



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:15 PM UTC

PDB ID : 7COG / pdb_00007cog
Title : Cholesterol esterase from Burkholderia stabilis (monoclinic crystal form)
Authors : Yasutake, Y.; Tamura, T.
Deposited on : 2020-08-04
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

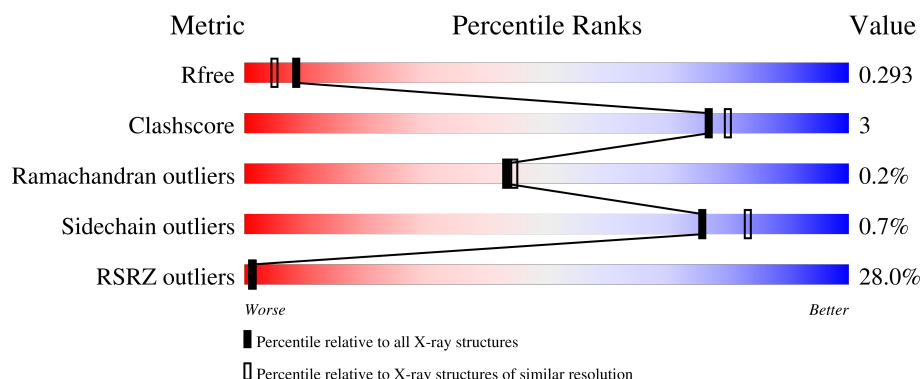
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	320	3% 94% 6%
1	B	320	65% 89% 10%
1	C	320	3% 95% 5%
1	D	320	40% 92% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9472 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 Alpha/beta hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total 2345	C 1473	N 400	O 469	S 3	0	0	0
1	B	320	Total 2345	C 1473	N 400	O 469	S 3	0	0	0
1	C	320	Total 2345	C 1473	N 400	O 469	S 3	0	0	0
1	D	320	Total 2345	C 1473	N 400	O 469	S 3	0	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	11	Total 11	O 11	0	0
3	C	29	Total 29	O 29	0	0
3	D	19	Total 19	O 19	0	0

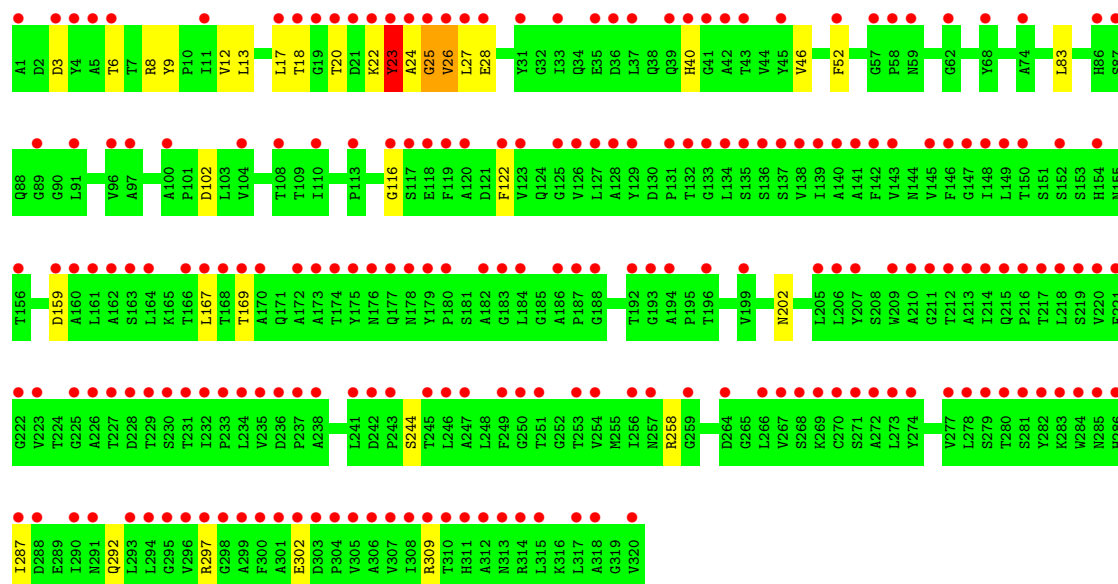
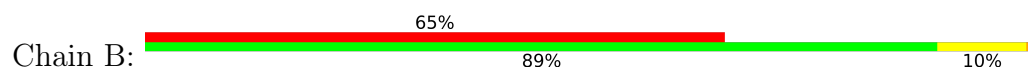
3 Residue-property plots [i](#)

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: Alpha/beta hydrolase



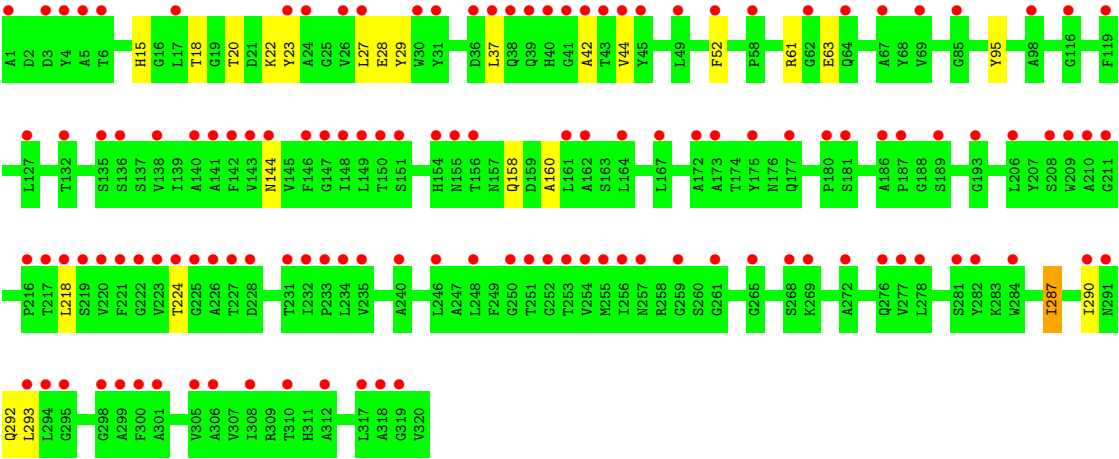
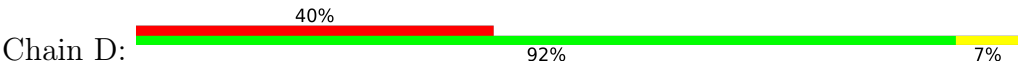
- Molecule 1: Alpha/beta hydrolase



- Molecule 1: Alpha/beta hydrolase



- Molecule 1: Alpha/beta hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	186.29Å 47.09Å 70.08Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	46.50 – 2.10 46.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.50-2.10) 99.5 (46.50-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.252 (Not available) , 0.293	Depositor DCC
R_{free} test set	3541 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.437 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9472	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0252e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.10	0/2393	0.31	0/3276
1	B	0.11	0/2393	0.34	2/3276 (0.1%)
1	C	0.09	0/2393	0.26	0/3276
1	D	0.09	0/2393	0.29	0/3276
All	All	0.10	0/9572	0.30	2/13104 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	GLY	CA-C-N	5.04	131.04	121.97
1	B	25	GLY	C-N-CA	5.04	131.04	121.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2345	0	2290	12	0
1	B	2345	0	2290	20	0
1	C	2345	0	2290	8	0
1	D	2345	0	2290	14	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	29	0	0	1	0
3	B	11	0	0	0	0
3	C	29	0	0	0	0
3	D	19	0	0	0	0
All	All	9472	0	9160	54	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 3.

All (54) 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:D:287:ILE:HG22	1:D:292:GLN:HB2	1.75	0.67
1:B:17:LEU:HG	1:B:18:THR:HG23	1.81	0.61
1:A:17:LEU:HG	1:A:18:THR:HG23	1.84	0.58
1:B:52:PHE:O	1:B:159:ASP:N	2.37	0.58
1:C:17:LEU:HD21	1:C:167:LEU:HD11	1.86	0.57
1:D:23:TYR:N	1:D:27:LEU:O	2.35	0.56
1:B:116:GLY:HA3	1:B:169:THR:HA	1.89	0.55
1:A:212:THR:O	1:A:215:GLN:NE2	2.38	0.54
1:B:287:ILE:HB	1:B:292:GLN:HB2	1.91	0.53
1:D:15:HIS:O	1:D:61:ARG:NH2	2.39	0.53
1:A:102:ASP:OD2	1:A:202:ASN:ND2	2.39	0.51
1:B:23:TYR:N	1:B:27:LEU:O	2.44	0.51
1:A:124:GLN:HB2	1:A:164:LEU:HD11	1.94	0.48
1:B:8:ARG:NH2	1:B:9:TYR:OH	2.47	0.48
1:B:102:ASP:OD2	1:B:202:ASN:ND2	2.34	0.47
1:C:117:SER:OG	1:C:266:LEU:O	2.27	0.47
1:B:25:GLY:O	1:B:26:VAL:HG13	2.15	0.47
1:C:216:PRO:HB3	1:C:256:ILE:HD12	1.96	0.47
1:A:178:ASN:ND2	3:A:502:HOH:O	2.40	0.46
1:A:1:ALA:HA	1:A:39:GLN:O	2.15	0.45
1:A:197:GLU:HG2	1:A:204:HIS:HB2	1.97	0.45
1:B:13:LEU:HD12	1:B:46:VAL:HG22	1.97	0.45
1:D:144:ASN:ND2	1:D:158:GLN:O	2.49	0.45
1:B:25:GLY:O	1:B:26:VAL:HG22	2.17	0.45
1:D:18:THR:HG22	1:D:52:PHE:CZ	2.52	0.44
1:C:228:ASP:OD1	1:C:230:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:HA	1:B:28:GLU:HA	1.99	0.44
1:D:52:PHE:HB3	1:D:160:ALA:HA	1.99	0.44
1:C:2:ASP:N	1:C:2:ASP:OD1	2.50	0.44
1:D:63:GLU:OE2	1:D:95:TYR:OH	2.28	0.44
1:B:12:VAL:HB	1:B:83:LEU:HD23	1.99	0.44
1:A:23:TYR:HB2	1:A:27:LEU:HB3	2.00	0.43
1:D:37:LEU:HB3	1:D:42:ALA:HB3	2.00	0.43
1:A:13:LEU:HB3	1:A:30:TRP:CE2	2.53	0.43
1:A:23:TYR:N	1:A:27:LEU:O	2.42	0.43
1:D:20:THR:O	1:D:29:TYR:HB2	2.19	0.43
1:C:210:ALA:HB3	1:C:280:THR:HG22	2.01	0.43
1:B:40:HIS:ND1	1:B:309:ARG:HD3	2.34	0.42
1:D:290:ILE:HG13	1:D:292:GLN:HG3	2.01	0.42
1:B:17:LEU:HD13	1:B:167:LEU:HD11	2.02	0.42
1:C:28:GLU:HG3	1:C:31:TYR:HA	2.01	0.42
1:C:263:ASN:HB3	1:C:268:SER:HA	2.00	0.42
1:B:3:ASP:HB2	1:B:6:THR:CG2	2.50	0.42
1:D:37:LEU:HB2	1:D:44:VAL:HG21	2.01	0.42
1:B:302:GLU:OE1	1:B:302:GLU:N	2.45	0.41
1:A:12:VAL:HB	1:A:83:LEU:HD23	2.02	0.41
1:D:22:LYS:HA	1:D:28:GLU:HA	2.02	0.41
1:B:244:SER:OG	1:B:287:ILE:HD11	2.21	0.41
1:D:292:GLN:HB3	1:D:293:LEU:HA	2.03	0.41
1:A:17:LEU:HD12	1:A:18:THR:H	1.86	0.41
1:B:18:THR:HG22	1:B:52:PHE:CE1	2.55	0.41
1:B:23:TYR:HB3	1:B:24:ALA:H	1.69	0.40
1:B:122:PHE:HB2	1:B:258:ARG:HD2	2.04	0.40
1:D:218:LEU:O	1:D:224:THR:HG23	2.22	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	318/320 (99%)	309 (97%)	9 (3%)	0	100	100
1	B	318/320 (99%)	299 (94%)	17 (5%)	2 (1%)	21	18
1	C	318/320 (99%)	312 (98%)	6 (2%)	0	100	100
1	D	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
All	All	1272/1280 (99%)	1226 (96%)	44 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	TYR
1	B	26	VAL

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	247/247 (100%)	245 (99%)	2 (1%)	73	81
1	B	247/247 (100%)	244 (99%)	3 (1%)	63	72
1	C	247/247 (100%)	246 (100%)	1 (0%)	84	89
1	D	247/247 (100%)	246 (100%)	1 (0%)	84	89
All	All	988/988 (100%)	981 (99%)	7 (1%)	76	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LEU
1	A	218	LEU
1	B	20	THR
1	B	23	TYR
1	B	297	ARG
1	C	18	THR
1	D	287	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	257	ASN
1	B	64	GLN
1	B	257	ASN
1	C	48	ASN
1	C	215	GLN
1	C	262	GLN
1	C	313	ASN
1	D	177	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 4 ligands modelled in this entry, 4 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 ⓘ

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	320/320 (100%)	0.45	11 (3%) 48 50	9, 15, 23, 34	0
1	B	320/320 (100%)	2.54	208 (65%) 0 0	18, 36, 45, 53	0
1	C	320/320 (100%)	0.64	11 (3%) 48 50	10, 17, 26, 39	0
1	D	320/320 (100%)	2.03	129 (40%) 0 1	19, 30, 41, 65	0
All	All	1280/1280 (100%)	1.41	359 (28%) 1 1	9, 23, 42, 65	0

All (359) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	THR	10.6
1	D	221	PHE	10.2
1	D	223	VAL	9.5
1	D	220	VAL	8.7
1	B	26	VAL	8.2
1	D	1	ALA	6.4
1	B	20	THR	6.3
1	B	25	GLY	6.2
1	D	219	SER	6.1
1	B	227	THR	6.1
1	B	146	PHE	5.9
1	B	24	ALA	5.7
1	B	220	VAL	5.4
1	B	17	LEU	5.3
1	A	222	GLY	5.3
1	A	220	VAL	5.2
1	B	300	PHE	5.2
1	B	133	GLY	5.2
1	B	1	ALA	5.1
1	C	1	ALA	4.8
1	D	272	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	139	ILE	4.7
1	B	266	LEU	4.7
1	B	154	HIS	4.7
1	D	218	LEU	4.7
1	B	233	PRO	4.7
1	B	280	THR	4.7
1	D	222	GLY	4.7
1	B	226	ALA	4.6
1	B	305	VAL	4.5
1	B	234	LEU	4.5
1	D	3	ASP	4.5
1	B	123	VAL	4.5
1	B	128	ALA	4.5
1	D	232	ILE	4.4
1	B	318	ALA	4.3
1	B	317	LEU	4.3
1	B	223	VAL	4.3
1	D	37	LEU	4.2
1	B	100	ALA	4.2
1	A	219	SER	4.2
1	D	261	GLY	4.1
1	B	222	GLY	4.1
1	D	234	LEU	4.1
1	B	175	TYR	4.1
1	B	249	PHE	4.1
1	B	257	ASN	4.0
1	B	149	LEU	4.0
1	B	4	TYR	4.0
1	D	6	THR	4.0
1	D	24	ALA	3.9
1	B	232	ILE	3.9
1	B	306	ALA	3.9
1	B	294	LEU	3.9
1	B	217	THR	3.9
1	D	227	THR	3.9
1	B	143	VAL	3.9
1	D	142	PHE	3.9
1	B	277	VAL	3.8
1	B	19	GLY	3.8
1	D	217	THR	3.8
1	B	281	SER	3.8
1	D	26	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	293	LEU	3.7
1	B	237	PRO	3.7
1	D	298	GLY	3.7
1	B	235	VAL	3.7
1	B	308	ILE	3.7
1	D	224	THR	3.7
1	B	131	PRO	3.6
1	B	267	VAL	3.6
1	B	307	VAL	3.6
1	B	214	ILE	3.6
1	A	218	LEU	3.6
1	B	218	LEU	3.6
1	B	282	TYR	3.6
1	D	305	VAL	3.5
1	B	120	ALA	3.5
1	A	223	VAL	3.5
1	B	148	ILE	3.5
1	D	300	PHE	3.5
1	B	134	LEU	3.5
1	D	138	VAL	3.5
1	D	318	ALA	3.5
1	B	207	TYR	3.5
1	B	304	PRO	3.4
1	D	143	VAL	3.4
1	B	127	LEU	3.4
1	D	149	LEU	3.4
1	B	311	HIS	3.4
1	B	23	TYR	3.4
1	B	188	GLY	3.4
1	D	67	ALA	3.4
1	D	282	TYR	3.4
1	D	154	HIS	3.3
1	B	132	THR	3.3
1	D	210	ALA	3.3
1	D	299	ALA	3.3
1	B	241	LEU	3.3
1	B	52	PHE	3.3
1	B	270	CYS	3.3
1	B	136	SER	3.3
1	B	129	TYR	3.3
1	B	238	ALA	3.3
1	B	22	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	245	THR	3.3
1	D	150	THR	3.3
1	B	243	PRO	3.3
1	D	233	PRO	3.3
1	B	122	PHE	3.3
1	B	253	THR	3.2
1	B	173	ALA	3.2
1	B	272	ALA	3.2
1	D	256	ILE	3.2
1	D	317	LEU	3.2
1	B	212	THR	3.2
1	D	211	GLY	3.2
1	B	213	ALA	3.2
1	D	140	ALA	3.2
1	B	256	ILE	3.2
1	D	141	ALA	3.2
1	D	162	ALA	3.2
1	B	209	TRP	3.1
1	D	186	ALA	3.1
1	B	91	LEU	3.1
1	B	179	TYR	3.1
1	B	219	SER	3.1
1	D	252	GLY	3.1
1	B	177	GLN	3.1
1	B	138	VAL	3.1
1	B	126	VAL	3.1
1	B	194	ALA	3.1
1	C	21	ASP	3.1
1	B	210	ALA	3.1
1	B	37	LEU	3.1
1	D	27	LEU	3.1
1	D	164	LEU	3.1
1	B	150	THR	3.0
1	D	257	ASN	3.0
1	B	161	LEU	3.0
1	B	137	SER	3.0
1	D	281	SER	3.0
1	B	313	ASN	3.0
1	B	5	ALA	3.0
1	D	248	LEU	3.0
1	B	135	SER	3.0
1	B	172	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	208	SER	3.0
1	D	226	ALA	3.0
1	B	278	LEU	3.0
1	B	312	ALA	2.9
1	D	173	ALA	2.9
1	B	57	GLY	2.9
1	B	183	GLY	2.9
1	B	192	THR	2.9
1	B	246	LEU	2.9
1	D	278	LEU	2.9
1	B	104	VAL	2.9
1	D	40	HIS	2.9
1	D	187	PRO	2.9
1	B	271	SER	2.9
1	B	42	ALA	2.9
1	B	97	ALA	2.9
1	B	301	ALA	2.9
1	B	174	THR	2.9
1	D	290	ILE	2.9
1	D	151	SER	2.9
1	B	162	ALA	2.9
1	B	259	GLY	2.9
1	D	225	GLY	2.9
1	B	250	GLY	2.8
1	B	303	ASP	2.8
1	B	184	LEU	2.8
1	B	206	LEU	2.8
1	D	30	TRP	2.8
1	A	224	THR	2.8
1	B	145	VAL	2.8
1	B	168	THR	2.8
1	B	225	GLY	2.8
1	B	186	ALA	2.8
1	B	310	THR	2.8
1	B	199	VAL	2.8
1	D	135	SER	2.8
1	B	41	GLY	2.8
1	B	141	ALA	2.8
1	C	75	ALA	2.8
1	D	175	TYR	2.8
1	D	294	LEU	2.8
1	D	209	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	221	PHE	2.7
1	B	27	LEU	2.7
1	D	49	LEU	2.7
1	A	217	THR	2.7
1	D	310	THR	2.7
1	D	308	ILE	2.7
1	B	163	SER	2.7
1	B	284	TRP	2.7
1	D	147	GLY	2.7
1	B	164	LEU	2.7
1	D	277	VAL	2.7
1	B	89	GLY	2.7
1	C	188	GLY	2.7
1	D	85	GLY	2.7
1	C	136	SER	2.7
1	B	299	ALA	2.6
1	B	119	PHE	2.6
1	B	166	THR	2.6
1	A	3	ASP	2.6
1	B	36	ASP	2.6
1	B	254	VAL	2.6
1	B	169	THR	2.6
1	B	176	ASN	2.6
1	D	42	ALA	2.6
1	D	43	THR	2.6
1	D	206	LEU	2.6
1	B	236	ASP	2.6
1	B	302	GLU	2.6
1	B	182	ALA	2.6
1	B	251	THR	2.6
1	D	231	THR	2.6
1	B	117	SER	2.6
1	B	296	VAL	2.6
1	D	69	VAL	2.6
1	D	148	ILE	2.6
1	B	125	GLY	2.6
1	B	147	GLY	2.6
1	B	231	THR	2.6
1	B	297	ARG	2.6
1	D	269	LYS	2.5
1	B	21	ASP	2.5
1	B	74	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	230	SER	2.5
1	D	146	PHE	2.5
1	B	298	GLY	2.5
1	B	283	LYS	2.5
1	A	102	ASP	2.5
1	D	132	THR	2.5
1	D	284	TRP	2.5
1	B	116	GLY	2.5
1	D	295	GLY	2.5
1	D	319	GLY	2.5
1	B	170	ALA	2.5
1	D	98	ALA	2.5
1	B	273	LEU	2.5
1	D	155	ASN	2.5
1	B	290	ILE	2.5
1	B	108	THR	2.4
1	B	152	SER	2.4
1	D	172	ALA	2.4
1	D	127	LEU	2.4
1	D	52	PHE	2.4
1	B	159	ASP	2.4
1	C	152	SER	2.4
1	D	268	SER	2.4
1	B	205	LEU	2.4
1	D	17	LEU	2.4
1	B	118	GLU	2.4
1	C	221	PHE	2.4
1	D	119	PHE	2.4
1	B	33	ILE	2.4
1	B	309	ARG	2.4
1	B	160	ALA	2.4
1	B	247	ALA	2.4
1	D	161	LEU	2.4
1	D	167	LEU	2.4
1	B	3	ASP	2.4
1	B	110	ILE	2.4
1	D	254	VAL	2.4
1	D	216	PRO	2.4
1	D	4	TYR	2.3
1	B	315	LEU	2.3
1	D	177	GLN	2.3
1	D	259	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	86	HIS	2.3
1	B	6	THR	2.3
1	B	39	GLN	2.3
1	B	140	ALA	2.3
1	D	116	GLY	2.3
1	B	287	ILE	2.3
1	B	229	THR	2.3
1	D	253	THR	2.3
1	D	144	ASN	2.3
1	D	291	ASN	2.3
1	C	78	ALA	2.3
1	B	228	ASP	2.3
1	C	57	GLY	2.3
1	B	96	VAL	2.3
1	B	113	PRO	2.3
1	D	251	THR	2.3
1	B	291	ASN	2.3
1	D	293	LEU	2.3
1	C	23	TYR	2.3
1	D	39	GLN	2.2
1	D	136	SER	2.2
1	B	156	THR	2.2
1	D	5	ALA	2.2
1	D	41	GLY	2.2
1	D	306	ALA	2.2
1	D	246	LEU	2.2
1	D	23	TYR	2.2
1	A	39	GLN	2.2
1	D	276	GLN	2.2
1	B	268	SER	2.2
1	B	279	SER	2.2
1	B	43	THR	2.2
1	B	180	PRO	2.2
1	B	320	VAL	2.2
1	D	228	ASP	2.2
1	D	250	GLY	2.2
1	B	28	GLU	2.2
1	B	286	HIS	2.2
1	B	274	TYR	2.2
1	B	87	SER	2.2
1	D	189	SER	2.2
1	B	59	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	156	THR	2.2
1	B	264	ASP	2.2
1	B	288	ASP	2.2
1	D	36	ASP	2.2
1	B	211	GLY	2.2
1	D	38	GLN	2.2
1	B	167	LEU	2.2
1	D	181	SER	2.2
1	B	31	TYR	2.2
1	D	180	PRO	2.1
1	B	142	PHE	2.1
1	C	97	ALA	2.1
1	B	314	ARG	2.1
1	B	45	TYR	2.1
1	B	285	ASN	2.1
1	D	45	TYR	2.1
1	B	187	PRO	2.1
1	B	178	ASN	2.1
1	B	40	HIS	2.1
1	B	193	GLY	2.1
1	B	295	GLY	2.1
1	D	62	GLY	2.1
1	B	269	LYS	2.1
1	D	301	ALA	2.1
1	D	255	MET	2.1
1	B	242	ASP	2.1
1	B	216	PRO	2.1
1	D	58	PRO	2.1
1	B	11	ILE	2.1
1	D	44	VAL	2.1
1	D	240	ALA	2.1
1	D	312	ALA	2.1
1	B	196	THR	2.0
1	B	62	GLY	2.0
1	B	68	TYR	2.0
1	D	193	GLY	2.0
1	D	265	GLY	2.0
1	A	221	PHE	2.0
1	B	35	GLU	2.0
1	D	235	VAL	2.0
1	B	215	GLN	2.0
1	D	64	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	58	PRO	2.0
1	D	31	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	CA	B	401	1/1	0.93	0.07	41,41,41,41	0
2	CA	A	401	1/1	0.94	0.05	19,19,19,19	0
2	CA	D	401	1/1	0.95	0.06	25,25,25,25	0
2	CA	C	401	1/1	0.96	0.07	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.