE	5.5
1	B	171	TYR	5.5
1	A	29	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	115	TRP	5.5
1	B	306	ALA	5.5
1	B	198	LEU	5.4
1	B	156	VAL	5.3
1	B	274	PHE	5.3
1	A	416	PRO	5.3
1	A	293	ASN	5.3
1	A	303	LEU	5.2
1	B	82	PHE	5.2
1	A	439	ASN	5.2
1	A	207	TRP	5.1
1	A	408	THR	5.1
1	B	112	VAL	5.1
1	A	309	ILE	5.1
1	A	31	THR	5.0
1	A	391	GLY	5.0
1	A	324	TRP	5.0
1	B	30	SER	5.0
1	A	359	PHE	5.0
1	A	393	PHE	5.0
1	A	332	TYR	4.9
1	A	94	THR	4.9
1	B	246	ALA	4.9
1	B	143	TRP	4.9
1	B	219	TYR	4.9
1	B	89	LEU	4.9
1	B	109	ALA	4.9
1	B	456	VAL	4.8
1	A	370	ILE	4.8
1	A	390	THR	4.7
1	B	235	PHE	4.7
1	B	417	ALA	4.7
1	B	447	LEU	4.7
1	A	392	LYS	4.7
1	B	172	LEU	4.6
1	A	239	MET	4.6
1	A	424	THR	4.6
1	B	212	LEU	4.6
1	B	445	PHE	4.6
1	B	284	ILE	4.5
1	A	249	SER	4.5
1	A	62	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	33	THR	4.5
1	B	390	THR	4.5
1	A	198	LEU	4.5
1	B	77	THR	4.4
1	A	292	MET	4.4
1	A	128	ALA	4.4
1	B	46	PHE	4.4
1	B	393	PHE	4.4
1	A	42	THR	4.4
1	A	452	ILE	4.4
1	A	221	VAL	4.3
1	B	414	PHE	4.3
1	A	461	SER	4.3
1	A	84	ILE	4.3
1	A	331	THR	4.3
1	A	34	VAL	4.3
1	A	145	PRO	4.3
1	A	48	VAL	4.3
1	A	215	PHE	4.3
1	A	362	PHE	4.3
1	A	247	ILE	4.2
1	B	247	ILE	4.2
1	A	245	TYR	4.2
1	A	271	TYR	4.2
1	B	332	TYR	4.2
1	B	440	ASN	4.2
1	A	61	LEU	4.2
1	B	187	ILE	4.2
1	A	172	LEU	4.2
1	A	315	ILE	4.2
1	A	246	ALA	4.1
1	B	168	TYR	4.1
1	B	327	ALA	4.1
1	A	139	LEU	4.1
1	A	413	GLY	4.1
1	B	184	GLY	4.1
1	B	139	LEU	4.0
1	A	299	ILE	4.0
1	A	79	GLY	4.0
1	B	379	ASN	4.0
1	B	441	SER	4.0
1	A	458	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	51	ALA	4.0
1	B	32	VAL	4.0
1	B	376	PRO	4.0
1	A	302	GLY	4.0
1	A	279	SER	3.9
1	B	146	PRO	3.9
1	B	285	TRP	3.9
1	A	69	ILE	3.9
1	A	105	THR	3.9
1	B	388	PRO	3.9
1	A	385	TYR	3.9
1	B	248	ASN	3.9
1	A	36	TRP	3.9
1	B	148	TRP	3.9
1	B	181	SER	3.9
1	B	430	LEU	3.9
1	A	64	THR	3.9
1	A	231	ALA	3.9
1	B	129	ILE	3.9
1	B	190	ILE	3.9
1	B	254	ILE	3.9
1	B	342	LEU	3.9
1	B	276	THR	3.8
1	A	43	ILE	3.8
1	A	411	LEU	3.8
1	B	416	PRO	3.8
1	A	88	ILE	3.8
1	B	38	THR	3.8
1	A	388	PRO	3.8
1	A	241	PHE	3.8
1	B	329	PHE	3.8
1	A	37	ASP	3.7
1	B	233	VAL	3.7
1	A	343	ASN	3.7
1	B	389	LYS	3.7
1	B	427	THR	3.7
1	A	379	ASN	3.7
1	A	168	TYR	3.7
1	B	133	TYR	3.7
1	A	281	GLY	3.7
1	B	175	HIS	3.6
1	A	444	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	133	TYR	3.6
1	B	202	TYR	3.6
1	A	190	ILE	3.6
1	B	192	ILE	3.6
1	B	411	LEU	3.6
1	B	410	THR	3.6
1	A	46	PHE	3.6
1	A	95	TRP	3.6
1	A	306	ALA	3.6
1	A	350	ALA	3.6
1	B	185	ILE	3.6
1	A	162	THR	3.6
1	B	424	THR	3.6
1	B	83	SER	3.6
1	B	344	SER	3.6
1	B	268	GLY	3.6
1	A	85	PHE	3.5
1	B	271	TYR	3.5
1	B	347	TYR	3.5
1	B	289	VAL	3.5
1	B	124	PRO	3.5
1	A	415	SER	3.5
1	B	370	ILE	3.5
1	A	334	GLY	3.5
1	A	449	PRO	3.5
1	B	273	PRO	3.5
1	A	414	PHE	3.5
1	A	378	SER	3.5
1	B	142	VAL	3.5
1	B	270	SER	3.4
1	B	165	TYR	3.4
1	B	343	ASN	3.4
1	B	354	TYR	3.4
1	A	419	VAL	3.4
1	B	377	VAL	3.4
1	A	76	THR	3.4
1	B	290	SER	3.4
1	A	72	LEU	3.4
1	B	381	TYR	3.4
1	A	136	ASP	3.4
1	B	153	GLY	3.4
1	A	402	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	189	HIS	3.4
1	A	63[A]	GLU	3.4
1	B	78	ASP	3.3
1	B	442[A]	SER	3.3
1	A	437	THR	3.3
1	B	223	THR	3.3
1	A	185	ILE	3.3
1	A	192	ILE	3.3
1	B	229	ILE	3.3
1	A	115	TRP	3.3
1	B	113	TRP	3.3
1	A	92	GLY	3.3
1	B	140	TYR	3.3
1	B	183	PHE	3.3
1	B	234	VAL	3.3
1	A	328	CYS	3.3
1	A	457	GLY	3.3
1	A	430	LEU	3.3
1	A	323	TYR	3.3
1	A	438	VAL	3.3
1	B	438	VAL	3.3
1	B	138	ILE	3.3
1	B	363	ILE	3.3
1	B	413	GLY	3.3
1	B	37	ASP	3.2
1	A	102	PRO	3.2
1	A	78	ASP	3.2
1	A	356	ILE	3.2
1	B	104	LYS	3.2
1	A	440	ASN	3.2
1	B	160	LEU	3.2
1	B	120	ASP	3.2
1	A	313	MET	3.2
1	A	423	THR	3.2
1	B	277	THR	3.2
1	B	437	THR	3.2
1	A	442[B]	SER	3.2
1	A	222	PRO	3.2
1	A	321	TRP	3.2
1	A	404	LYS	3.2
1	B	422	TYR	3.1
1	B	454	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	135	VAL	3.1
1	B	241	PHE	3.1
1	B	136	ASP	3.1
1	B	88	ILE	3.1
1	B	457	GLY	3.1
1	B	207	TRP	3.1
1	A	223	THR	3.1
1	A	275	THR	3.1
1	B	188	THR	3.1
1	A	229	ILE	3.1
1	B	111	ASP	3.1
1	A	459	THR	3.1
1	B	179	TYR	3.1
1	A	235	PHE	3.1
1	B	369	ARG	3.0
1	A	436	ILE	3.0
1	A	264	ALA	3.0
1	A	298	THR	3.0
1	B	73	LEU	3.0
1	A	197	ASN	3.0
1	A	285	TRP	3.0
1	A	325	TRP	3.0
1	B	367	TRP	3.0
1	A	347	TYR	3.0
1	B	245	TYR	3.0
1	A	280	LYS	3.0
1	B	226	LYS	3.0
1	A	82	PHE	3.0
1	A	38	THR	3.0
1	A	297	THR	3.0
1	B	459	THR	3.0
1	A	147	ALA	3.0
1	A	284	ILE	3.0
1	B	279	SER	3.0
1	A	143	TRP	3.0
1	A	380	VAL	3.0
1	B	400	ASN	3.0
1	A	89	LEU	3.0
1	A	86	ARG	2.9
1	A	111	ASP	2.9
1	A	175	HIS	2.9
1	A	196	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	443	PHE	2.9
1	A	353	LEU	2.9
1	A	371	GLU	2.9
1	B	69	ILE	2.9
1	B	341	ASP	2.9
1	A	154	SER	2.9
1	B	162	THR	2.9
1	A	354	TYR	2.9
1	A	377	VAL	2.9
1	B	209	PRO	2.9
1	A	40	TYR	2.9
1	A	267	TYR	2.9
1	A	396	VAL	2.9
1	A	224	PHE	2.8
1	A	447	LEU	2.8
1	A	58	ILE	2.8
1	A	176	ILE	2.8
1	A	214	ILE	2.8
1	B	84	ILE	2.8
1	B	214	ILE	2.8
1	B	407	ILE	2.8
1	B	436	ILE	2.8
1	A	248	ASN	2.8
1	A	236	ALA	2.8
1	B	255	ALA	2.8
1	A	134	GLY	2.8
1	A	256	VAL	2.8
1	B	48	VAL	2.8
1	A	260	ASP	2.8
1	A	74	PHE	2.8
1	B	52	PHE	2.8
1	A	305	TRP	2.8
1	B	152	ASN	2.8
1	A	108	PRO	2.8
1	B	159	SER	2.8
1	A	66	GLN	2.8
1	A	70	TYR	2.8
1	A	112	VAL	2.8
1	A	152	ASN	2.8
1	B	141	THR	2.8
1	B	303	LEU	2.8
1	A	146	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	395	ILE	2.8
1	B	43	ILE	2.8
1	B	251	ASN	2.7
1	B	345	LYS	2.7
1	A	410	THR	2.7
1	A	420	THR	2.7
1	A	118	SER	2.7
1	B	434	SER	2.7
1	A	155	VAL	2.7
1	B	256	VAL	2.7
1	B	458	ASP	2.7
1	A	337	LEU	2.7
1	B	415	SER	2.7
1	A	454	THR	2.7
1	B	266	ASN	2.7
1	A	160	LEU	2.7
1	A	446	GLU	2.7
1	A	376	PRO	2.7
1	B	117	GLU	2.7
1	A	342	LEU	2.7
1	B	72	LEU	2.7
1	A	445	PHE	2.6
1	B	147	ALA	2.6
1	B	350	ALA	2.6
1	B	39	THR	2.6
1	A	251	ASN	2.6
1	B	116	ASN	2.6
1	A	398	ILE	2.6
1	B	253	PRO	2.6
1	A	369	ARG	2.6
1	B	378	SER	2.6
1	A	448	ALA	2.6
1	B	173	ALA	2.6
1	B	408	THR	2.6
1	B	99	ASP	2.6
1	B	322	PHE	2.6
1	A	434	SER	2.6
1	A	407	ILE	2.6
1	A	412	LYS	2.6
1	B	267	TYR	2.6
1	B	61	LEU	2.6
1	B	220	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	230	THR	2.6
1	A	441	SER	2.6
1	A	443	PHE	2.6
1	B	312	PHE	2.6
1	B	293	ASN	2.6
1	B	299	ILE	2.6
1	A	35	ASP	2.5
1	B	36	TRP	2.5
1	A	170	THR	2.5
1	A	202	TYR	2.5
1	B	151	THR	2.5
1	A	451	SER	2.5
1	A	300	ASN	2.5
1	A	123	ILE	2.5
1	A	261	ILE	2.5
1	A	403	SER	2.5
1	A	200	THR	2.5
1	A	206	ARG	2.5
1	A	397	ALA	2.5
1	A	233	VAL	2.5
1	B	227	GLU	2.5
1	A	263	GLY	2.5
1	B	215	PHE	2.5
1	B	224	PHE	2.5
1	B	455	PHE	2.5
1	A	368	GLN	2.5
1	A	114	ASP	2.5
1	A	169	ALA	2.5
1	B	384	ALA	2.5
1	A	250	LEU	2.5
1	A	234	VAL	2.5
1	A	348	LYS	2.5
1	B	383	THR	2.4
1	B	74	PHE	2.4
1	A	96	GLY	2.4
1	B	297	THR	2.4
1	B	346	THR	2.4
1	A	330	LYS	2.4
1	A	131	SER	2.4
1	A	363	ILE	2.4
1	B	126	ILE	2.4
1	A	460	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	97	ASN	2.4
1	B	97	ASN	2.4
1	A	381	TYR	2.4
1	A	422	TYR	2.4
1	A	39	THR	2.4
1	A	291	ASP	2.4
1	B	71	ASP	2.4
1	B	121	ASP	2.4
1	A	45	GLY	2.4
1	B	452	ILE	2.3
1	A	212	LEU	2.3
1	A	346	THR	2.3
1	B	40	TYR	2.3
1	A	60	ARG	2.3
1	A	217	ARG	2.3
1	B	433	GLY	2.3
1	A	173	ALA	2.3
1	B	58	ILE	2.3
1	B	269	SER	2.3
1	B	309	ILE	2.3
1	A	289	VAL	2.3
1	B	34	VAL	2.3
1	B	435	ASP	2.3
1	A	228	ASN	2.3
1	B	56	ASN	2.3
1	B	47	GLY	2.3
1	B	134	GLY	2.3
1	B	401	GLY	2.3
1	B	70	TYR	2.3
1	B	323	TYR	2.3
1	A	218	ASP	2.3
1	B	114	ASP	2.3
1	A	77	THR	2.2
1	A	367	TRP	2.2
1	B	158	GLY	2.2
1	B	353	LEU	2.2
1	A	258	ARG	2.2
1	A	428	GLN	2.2
1	B	137	GLN	2.2
1	A	117	GLU	2.2
1	B	57	ASN	2.2
1	B	228	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	2.2
1	B	404	LYS	2.2
1	A	109	ALA	2.2
1	A	327	ALA	2.2
1	B	264	ALA	2.2
1	A	230	THR	2.2
1	B	275	THR	2.2
1	B	420	THR	2.2
1	A	44	ASP	2.2
1	A	186	GLU	2.2
1	A	344	SER	2.2
1	A	345	LYS	2.2
1	A	389	LYS	2.2
1	B	362	PHE	2.2
1	A	167	ALA	2.2
1	A	383	THR	2.2
1	A	384	ALA	2.2
1	B	59	ALA	2.2
1	B	298	THR	2.2
1	B	316	THR	2.2
1	B	423	THR	2.2
1	B	453	THR	2.2
1	A	56	ASN	2.2
1	A	148	TRP	2.1
1	B	325	TRP	2.1
1	A	137	GLN	2.1
1	B	391	GLY	2.1
1	B	98	ALA	2.1
1	B	236	ALA	2.1
1	B	444	SER	2.1
1	B	164	LYS	2.1
1	B	102	PRO	2.1
1	A	316	THR	2.1
1	A	455	PHE	2.1
1	B	425	SER	2.1
1	A	67	ASN	2.1
1	A	178	ASN	2.1
1	B	385	TYR	2.1
1	A	120	ASP	2.1
1	B	75	SER	2.1
1	A	295	ASN	2.1
1	B	110	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	405	GLN	2.1
1	A	99	ASP	2.1
1	A	312	PHE	2.1
1	A	140	TYR	2.1
1	A	253	PRO	2.1
1	B	365	PRO	2.1
1	A	213	ARG	2.0
1	A	400	ASN	2.0
1	A	184	GLY	2.0
1	A	268	GLY	2.0
1	B	186	GLU	2.0
1	B	320	ALA	2.0
1	B	258	ARG	2.0
1	A	199	GLU	2.0
1	A	126	ILE	2.0
1	A	181	SER	2.0
1	A	201	SER	2.0
1	B	305	TRP	2.0
1	B	358	GLN	2.0
1	B	62	GLY	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(Å ²)	Q<0.9
2	CL	A	509	1/1	0.88	0.26	68,68,68,68	0
2	CL	A	503	1/1	0.90	0.18	52,52,52,52	0
2	CL	A	514	1/1	0.91	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	501	1/1	0.91	0.26	33,33,33,33	0
3	ACT	B	509	4/4	0.91	0.24	24,24,26,27	0
3	ACT	A	516	4/4	0.92	0.18	17,18,20,21	0
2	CL	A	510	1/1	0.93	0.17	50,50,50,50	0
2	CL	B	505	1/1	0.94	0.11	38,38,38,38	0
2	CL	A	515	1/1	0.95	0.15	26,26,26,26	0
2	CL	A	507	1/1	0.95	0.10	23,23,23,23	0
2	CL	A	511	1/1	0.95	0.17	33,33,33,33	0
2	CL	A	513	1/1	0.95	0.17	49,49,49,49	0
2	CL	A	501	1/1	0.95	0.12	39,39,39,39	0
2	CL	A	505	1/1	0.96	0.20	29,29,29,29	0
2	CL	B	506	1/1	0.96	0.08	27,27,27,27	0
2	CL	A	512	1/1	0.96	0.12	40,40,40,40	0
3	ACT	A	517	4/4	0.96	0.15	21,21,22,22	0
2	CL	A	502	1/1	0.96	0.12	31,31,31,31	0
2	CL	B	504	1/1	0.97	0.23	39,39,39,39	0
2	CL	A	508	1/1	0.97	0.12	22,22,22,22	0
2	CL	A	506	1/1	0.97	0.21	45,45,45,45	0
2	CL	A	504	1/1	0.97	0.20	48,48,48,48	0
2	CL	B	502	1/1	0.97	0.17	23,23,23,23	0
2	CL	B	503	1/1	0.97	0.09	24,24,24,24	0
2	CL	B	508	1/1	0.98	0.24	45,45,45,45	0
2	CL	B	507	1/1	0.98	0.28	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.