Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 11:21 PM EDT

PDB ID	:	7N6H
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:

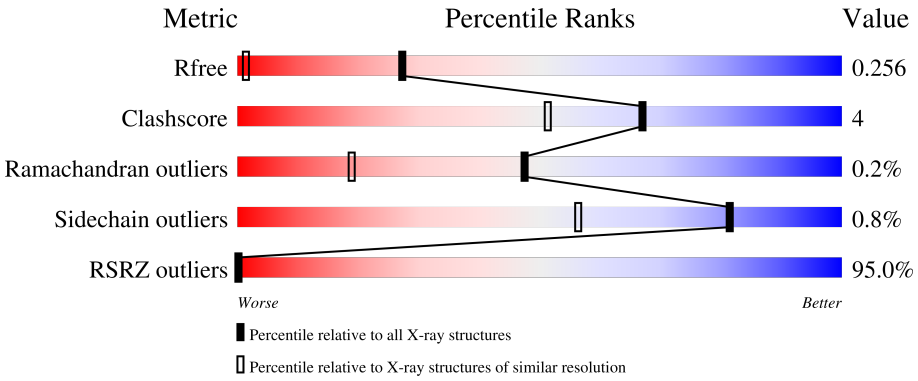
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (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 <=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	92% 89% 9%
1	B	444	93% 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	504	-	-	-	X
2	CL	A	506	-	-	-	X
2	CL	A	508	-	-	X	-
2	CL	A	511	-	-	-	X
2	CL	A	515	-	-	X	-
2	CL	B	503	-	-	X	-
2	CL	B	507	-	-	-	X

2 Entry composition (i)

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 (three-letter code: CL) (formula: Cl).

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

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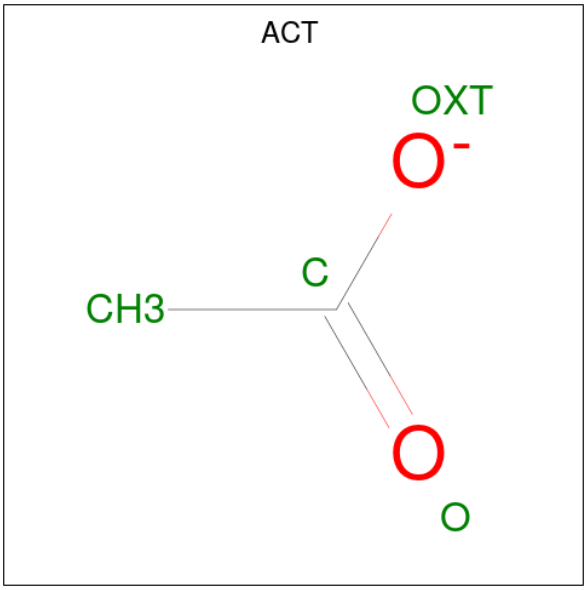
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	8	Total Cl 8 8	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is water.

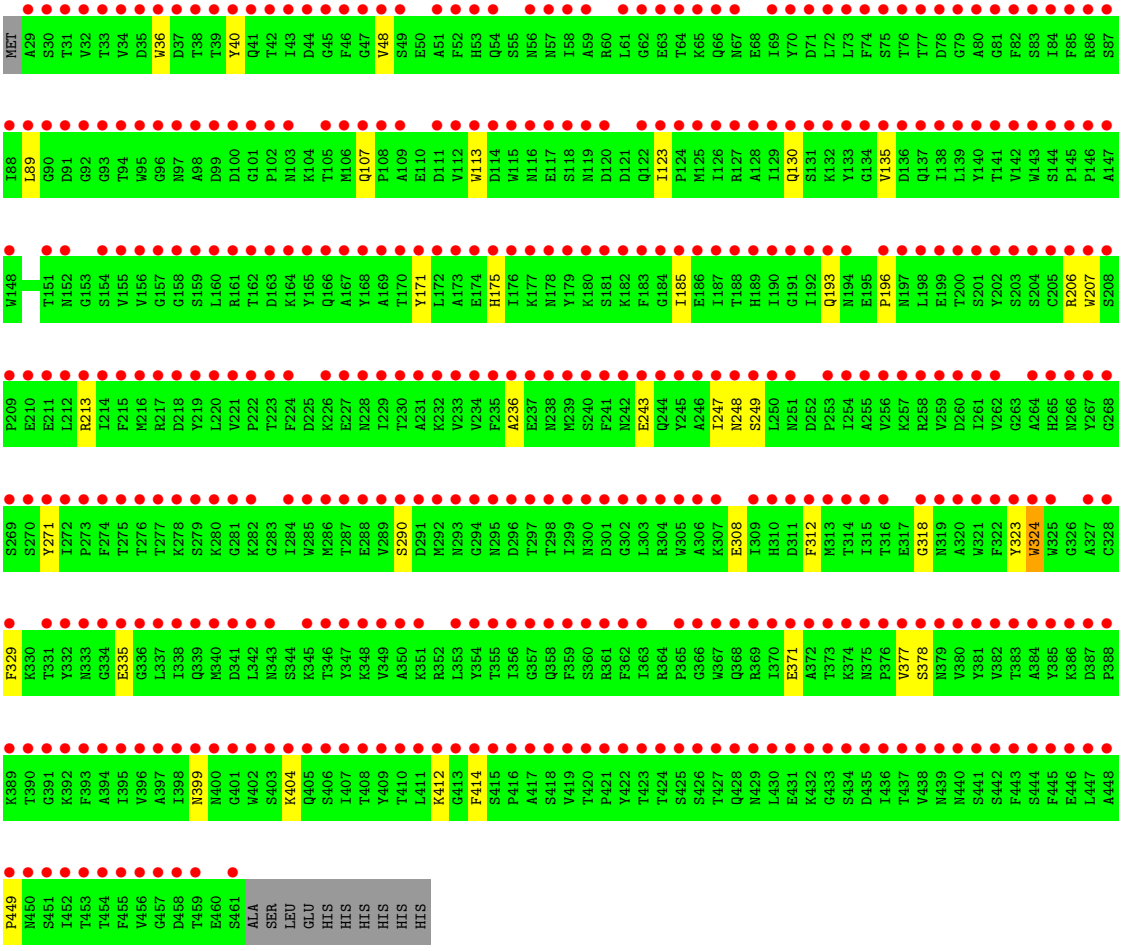
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	388	Total O 388 388	0	0
4	B	329	Total O 329 329	0	0

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.

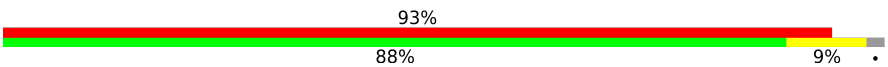
• Molecule 1: AcXbh30A

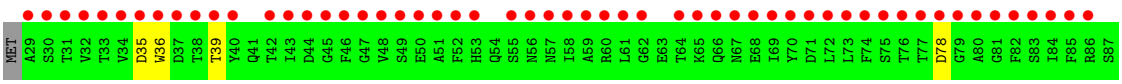
Chain A:

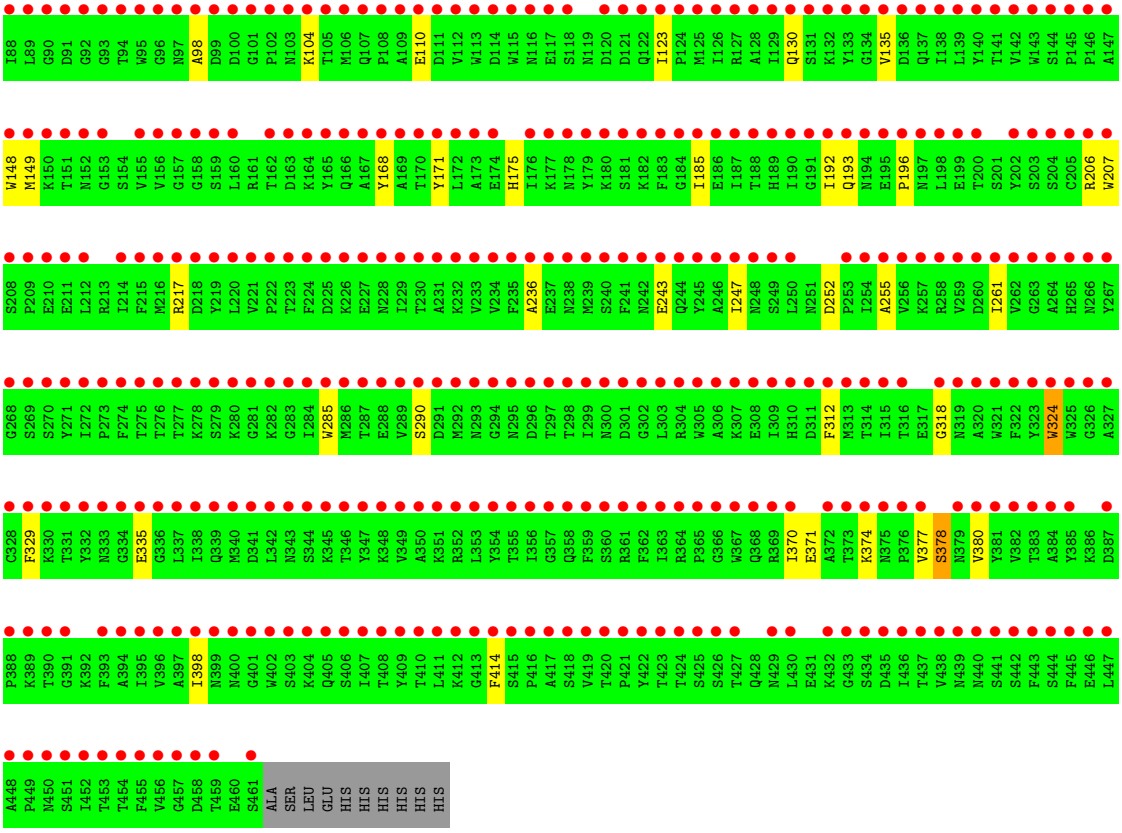


• Molecule 1: AcXbh30A

Chain B:






I88 L89 G90 D91 G92 G93 T94 W95 G96 N97 A98 D99 D100 G101 P102 N103 K104 T105 M106 Q107 P108 A109 E110 D111 V112 W113 D114 W115 N116 E117 S118 N119 D120 D121 Q122 I123 P124 M125 I126 R127 A128 I129 Q130 S131 K132 Y133 G134 V135 D136 Q137 I138 L139 Y140 T141 V142 W143 S144 P145 P146 A147
W148 M149 K150 T151 N152 G153 S154 V155 V156 G157 G158 S159 L160 R161 T162 D163 K164 Y165 Q166 A167 Y168 A169 T170 Y171 L172 A173 E174 H175 I176 K177 N178 Y179 K180 S181 K182 F183 G184 I185 E186 I187 T188 H189 I190 G191 I192 Q193 N194 E195 P196 N197 L198 E199 T200 S201 Y202 S203 S204 C205 R206 W207
S208 P209 E210 E211 L212 R213 I214 F215 M216 R217 D218 Y219 L220 V221 P222 T223 F224 D225 K226 E227 N228 I229 T230 A231 K232 V233 V234 F235 A236 E237 N238 M239 S240 F241 N242 E243 Q244 Y245 A246 I247 N248 S249 L250 N251 D252 P253 I254 A255 V256 K257 R258 V259 D260 I261 V262 G263 A264 H265 N266 Y267
G268 S269 S270 Y271 I272 P273 F274 T275 T276 T277 K278 S279 K280 G281 K282 G283 I284 W285 M286 T287 E288 V289 S290 D291 M292 N293 G294 N295 D296 T297 T298 I299 N300 D301 G302 L303 R304 W305 A306 K307 E308 I309 H310 D311 F312 N313 T314 I315 T316 E317 G318 N319 A320 W321 F322 Y323 W324 W325 G326 A327
C328 F329 K330 T331 Y332 N333 G334 E335 G336 L337 I338 Q339 M340 D341 L342 N343 S344 K345 T346 Y347 K348 V349 A350 K351 R352 L353 Y354 T355 I356 G357 Q358 F359 S360 R361 F362 I363 R364 P365 G366 W367 Q368 R369 I370 E371 A372 T373 K374 N375 P376 V377 S378 N379 V380 Y381 V382 T383 A384 Y385 K386 D387
P388 K389 T390 G391 K392 F393 A394 I395 V396 A397 I398 N399 N400 G401 W402 S403 K404 Q405 S406 I407 T408 Y409 T410 L411 K412 G413 F414 S415 P416 A417 S418 V419 T420 P421 Y422 T423 T424 S425 S426 T427 Q428 N429 L430 E431 K432 G433 S434 D435 T436 T437 V438 N439 N440 S441 S442 F443 S444 F445 E446 L447
A448 P449 N450 S451 I452 T453 T454 F455 V456 G457 D458 T459 E460 S461 ALA SER LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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) 96.2 (41.18-1.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.51 (at 1.28Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.202 , 0.254 0.203 , 0.256	Depositor DCC
R_{free} test set	10529 reflections (4.98%)	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)	0.31 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.387 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/3544	0.47	0/4821
1	B	0.24	0/3533	0.46	0/4806
All	All	0.24	0/7077	0.47	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: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:A:249:SER:OG	2:A:508:CL:CL	2.61	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 (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	433/444 (98%)	418 (96%)	14 (3%)	1 (0%)	47	19
1	B	432/444 (97%)	418 (97%)	13 (3%)	1 (0%)	47	19
All	All	865/888 (97%)	836 (97%)	27 (3%)	2 (0%)	47	19

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%)	373 (99%)	3 (1%)	81 56
1	B	374/384 (97%)	371 (99%)	3 (1%)	81 56
All	All	750/768 (98%)	744 (99%)	6 (1%)	81 56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	A	324	TRP
1	A	329	PHE
1	B	324	TRP
1	B	329	PHE
1	B	378	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

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	B	509	-	3,3,3	1.28	0	3,3,3	1.27	0
3	ACT	A	516	-	3,3,3	1.27	0	3,3,3	1.41	0
3	ACT	A	517	-	3,3,3	1.25	0	3,3,3	1.32	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, 95^{th} 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%)	4.62	410 (94%)	0	0	10, 15, 21, 38	0
1	B	433/444 (97%)	4.76	413 (95%)	0	0	9, 14, 21, 34	0
All	All	866/888 (97%)	4.69	823 (95%)	0	0	9, 15, 21, 38	0

All (823) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	ALA	36.8
1	B	306	ALA	14.5
1	B	146	PRO	12.5
1	B	246	ALA	11.7
1	B	329	PHE	11.5
1	A	338	ILE	11.2
1	B	402	TRP	11.2
1	A	293	ASN	11.0
1	A	135	VAL	11.0
1	B	219	TYR	10.7
1	B	456	VAL	10.5
1	A	359	PHE	10.5
1	B	108	PRO	10.4
1	A	279	SER	10.4
1	B	190	ILE	10.2
1	B	82	PHE	10.1
1	A	315	ILE	10.0
1	A	198	LEU	9.9
1	B	417	ALA	9.7
1	B	347	TYR	9.7
1	B	299	ILE	9.7
1	A	241	PHE	9.6
1	A	33	THR	9.6
1	B	430	LEU	9.6

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Mol	Chain	Res	Type	RSRZ
1	B	247	ILE	9.5
1	B	156	VAL	9.5
1	B	411	LEU	9.5
1	A	259	VAL	9.5
1	A	324	TRP	9.5
1	A	247	ILE	9.4
1	B	370	ILE	9.4
1	B	327	ALA	9.4
1	B	52	PHE	9.3
1	B	285	TRP	9.3
1	B	84	ILE	9.3
1	B	284	ILE	9.3
1	A	207	TRP	9.2
1	A	168	TYR	9.2
1	B	112	VAL	9.1
1	B	187	ILE	9.0
1	B	409	TYR	9.0
1	A	129	ILE	8.9
1	B	70	TYR	8.8
1	A	274	PHE	8.8
1	B	427	THR	8.7
1	A	40	TYR	8.7
1	A	74	PHE	8.7
1	B	38	THR	8.7
1	A	48	VAL	8.6
1	A	32	VAL	8.6
1	B	188	THR	8.5
1	A	138	ILE	8.5
1	B	212	LEU	8.4
1	B	223	THR	8.4
1	A	299	ILE	8.4
1	A	133	TYR	8.3
1	A	43	ILE	8.3
1	B	303	LEU	8.2
1	B	148	TRP	8.2
1	A	123	ILE	8.2
1	B	381	TYR	8.2
1	A	221	VAL	8.2
1	A	271	TYR	8.2
1	A	105	THR	8.2
1	A	155	VAL	8.1
1	A	367	TRP	8.1

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Mol	Chain	Res	Type	RSRZ
1	B	254	ILE	8.1
1	A	419	VAL	8.1
1	A	46	PHE	8.1
1	A	215	PHE	8.1
1	B	179	TYR	8.1
1	B	89	LEU	8.0
1	B	389	LYS	8.0
1	B	123	ILE	8.0
1	A	250	LEU	8.0
1	A	172	LEU	7.9
1	B	309	ILE	7.8
1	B	46	PHE	7.8
1	A	439	ASN	7.8
1	B	233	VAL	7.8
1	A	170	THR	7.7
1	B	31	THR	7.7
1	B	445	PHE	7.7
1	B	271	TYR	7.7
1	B	207	TRP	7.6
1	A	303	LEU	7.6
1	B	151	THR	7.6
1	A	321	TRP	7.6
1	A	224	PHE	7.6
1	A	145	PRO	7.6
1	A	455	PHE	7.5
1	B	274	PHE	7.5
1	A	402	TRP	7.5
1	A	456[A]	VAL	7.5
1	B	261	ILE	7.4
1	B	443	PHE	7.4
1	B	165	TYR	7.4
1	A	222	PRO	7.4
1	A	160	LEU	7.4
1	A	390	THR	7.4
1	B	133	TYR	7.4
1	B	202	TYR	7.3
1	A	331	THR	7.3
1	A	452	ILE	7.3
1	B	43	ILE	7.3
1	A	118	SER	7.2
1	B	270	SER	7.2
1	A	461	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	48	VAL	7.2
1	A	309	ILE	7.1
1	B	436	ILE	7.1
1	A	61	LEU	7.1
1	A	285	TRP	7.1
1	A	142	VAL	7.1
1	A	64	THR	7.1
1	A	261	ILE	7.1
1	B	116	ASN	7.1
1	A	393	PHE	7.1
1	A	408	THR	7.1
1	B	290	SER	7.0
1	A	231	ALA	7.0
1	B	235	PHE	7.0
1	B	414	PHE	7.0
1	A	412	LYS	7.0
1	A	329	PHE	7.0
1	A	31	THR	7.0
1	A	176	ILE	6.9
1	A	113	TRP	6.9
1	B	115	TRP	6.9
1	B	437	THR	6.9
1	A	29	ALA	6.9
1	A	430	LEU	6.9
1	B	424	THR	6.8
1	B	109	ALA	6.8
1	A	438	VAL	6.8
1	B	143	TRP	6.8
1	A	391	GLY	6.8
1	B	214	ILE	6.8
1	A	305	TRP	6.8
1	B	59	ALA	6.8
1	A	92	GLY	6.7
1	A	69	ILE	6.7
1	A	354	TYR	6.7
1	B	367	TRP	6.7
1	A	66	GLN	6.6
1	A	89	LEU	6.6
1	B	236	ALA	6.6
1	A	34	VAL	6.6
1	B	362	PHE	6.6
1	A	30	SER	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	441	SER	6.5
1	A	394	ALA	6.5
1	A	322	PHE	6.5
1	A	76	THR	6.5
1	A	229	ILE	6.5
1	A	459	THR	6.5
1	B	51	ALA	6.5
1	A	414	PHE	6.5
1	B	230	THR	6.5
1	A	185	ILE	6.5
1	B	415	SER	6.5
1	B	452	ILE	6.5
1	B	171	TYR	6.4
1	B	83	SER	6.4
1	B	384	ALA	6.4
1	A	85	PHE	6.4
1	B	438	VAL	6.4
1	A	323	TYR	6.4
1	B	312	PHE	6.3
1	B	245	TYR	6.3
1	A	334	GLY	6.3
1	A	246	ALA	6.3
1	A	353	LEU	6.3
1	B	328	CYS	6.3
1	B	126	ILE	6.3
1	B	234	VAL	6.3
1	A	36	TRP	6.3
1	B	162	THR	6.2
1	A	70	TYR	6.2
1	A	173	ALA	6.2
1	A	58	ILE	6.2
1	A	254	ILE	6.2
1	A	275	THR	6.2
1	A	381	TYR	6.2
1	A	398	ILE	6.2
1	B	305	TRP	6.2
1	A	267	TYR	6.2
1	B	94	THR	6.2
1	B	58	ILE	6.2
1	B	363	ILE	6.2
1	A	42	THR	6.1
1	A	190	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	138	ILE	6.1
1	B	137	GLN	6.1
1	A	297	THR	6.1
1	B	267	TYR	6.1
1	B	224	PHE	6.1
1	B	356	ILE	6.1
1	B	250	LEU	6.0
1	B	322	PHE	6.0
1	A	192	ILE	6.0
1	A	363	ILE	6.0
1	B	36	TRP	6.0
1	A	239	MET	6.0
1	A	328	CYS	6.0
1	A	385	TYR	6.0
1	B	379	ASN	6.0
1	A	188	THR	6.0
1	A	139	LEU	5.9
1	B	73	LEU	5.9
1	B	447	LEU	5.9
1	B	416	PRO	5.9
1	A	316	THR	5.9
1	B	152	ASN	5.9
1	A	214	ILE	5.9
1	B	229	ILE	5.9
1	A	262	VAL	5.9
1	B	241	PHE	5.9
1	B	47	GLY	5.9
1	B	192	ILE	5.9
1	B	176	ILE	5.8
1	A	349	VAL	5.8
1	B	159	SER	5.8
1	B	102	PRO	5.8
1	A	422	TYR	5.8
1	B	141	THR	5.8
1	B	344	SER	5.8
1	A	410	THR	5.8
1	A	416	PRO	5.8
1	A	202	TYR	5.8
1	A	362	PHE	5.8
1	B	226	LYS	5.7
1	B	56	ASN	5.7
1	B	139	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	226	LYS	5.7
1	B	273	PRO	5.7
1	A	445	PHE	5.7
1	A	156	VAL	5.7
1	B	142	VAL	5.7
1	A	115	TRP	5.6
1	A	253	PRO	5.6
1	B	342	LEU	5.6
1	B	180	LYS	5.6
1	B	32	VAL	5.6
1	B	343	ASN	5.6
1	A	403	SER	5.6
1	B	323	TYR	5.6
1	B	272	ILE	5.5
1	A	234	VAL	5.5
1	B	454	THR	5.5
1	A	189	HIS	5.5
1	A	384	ALA	5.5
1	A	337	LEU	5.5
1	A	82	PHE	5.5
1	A	178	ASN	5.5
1	A	370	ILE	5.5
1	B	423	THR	5.5
1	A	233	VAL	5.5
1	B	34	VAL	5.5
1	B	78	ASP	5.5
1	A	378	SER	5.4
1	A	443	PHE	5.4
1	B	74	PHE	5.4
1	B	183	PHE	5.4
1	A	447	LEU	5.4
1	B	220	LEU	5.4
1	B	297	THR	5.4
1	A	171	TYR	5.4
1	B	385	TYR	5.4
1	A	98	ALA	5.4
1	A	84	ILE	5.4
1	A	284	ILE	5.4
1	B	407	ILE	5.4
1	B	461	SER	5.4
1	A	449	PRO	5.4
1	B	332	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	343	ASN	5.4
1	B	324	TRP	5.4
1	B	353	LEU	5.4
1	B	88	ILE	5.4
1	B	99	ASP	5.4
1	A	264	ALA	5.4
1	B	354	TYR	5.3
1	B	77	THR	5.3
1	B	289	VAL	5.3
1	B	396	VAL	5.3
1	B	375	ASN	5.3
1	A	356	ILE	5.3
1	B	395	ILE	5.3
1	B	129	ILE	5.3
1	B	315	ILE	5.3
1	B	98	ALA	5.3
1	B	397	ALA	5.3
1	A	80	ALA	5.3
1	A	86	ARG	5.2
1	B	140	TYR	5.2
1	B	376	PRO	5.2
1	B	337	LEU	5.2
1	B	393	PHE	5.2
1	B	136	ASP	5.2
1	A	448	ALA	5.2
1	A	292	MET	5.2
1	A	143	TRP	5.2
1	A	235	PHE	5.2
1	B	341	ASP	5.2
1	B	57	ASN	5.2
1	A	272	ILE	5.1
1	A	169	ALA	5.1
1	A	401	GLY	5.1
1	A	199	GLU	5.1
1	A	72	LEU	5.1
1	A	399	ASN	5.1
1	A	162	THR	5.0
1	A	268	GLY	5.0
1	B	383	THR	5.0
1	A	289	VAL	5.0
1	B	377	VAL	5.0
1	B	325	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	455	PHE	5.0
1	A	38	THR	5.0
1	B	147	ALA	5.0
1	A	396	VAL	5.0
1	B	61	LEU	5.0
1	A	245	TYR	5.0
1	A	258	ARG	5.0
1	B	369	ARG	5.0
1	A	458	ASP	5.0
1	B	406	SER	5.0
1	B	145	PRO	5.0
1	A	52	PHE	5.0
1	B	95	TRP	5.0
1	B	390	THR	5.0
1	B	422	TYR	5.0
1	B	350	ALA	5.0
1	A	131	SER	4.9
1	A	73	LEU	4.9
1	A	212	LEU	4.9
1	B	259	VAL	4.9
1	B	355	THR	4.9
1	B	69	ILE	4.9
1	A	257	LYS	4.9
1	A	436	ILE	4.9
1	B	321	TRP	4.9
1	B	446	GLU	4.9
1	B	135	VAL	4.9
1	A	375	ASN	4.8
1	A	183	PHE	4.8
1	A	75	SER	4.8
1	A	347	TYR	4.8
1	A	409	TYR	4.8
1	B	168	TYR	4.8
1	A	126	ILE	4.8
1	A	294	GLY	4.8
1	B	253	PRO	4.8
1	A	111	ASP	4.8
1	A	206	ARG	4.8
1	A	213	ARG	4.8
1	A	96	GLY	4.8
1	B	433	GLY	4.8
1	B	388	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	141	THR	4.7
1	B	338	ILE	4.7
1	A	256	VAL	4.7
1	A	423	THR	4.7
1	B	453	THR	4.7
1	A	218	ASP	4.7
1	A	187	ILE	4.7
1	B	174	GLU	4.7
1	A	140	TYR	4.7
1	A	228	ASN	4.7
1	A	437	THR	4.7
1	A	397	ALA	4.7
1	B	92	GLY	4.7
1	A	37	ASP	4.7
1	A	196	PRO	4.6
1	B	398	ILE	4.6
1	A	444	SER	4.6
1	A	95	TRP	4.6
1	B	359	PHE	4.6
1	A	281	GLY	4.6
1	A	165	TYR	4.6
1	A	382	VAL	4.6
1	B	382	VAL	4.6
1	A	205	CYS	4.6
1	A	134	GLY	4.6
1	B	185	ILE	4.6
1	A	388	PRO	4.6
1	A	266	ASN	4.5
1	A	377	VAL	4.5
1	B	440	ASN	4.5
1	B	30	SER	4.5
1	B	181	SER	4.5
1	A	350	ALA	4.5
1	B	62	GLY	4.5
1	B	404	LYS	4.5
1	B	298	THR	4.5
1	B	215	PHE	4.5
1	B	40	TYR	4.5
1	B	79	GLY	4.5
1	A	78	ASP	4.5
1	B	292	MET	4.5
1	A	148	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	159	SER	4.4
1	B	333	ASN	4.4
1	A	366	GLY	4.4
1	A	314	THR	4.4
1	B	262	VAL	4.4
1	B	401	GLY	4.4
1	A	383	THR	4.4
1	A	407	ILE	4.4
1	B	113	TRP	4.4
1	A	219	TYR	4.4
1	B	434	SER	4.4
1	A	249	SER	4.3
1	A	197	ASN	4.3
1	B	194	ASN	4.3
1	B	295	ASN	4.3
1	A	411	LEU	4.3
1	A	298	THR	4.3
1	B	127	ARG	4.3
1	B	380	VAL	4.3
1	B	346	THR	4.3
1	A	346	THR	4.2
1	A	400	ASN	4.2
1	B	320	ALA	4.2
1	A	442[B]	SER	4.2
1	A	77	THR	4.2
1	A	163	ASP	4.2
1	A	373	THR	4.2
1	B	85	PHE	4.2
1	B	131	SER	4.2
1	B	76	THR	4.2
1	B	172	LEU	4.2
1	B	319	ASN	4.2
1	B	118	SER	4.2
1	B	42	THR	4.2
1	A	371	GLU	4.2
1	A	128	ALA	4.1
1	B	80	ALA	4.1
1	B	222	PRO	4.1
1	A	119	ASN	4.1
1	B	368	GLN	4.1
1	B	97	ASN	4.1
1	B	198	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	VAL	4.1
1	A	454	THR	4.1
1	A	97	ASN	4.1
1	B	169	ALA	4.1
1	A	389	LYS	4.1
1	A	428	GLN	4.1
1	B	279	SER	4.1
1	B	451	SER	4.1
1	B	128	ALA	4.1
1	A	335	GLU	4.1
1	A	340	MET	4.1
1	B	65	LYS	4.1
1	A	223	THR	4.1
1	B	39	THR	4.1
1	A	269	SER	4.0
1	A	217	ARG	4.0
1	A	395	ILE	4.0
1	A	342	LEU	4.0
1	B	72	LEU	4.0
1	B	255	ALA	4.0
1	B	403	SER	4.0
1	A	227	GLU	4.0
1	B	121	ASP	4.0
1	A	313	MET	4.0
1	B	160	LEU	4.0
1	A	440	ASN	4.0
1	A	325	TRP	4.0
1	A	312	PHE	4.0
1	A	392	LYS	4.0
1	A	181	SER	4.0
1	B	75	SER	4.0
1	B	110	GLU	4.0
1	A	35	ASP	4.0
1	B	256	VAL	3.9
1	B	64	THR	3.9
1	A	327	ALA	3.9
1	A	361	ARG	3.9
1	A	220	LEU	3.9
1	A	424	THR	3.9
1	B	117	GLU	3.9
1	B	310	HIS	3.9
1	A	300	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	275	THR	3.9
1	B	287	THR	3.9
1	A	45	GLY	3.9
1	B	93	GLY	3.9
1	B	365	PRO	3.9
1	A	136	ASP	3.9
1	A	265	HIS	3.9
1	A	114	ASP	3.9
1	B	426	SER	3.9
1	B	442[A]	SER	3.9
1	B	358	GLN	3.9
1	A	103	ASN	3.9
1	B	125	MET	3.8
1	B	248	ASN	3.8
1	A	161	ARG	3.8
1	A	376	PRO	3.8
1	B	228	ASN	3.8
1	A	276	THR	3.8
1	B	425	SER	3.8
1	B	124	PRO	3.8
1	B	33	THR	3.8
1	B	316	THR	3.8
1	A	47	GLY	3.8
1	A	191	GLY	3.8
1	B	400	ASN	3.8
1	B	448	ALA	3.7
1	A	102	PRO	3.7
1	A	194	ASN	3.7
1	A	255	ALA	3.7
1	A	286	MET	3.7
1	B	37	ASP	3.7
1	A	248	ASN	3.7
1	B	68	GLU	3.7
1	B	107	GLN	3.7
1	A	109	ALA	3.7
1	B	173	ALA	3.7
1	B	231	ALA	3.7
1	A	251	ASN	3.7
1	B	300	ASN	3.7
1	B	60	ARG	3.7
1	B	221	VAL	3.7
1	A	151	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	THR	3.7
1	B	308	GLU	3.7
1	A	260	ASP	3.7
1	B	203	SER	3.7
1	A	112	VAL	3.6
1	A	116	ASN	3.6
1	A	179	TYR	3.6
1	A	332	TYR	3.6
1	A	108	PRO	3.6
1	A	320	ALA	3.6
1	A	345	LYS	3.6
1	B	266	ASN	3.6
1	B	217	ARG	3.6
1	B	296	ASP	3.6
1	A	368	GLN	3.6
1	B	374	LYS	3.6
1	A	434	SER	3.6
1	B	269	SER	3.6
1	B	439	ASN	3.6
1	B	364	ARG	3.6
1	B	286	MET	3.6
1	A	39	THR	3.6
1	A	336	GLY	3.6
1	B	331	THR	3.6
1	A	71	ASP	3.6
1	A	182	LYS	3.6
1	A	372	ALA	3.6
1	B	182	LYS	3.6
1	A	79	GLY	3.5
1	B	177	LYS	3.5
1	A	236	ALA	3.5
1	A	421	PRO	3.5
1	A	203	SER	3.5
1	B	71	ASP	3.5
1	A	63[A]	GLU	3.5
1	A	124	PRO	3.5
1	B	293	ASN	3.5
1	B	449	PRO	3.5
1	B	450	ASN	3.5
1	A	240	SER	3.5
1	B	114	ASP	3.5
1	A	175	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	3.5
1	B	153	GLY	3.5
1	A	117	GLU	3.5
1	B	55	SER	3.5
1	B	276	THR	3.5
1	A	209	PRO	3.5
1	B	67	ASN	3.4
1	A	355	THR	3.4
1	B	301	ASP	3.4
1	B	302	GLY	3.4
1	B	122	GLN	3.4
1	B	186	GLU	3.4
1	A	360	SER	3.4
1	A	291	ASP	3.4
1	A	357	GLY	3.4
1	B	200	THR	3.4
1	A	93	GLY	3.4
1	B	336	GLY	3.4
1	B	373	THR	3.4
1	A	83	SER	3.4
1	B	225	ASP	3.4
1	A	201	SER	3.4
1	A	290	SER	3.4
1	B	444	SER	3.4
1	B	413	GLY	3.3
1	A	147	ALA	3.3
1	A	369	ARG	3.3
1	B	361	ARG	3.3
1	A	88	ILE	3.3
1	B	408	THR	3.3
1	B	265	HIS	3.3
1	B	405	GLN	3.3
1	B	209	PRO	3.3
1	B	195	GLU	3.3
1	A	65	LYS	3.3
1	A	216	MET	3.3
1	B	53	HIS	3.3
1	B	193	GLN	3.3
1	B	457	GLY	3.3
1	A	208	SER	3.3
1	A	426	SER	3.3
1	B	304	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	51	ALA	3.3
1	B	349	VAL	3.3
1	A	56	ASN	3.3
1	A	310	HIS	3.3
1	B	257	LYS	3.3
1	B	458	ASP	3.3
1	A	295	ASN	3.3
1	B	372	ALA	3.3
1	B	313	MET	3.3
1	A	91	ASP	3.2
1	A	365	PRO	3.2
1	B	238	ASN	3.2
1	B	412	LYS	3.2
1	A	306	ALA	3.2
1	B	339	GLN	3.2
1	A	177	LYS	3.2
1	A	277	THR	3.2
1	B	258	ARG	3.2
1	A	441	SER	3.2
1	B	240	SER	3.2
1	B	263	GLY	3.2
1	A	204	SER	3.2
1	A	425	SER	3.2
1	A	62	GLY	3.2
1	A	174	GLU	3.2
1	B	239	MET	3.2
1	B	264	ALA	3.2
1	B	196	PRO	3.1
1	A	333	ASN	3.1
1	A	420	THR	3.1
1	A	404	LYS	3.1
1	B	164	LYS	3.1
1	A	406	SER	3.1
1	A	94	THR	3.1
1	B	314	THR	3.1
1	B	348	LYS	3.1
1	B	144	SER	3.1
1	B	419	VAL	3.1
1	B	86	ARG	3.1
1	A	167	ALA	3.1
1	A	302	GLY	3.1
1	A	57	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLU	3.1
1	A	432	LYS	3.1
1	B	134	GLY	3.0
1	B	334	GLY	3.0
1	A	137	GLN	3.0
1	A	152	ASN	3.0
1	B	340	MET	3.0
1	B	105	THR	3.0
1	B	249	SER	3.0
1	B	399	ASN	3.0
1	A	200	THR	3.0
1	A	318	GLY	3.0
1	B	103	ASN	3.0
1	A	180	LYS	3.0
1	A	270	SER	3.0
1	B	45	GLY	3.0
1	B	204	SER	3.0
1	B	278	LYS	3.0
1	A	358	GLN	3.0
1	A	186	GLU	2.9
1	B	237	GLU	2.9
1	A	307	LYS	2.9
1	A	374	LYS	2.9
1	B	163	ASP	2.9
1	A	244	GLN	2.9
1	B	244	GLN	2.9
1	B	394	ALA	2.9
1	A	90	GLY	2.9
1	B	184	GLY	2.9
1	B	421	PRO	2.9
1	B	120	ASP	2.9
1	A	106	MET	2.8
1	B	366	GLY	2.8
1	A	44	ASP	2.8
1	A	193	GLN	2.8
1	A	417	ALA	2.8
1	B	387	ASP	2.8
1	B	158	GLY	2.8
1	A	304	ARG	2.8
1	B	211	GLU	2.8
1	B	91	ASP	2.8
1	A	184	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	197	ASN	2.8
1	A	146	PRO	2.8
1	B	170	THR	2.8
1	B	459	THR	2.8
1	A	41	GLN	2.8
1	B	391	GLY	2.8
1	B	242	ASN	2.8
1	B	345	LYS	2.8
1	A	405	GLN	2.8
1	A	132	LYS	2.7
1	A	230	THR	2.7
1	B	410	THR	2.7
1	B	81	GLY	2.7
1	B	167	ALA	2.7
1	A	232	LYS	2.7
1	A	351	LYS	2.7
1	B	104	LYS	2.7
1	A	158	GLY	2.7
1	A	301	ASP	2.7
1	A	387	ASP	2.7
1	A	451	SER	2.7
1	B	157	GLY	2.7
1	B	357	GLY	2.7
1	B	106	MET	2.7
1	B	429	ASN	2.7
1	B	205	CYS	2.7
1	A	130	GLN	2.7
1	B	307	LYS	2.6
1	A	164	LYS	2.6
1	A	242	ASN	2.6
1	A	280	LYS	2.6
1	B	216	MET	2.6
1	A	59	ALA	2.6
1	A	450	ASN	2.6
1	A	427	THR	2.6
1	B	420	THR	2.6
1	B	291	ASP	2.6
1	B	178	ASN	2.6
1	B	288	GLU	2.6
1	B	330	LYS	2.6
1	A	287	THR	2.6
1	B	326	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASP	2.6
1	B	49	SER	2.6
1	B	166	GLN	2.6
1	B	243	GLU	2.6
1	A	429	ASN	2.6
1	A	157	GLY	2.5
1	A	446	GLU	2.5
1	B	280	LYS	2.5
1	A	238	ASN	2.5
1	A	379	ASN	2.5
1	A	166	GLN	2.5
1	A	341	ASP	2.5
1	B	66	GLN	2.5
1	A	211	GLU	2.5
1	B	35	ASP	2.5
1	B	199	GLU	2.5
1	B	132	LYS	2.5
1	A	99	ASP	2.5
1	A	296	ASP	2.5
1	A	87	SER	2.5
1	A	415	SER	2.5
1	B	149	MET	2.5
1	B	281	GLY	2.5
1	B	432	LYS	2.5
1	A	435	ASP	2.5
1	A	319	ASN	2.4
1	B	318	GLY	2.4
1	A	278	LYS	2.4
1	B	100	ASP	2.4
1	B	360	SER	2.4
1	A	273	PRO	2.4
1	B	150	LYS	2.4
1	B	208	SER	2.4
1	A	243	GLU	2.3
1	A	433	GLY	2.3
1	B	227	GLU	2.3
1	A	49	SER	2.3
1	A	282	LYS	2.3
1	B	155	VAL	2.3
1	B	191	GLY	2.3
1	A	154	SER	2.3
1	B	418	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	453	THR	2.3
1	B	260	ASP	2.3
1	A	386	LYS	2.3
1	B	282	LYS	2.3
1	A	53	HIS	2.3
1	B	210	GLU	2.3
1	B	232	LYS	2.3
1	A	54	GLN	2.3
1	A	67	ASN	2.3
1	A	101	GLY	2.3
1	B	44	ASP	2.2
1	A	125	MET	2.2
1	B	50	GLU	2.2
1	A	311	ASP	2.2
1	B	218	ASP	2.2
1	A	457	GLY	2.2
1	B	283	GLY	2.2
1	A	431	GLU	2.2
1	B	435	ASP	2.2
1	A	144	SER	2.2
1	A	413	GLY	2.2
1	A	418	SER	2.2
1	B	351	LYS	2.2
1	B	189	HIS	2.2
1	B	352	ARG	2.2
1	B	111	ASP	2.2
1	B	268	GLY	2.2
1	A	348	LYS	2.2
1	A	288	GLU	2.1
1	B	335	GLU	2.1
1	B	90	GLY	2.1
1	A	127	ARG	2.1
1	B	311	ASP	2.1
1	A	210	GLU	2.1
1	B	130	GLN	2.1
1	B	206	ARG	2.1
1	A	120	ASP	2.1
1	B	96	GLY	2.1
1	B	294	GLY	2.1
1	A	339	GLN	2.0
1	A	107	GLN	2.0
1	A	122	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	101	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 monosaccharides 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, 95^{th} 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	ACT	A	517	4/4	0.30	0.31	21,21,22,22	0
3	ACT	A	516	4/4	0.33	0.29	17,18,20,21	0
2	CL	A	511	1/1	0.37	0.49	33,33,33,33	0
2	CL	A	506	1/1	0.39	0.45	45,45,45,45	0
2	CL	A	501	1/1	0.46	0.29	39,39,39,39	0
2	CL	A	509	1/1	0.48	0.38	68,68,68,68	0
2	CL	A	502	1/1	0.49	0.15	31,31,31,31	0
2	CL	A	513	1/1	0.49	0.22	49,49,49,49	0
2	CL	A	503	1/1	0.51	0.20	52,52,52,52	0
3	ACT	B	509	4/4	0.61	0.31	24,24,26,27	0
2	CL	A	510	1/1	0.64	0.20	50,50,50,50	0
2	CL	B	507	1/1	0.66	0.54	79,79,79,79	0
2	CL	B	506	1/1	0.66	0.20	27,27,27,27	0
2	CL	A	507	1/1	0.67	0.33	23,23,23,23	0
2	CL	B	501	1/1	0.72	0.25	33,33,33,33	0
2	CL	B	505	1/1	0.73	0.25	38,38,38,38	0
2	CL	A	505	1/1	0.73	0.11	29,29,29,29	0
2	CL	A	514	1/1	0.74	0.21	45,45,45,45	0
2	CL	B	502	1/1	0.74	0.10	23,23,23,23	0
2	CL	A	512	1/1	0.75	0.22	40,40,40,40	0
2	CL	A	504	1/1	0.76	0.46	48,48,48,48	0
2	CL	A	515	1/1	0.78	0.21	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	508	1/1	0.81	0.17	22,22,22,22	0
2	CL	B	504	1/1	0.82	0.24	39,39,39,39	0
2	CL	B	508	1/1	0.88	0.16	45,45,45,45	0
2	CL	B	503	1/1	0.91	0.06	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.