



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:16 AM UTC

PDB ID : 4OD4 / pdb_00004od4
Title : Apo structure of a UbiA homolog from Aeropyrum pernix K1
Authors : Li, W.; Cheng, W.
Deposited on : 2014-01-09
Resolution : 3.30 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:

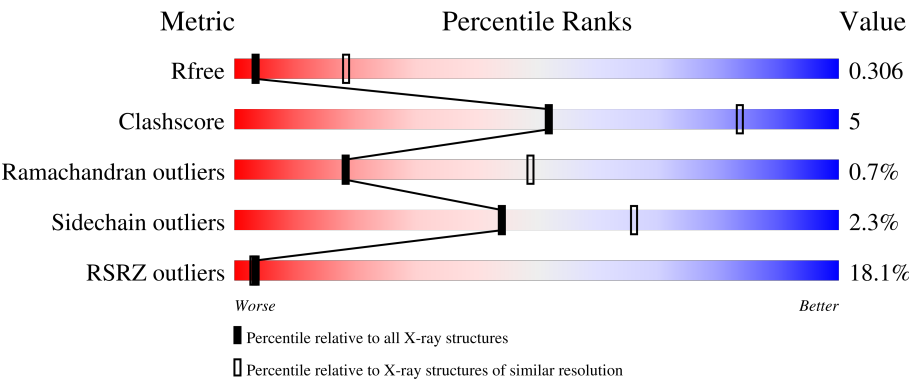
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	303	13% 80%11%9%
1	B	303	18% 80%10%9%
1	C	303	13% 80%10%9%
1	D	303	12% 81%10%9%
1	E	303	24% 80%10%9%

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Mol	Chain	Length	Quality of chain
1	F	303	19% 79% 11% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12036 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 4-hydroxybenzoate octaprenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2006	1320	333	346	7			
1	B	275	Total	C	N	O	S	0	0	0
			2006	1320	333	346	7			
1	C	275	Total	C	N	O	S	0	0	0
			2006	1320	333	346	7			
1	D	275	Total	C	N	O	S	0	0	0
			2006	1320	333	346	7			
1	E	275	Total	C	N	O	S	0	0	0
			2006	1320	333	346	7			
1	F	275	Total	C	N	O	S	0	0	0
			2006	1320	333	346	7			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP Q9YBM8
A	-17	GLY	-	expression tag	UNP Q9YBM8
A	-16	SER	-	expression tag	UNP Q9YBM8
A	-15	SER	-	expression tag	UNP Q9YBM8
A	-14	HIS	-	expression tag	UNP Q9YBM8
A	-13	HIS	-	expression tag	UNP Q9YBM8
A	-12	HIS	-	expression tag	UNP Q9YBM8
A	-11	HIS	-	expression tag	UNP Q9YBM8
A	-10	HIS	-	expression tag	UNP Q9YBM8
A	-9	HIS	-	expression tag	UNP Q9YBM8
A	-8	SER	-	expression tag	UNP Q9YBM8
A	-7	SER	-	expression tag	UNP Q9YBM8
A	-6	GLY	-	expression tag	UNP Q9YBM8
A	-5	LEU	-	expression tag	UNP Q9YBM8
A	-4	VAL	-	expression tag	UNP Q9YBM8
A	-3	PRO	-	expression tag	UNP Q9YBM8
A	-2	ALA	-	expression tag	UNP Q9YBM8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9YBM8
A	0	SER	-	expression tag	UNP Q9YBM8
B	-18	MET	-	expression tag	UNP Q9YBM8
B	-17	GLY	-	expression tag	UNP Q9YBM8
B	-16	SER	-	expression tag	UNP Q9YBM8
B	-15	SER	-	expression tag	UNP Q9YBM8
B	-14	HIS	-	expression tag	UNP Q9YBM8
B	-13	HIS	-	expression tag	UNP Q9YBM8
B	-12	HIS	-	expression tag	UNP Q9YBM8
B	-11	HIS	-	expression tag	UNP Q9YBM8
B	-10	HIS	-	expression tag	UNP Q9YBM8
B	-9	HIS	-	expression tag	UNP Q9YBM8
B	-8	SER	-	expression tag	UNP Q9YBM8
B	-7	SER	-	expression tag	UNP Q9YBM8
B	-6	GLY	-	expression tag	UNP Q9YBM8
B	-5	LEU	-	expression tag	UNP Q9YBM8
B	-4	VAL	-	expression tag	UNP Q9YBM8
B	-3	PRO	-	expression tag	UNP Q9YBM8
B	-2	ALA	-	expression tag	UNP Q9YBM8
B	-1	GLY	-	expression tag	UNP Q9YBM8
B	0	SER	-	expression tag	UNP Q9YBM8
C	-18	MET	-	expression tag	UNP Q9YBM8
C	-17	GLY	-	expression tag	UNP Q9YBM8
C	-16	SER	-	expression tag	UNP Q9YBM8
C	-15	SER	-	expression tag	UNP Q9YBM8
C	-14	HIS	-	expression tag	UNP Q9YBM8
C	-13	HIS	-	expression tag	UNP Q9YBM8
C	-12	HIS	-	expression tag	UNP Q9YBM8
C	-11	HIS	-	expression tag	UNP Q9YBM8
C	-10	HIS	-	expression tag	UNP Q9YBM8
C	-9	HIS	-	expression tag	UNP Q9YBM8
C	-8	SER	-	expression tag	UNP Q9YBM8
C	-7	SER	-	expression tag	UNP Q9YBM8
C	-6	GLY	-	expression tag	UNP Q9YBM8
C	-5	LEU	-	expression tag	UNP Q9YBM8
C	-4	VAL	-	expression tag	UNP Q9YBM8
C	-3	PRO	-	expression tag	UNP Q9YBM8
C	-2	ALA	-	expression tag	UNP Q9YBM8
C	-1	GLY	-	expression tag	UNP Q9YBM8
C	0	SER	-	expression tag	UNP Q9YBM8
D	-18	MET	-	expression tag	UNP Q9YBM8
D	-17	GLY	-	expression tag	UNP Q9YBM8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q9YBM8
D	-15	SER	-	expression tag	UNP Q9YBM8
D	-14	HIS	-	expression tag	UNP Q9YBM8
D	-13	HIS	-	expression tag	UNP Q9YBM8
D	-12	HIS	-	expression tag	UNP Q9YBM8
D	-11	HIS	-	expression tag	UNP Q9YBM8
D	-10	HIS	-	expression tag	UNP Q9YBM8
D	-9	HIS	-	expression tag	UNP Q9YBM8
D	-8	SER	-	expression tag	UNP Q9YBM8
D	-7	SER	-	expression tag	UNP Q9YBM8
D	-6	GLY	-	expression tag	UNP Q9YBM8
D	-5	LEU	-	expression tag	UNP Q9YBM8
D	-4	VAL	-	expression tag	UNP Q9YBM8
D	-3	PRO	-	expression tag	UNP Q9YBM8
D	-2	ALA	-	expression tag	UNP Q9YBM8
D	-1	GLY	-	expression tag	UNP Q9YBM8
D	0	SER	-	expression tag	UNP Q9YBM8
E	-18	MET	-	expression tag	UNP Q9YBM8
E	-17	GLY	-	expression tag	UNP Q9YBM8
E	-16	SER	-	expression tag	UNP Q9YBM8
E	-15	SER	-	expression tag	UNP Q9YBM8
E	-14	HIS	-	expression tag	UNP Q9YBM8
E	-13	HIS	-	expression tag	UNP Q9YBM8
E	-12	HIS	-	expression tag	UNP Q9YBM8
E	-11	HIS	-	expression tag	UNP Q9YBM8
E	-10	HIS	-	expression tag	UNP Q9YBM8
E	-9	HIS	-	expression tag	UNP Q9YBM8
E	-8	SER	-	expression tag	UNP Q9YBM8
E	-7	SER	-	expression tag	UNP Q9YBM8
E	-6	GLY	-	expression tag	UNP Q9YBM8
E	-5	LEU	-	expression tag	UNP Q9YBM8
E	-4	VAL	-	expression tag	UNP Q9YBM8
E	-3	PRO	-	expression tag	UNP Q9YBM8
E	-2	ALA	-	expression tag	UNP Q9YBM8
E	-1	GLY	-	expression tag	UNP Q9YBM8
E	0	SER	-	expression tag	UNP Q9YBM8
F	-18	MET	-	expression tag	UNP Q9YBM8
F	-17	GLY	-	expression tag	UNP Q9YBM8
F	-16	SER	-	expression tag	UNP Q9YBM8
F	-15	SER	-	expression tag	UNP Q9YBM8
F	-14	HIS	-	expression tag	UNP Q9YBM8
F	-13	HIS	-	expression tag	UNP Q9YBM8

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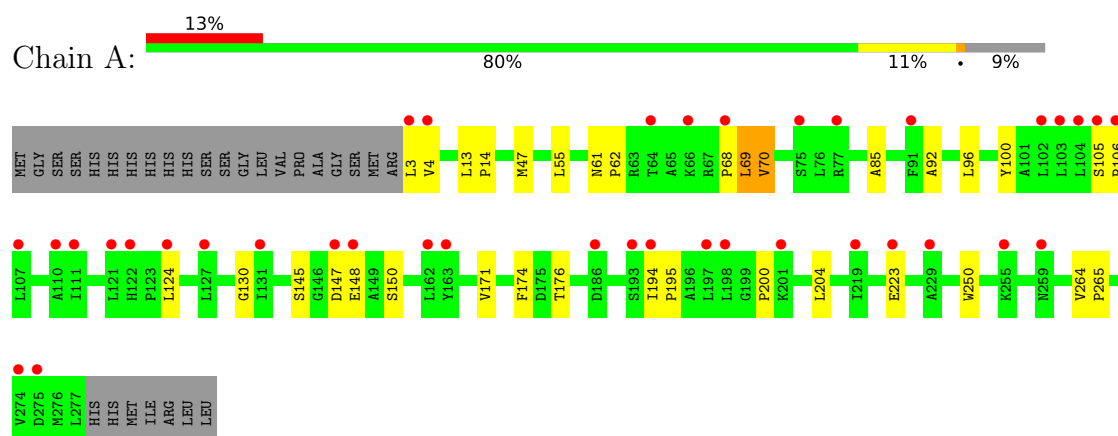
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	HIS	-	expression tag	UNP Q9YBM8
F	-11	HIS	-	expression tag	UNP Q9YBM8
F	-10	HIS	-	expression tag	UNP Q9YBM8
F	-9	HIS	-	expression tag	UNP Q9YBM8
F	-8	SER	-	expression tag	UNP Q9YBM8
F	-7	SER	-	expression tag	UNP Q9YBM8
F	-6	GLY	-	expression tag	UNP Q9YBM8
F	-5	LEU	-	expression tag	UNP Q9YBM8
F	-4	VAL	-	expression tag	UNP Q9YBM8
F	-3	PRO	-	expression tag	UNP Q9YBM8
F	-2	ALA	-	expression tag	UNP Q9YBM8
F	-1	GLY	-	expression tag	UNP Q9YBM8
F	0	SER	-	expression tag	UNP Q9YBM8

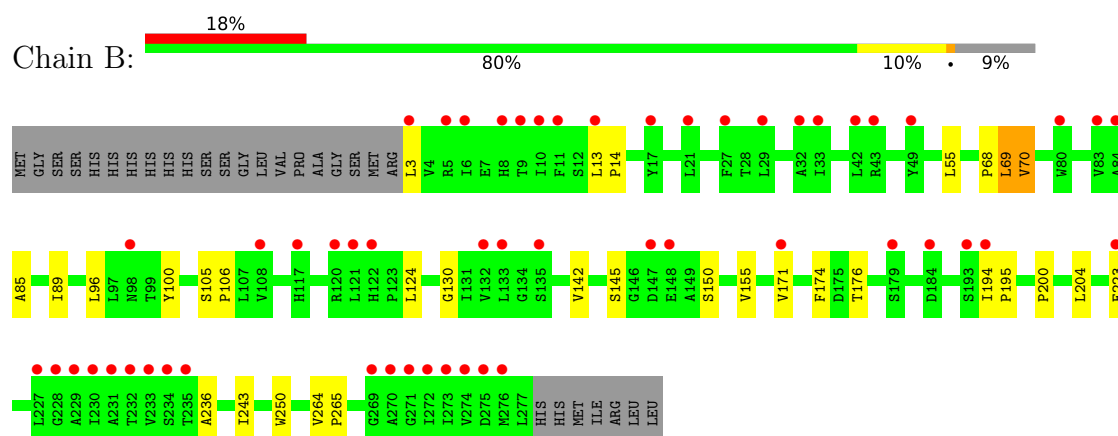
3 Residue-property plots

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.

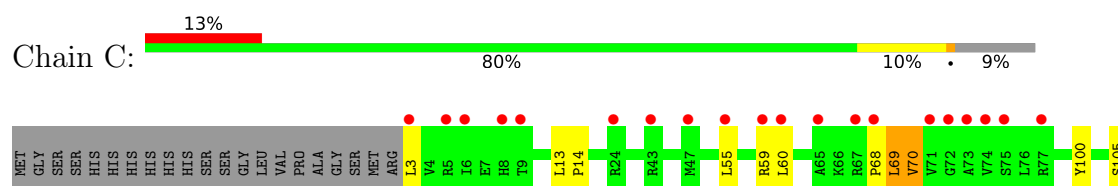
- Molecule 1: 4-hydroxybenzoate octaprenyltransferase

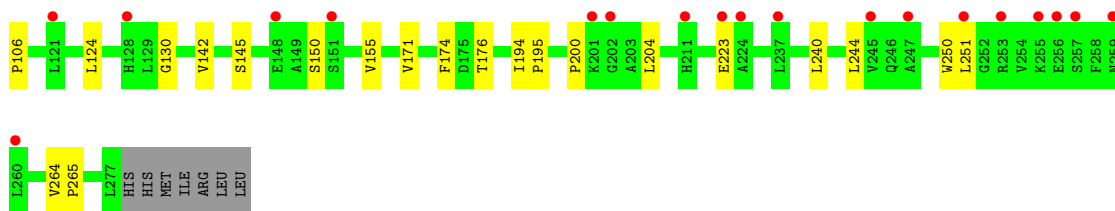


- Molecule 1: 4-hydroxybenzoate octaprenyltransferase

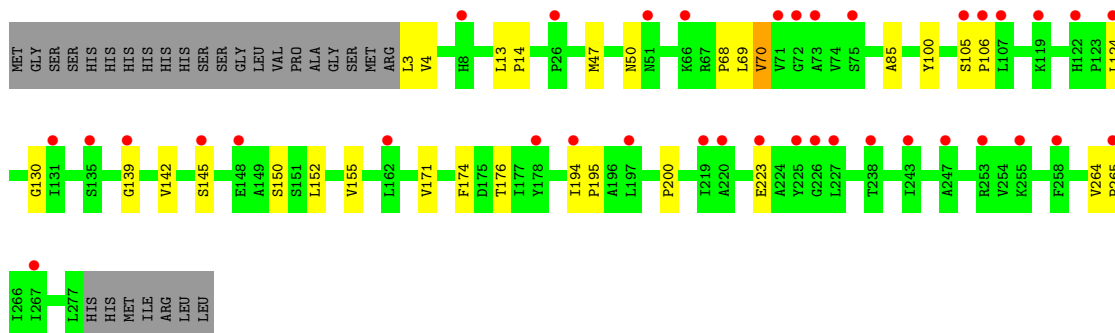
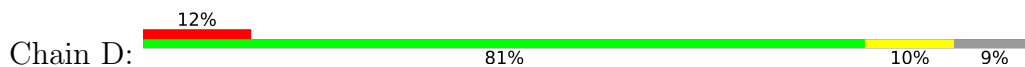


- Molecule 1: 4-hydroxybenzoate octaprenyltransferase

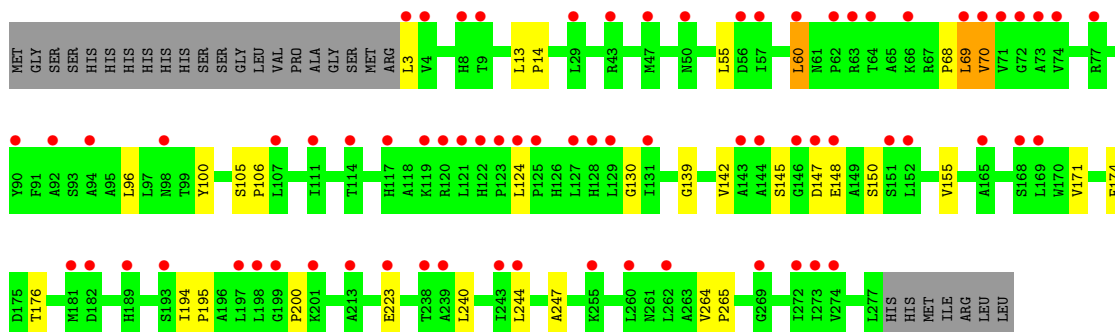
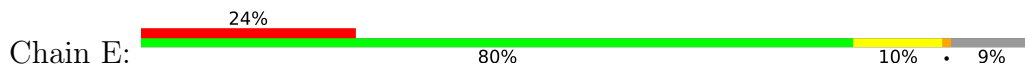




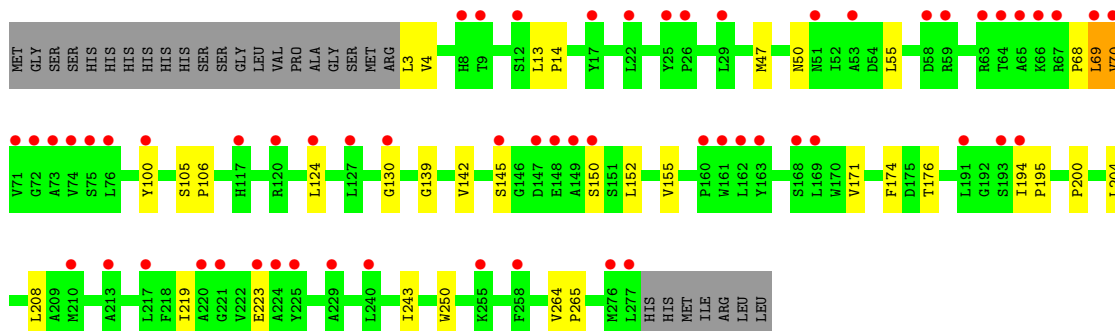
• Molecule 1: 4-hydroxybenzoate octaprenyltransferase



• Molecule 1: 4-hydroxybenzoate octaprenyltransferase



• Molecule 1: 4-hydroxybenzoate octaprenyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.09Å 123.07Å 423.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 3.30 49.78 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.78-3.30) 99.1 (49.78-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.272 , 0.303 0.279 , 0.306	Depositor DCC
R_{free} test set	2824 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12036	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/2050	0.79	1/2809 (0.0%)
1	B	0.44	0/2050	0.79	1/2809 (0.0%)
1	C	0.45	0/2050	0.79	1/2809 (0.0%)
1	D	0.42	0/2050	0.80	1/2809 (0.0%)
1	E	0.44	0/2050	0.80	1/2809 (0.0%)
1	F	0.44	0/2050	0.80	1/2809 (0.0%)
All	All	0.44	0/12300	0.80	6/16854 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	VAL	N-CA-C	-10.10	102.05	111.45
1	F	70	VAL	N-CA-C	-9.91	102.24	111.45
1	D	70	VAL	N-CA-C	-9.54	102.58	111.45
1	A	70	VAL	N-CA-C	-9.51	102.60	111.45
1	C	70	VAL	N-CA-C	-9.23	102.86	111.45
1	E	70	VAL	N-CA-C	-9.10	102.98	111.45

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	2006	0	2089	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2006	0	2089	29	0
1	C	2006	0	2089	36	0
1	D	2006	0	2089	15	0
1	E	2006	0	2089	32	0
1	F	2006	0	2089	23	0
All	All	12036	0	12534	124	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 5.

All (124) 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:C:59:ARG:CB	1:E:60:LEU:HD22	2.18	0.73
1:C:59:ARG:HD3	1:E:60:LEU:HD22	1.72	0.71
1:C:59:ARG:CD	1:E:60:LEU:HD22	2.23	0.69
1:C:59:ARG:HB3	1:E:60:LEU:CD2	2.24	0.67
1:C:59:ARG:HB3	1:E:60:LEU:HD22	1.76	0.66
1:E:247:ALA:HB1	1:F:219:ILE:HD11	1.79	0.63
1:B:243:ILE:CG1	1:C:244:LEU:HD11	2.31	0.61
1:B:243:ILE:HG21	1:C:244:LEU:HD11	1.84	0.58
1:B:243:ILE:CG2	1:C:244:LEU:HD11	2.32	0.58
1:A:85:ALA:HB1	1:B:96:LEU:HD21	1.88	0.56
1:C:59:ARG:CB	1:E:60:LEU:CD2	2.83	0.55
1:C:130:GLY:HA2	1:C:171:VAL:HG21	1.88	0.55
1:E:130:GLY:HA2	1:E:171:VAL:HG21	1.88	0.55
1:B:130:GLY:HA2	1:B:171:VAL:HG21	1.87	0.55
1:D:130:GLY:HA2	1:D:171:VAL:HG21	1.88	0.55
1:E:244:LEU:HD11	1:F:243:ILE:HD12	1.88	0.55
1:C:264:VAL:HB	1:C:265:PRO:HD3	1.89	0.54
1:B:243:ILE:O	1:C:240:LEU:HD21	2.08	0.54
1:F:130:GLY:HA2	1:F:171:VAL:HG21	1.90	0.54
1:B:243:ILE:HD12	1:C:244:LEU:HD11	1.90	0.54
1:A:130:GLY:HA2	1:A:171:VAL:HG21	1.88	0.53
1:B:130:GLY:HA2	1:B:171:VAL:CG2	2.39	0.52
1:B:243:ILE:HG13	1:C:244:LEU:HD11	1.91	0.52
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.92	0.52
1:F:264:VAL:HB	1:F:265:PRO:HD3	1.92	0.52
1:C:130:GLY:HA2	1:C:171:VAL:CG2	2.40	0.52
1:E:130:GLY:HA2	1:E:171:VAL:CG2	2.40	0.51
1:A:130:GLY:HA2	1:A:171:VAL:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.93	0.50
1:D:130:GLY:HA2	1:D:171:VAL:CG2	2.41	0.50
1:E:264:VAL:HB	1:E:265:PRO:HD3	1.93	0.50
1:C:176:THR:HG23	1:C:194:ILE:CG2	2.42	0.50
1:F:130:GLY:HA2	1:F:171:VAL:CG2	2.41	0.50
1:E:100:TYR:OH	1:E:150:SER:O	2.30	0.50
1:B:264:VAL:HB	1:B:265:PRO:HD3	1.94	0.50
1:A:100:TYR:OH	1:A:150:SER:O	2.30	0.50
1:D:100:TYR:OH	1:D:150:SER:O	2.31	0.49
1:F:100:TYR:OH	1:F:150:SER:O	2.30	0.49
1:E:244:LEU:HD11	1:F:243:ILE:CD1	2.41	0.49
1:C:60:LEU:HD21	1:E:60:LEU:HD11	1.93	0.49
1:E:60:LEU:HD23	1:E:60:LEU:N	2.28	0.49
1:F:176:THR:HG23	1:F:194:ILE:CG2	2.43	0.48
1:C:100:TYR:OH	1:C:150:SER:O	2.32	0.48
1:A:171:VAL:HA	1:A:174:PHE:CE2	2.49	0.48
1:E:176:THR:HG23	1:E:194:ILE:CG2	2.44	0.47
1:F:171:VAL:HA	1:F:174:PHE:CE2	2.50	0.47
1:B:243:ILE:CD1	1:C:244:LEU:HD11	2.43	0.47
1:B:176:THR:HG23	1:B:194:ILE:CG2	2.45	0.47
1:B:171:VAL:HA	1:B:174:PHE:CE2	2.49	0.47
1:C:244:LEU:HD12	1:C:244:LEU:N	2.29	0.47
1:B:243:ILE:HG13	1:C:244:LEU:CG	2.45	0.47
1:B:100:TYR:OH	1:B:150:SER:O	2.32	0.46
1:B:243:ILE:HG13	1:C:244:LEU:HG	1.97	0.46
1:C:59:ARG:HH11	1:E:60:LEU:HB3	1.79	0.46
1:E:171:VAL:HA	1:E:174:PHE:CE2	2.50	0.46
1:A:176:THR:HG23	1:A:194:ILE:CG2	2.46	0.46
1:D:171:VAL:HA	1:D:174:PHE:CE2	2.50	0.46
1:D:176:THR:HG23	1:D:194:ILE:CG2	2.45	0.46
1:C:171:VAL:HA	1:C:174:PHE:CE2	2.52	0.45
1:A:68:PRO:C	1:A:70:VAL:H	2.24	0.45
1:D:68:PRO:C	1:D:70:VAL:H	2.25	0.45
1:C:174:PHE:C	1:C:174:PHE:CD1	2.95	0.45
1:E:68:PRO:C	1:E:70:VAL:H	2.25	0.44
1:B:68:PRO:C	1:B:70:VAL:H	2.25	0.44
1:A:4:VAL:HG23	1:A:47:MET:SD	2.57	0.44
1:B:243:ILE:HG13	1:C:244:LEU:CD1	2.48	0.44
1:C:68:PRO:C	1:C:70:VAL:H	2.25	0.44
1:E:240:LEU:HD12	1:F:208:LEU:HD11	1.99	0.44
1:D:174:PHE:C	1:D:174:PHE:CD1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:N	1:B:14:PRO:CD	2.80	0.44
1:E:105:SER:N	1:E:106:PRO:HD2	2.33	0.44
1:F:55:LEU:HD13	1:F:69:LEU:HD13	1.99	0.44
1:F:68:PRO:C	1:F:70:VAL:H	2.26	0.44
1:B:174:PHE:CD1	1:B:174:PHE:C	2.96	0.43
1:E:174:PHE:C	1:E:174:PHE:CD1	2.95	0.43
1:F:174:PHE:CD1	1:F:174:PHE:C	2.96	0.43
1:D:105:SER:N	1:D:106:PRO:HD2	2.33	0.43
1:E:147:ASP:HA	1:E:148:GLU:HA	1.85	0.43
1:A:92:ALA:HB1	1:B:89:ILE:CG2	2.48	0.43
1:A:174:PHE:CD1	1:A:174:PHE:C	2.96	0.43
1:C:55:LEU:HD13	1:C:69:LEU:HD13	2.01	0.43
1:F:105:SER:N	1:F:106:PRO:HD2	2.34	0.43
1:A:55:LEU:HD13	1:A:69:LEU:HD13	2.01	0.43
1:D:4:VAL:HG23	1:D:47:MET:SD	2.59	0.42
1:A:204:LEU:HB3	1:A:250:TRP:CZ2	2.53	0.42
1:B:105:SER:N	1:B:106:PRO:HD2	2.34	0.42
1:C:105:SER:N	1:C:106:PRO:HD2	2.34	0.42
1:D:85:ALA:HB1	1:E:96:LEU:HD21	2.01	0.42
1:A:96:LEU:HD21	1:B:85:ALA:HB1	2.02	0.42
1:B:204:LEU:HB3	1:B:250:TRP:CZ2	2.55	0.42
1:B:236:ALA:HB2	1:C:251:LEU:HD13	2.02	0.42
1:D:13:LEU:N	1:D:14:PRO:CD	2.82	0.42
1:A:194:ILE:N	1:A:195:PRO:HD2	2.35	0.42
1:B:243:ILE:HG21	1:C:244:LEU:CD1	2.49	0.42
1:E:13:LEU:N	1:E:14:PRO:CD	2.83	0.42
1:F:152:LEU:HA	1:F:155:VAL:HG12	2.02	0.42
1:C:13:LEU:N	1:C:14:PRO:CD	2.83	0.41
1:C:204:LEU:HB3	1:C:250:TRP:CZ2	2.55	0.41
1:F:204:LEU:HB3	1:F:250:TRP:CZ2	2.55	0.41
1:B:55:LEU:HD13	1:B:69:LEU:HD13	2.02	0.41
1:C:142:VAL:HG12	1:C:155:VAL:HG22	2.03	0.41
1:F:194:ILE:N	1:F:195:PRO:HD2	2.35	0.41
1:D:194:ILE:N	1:D:195:PRO:HD2	2.36	0.41
1:F:13:LEU:N	1:F:14:PRO:CD	2.83	0.41
1:B:194:ILE:N	1:B:195:PRO:HD2	2.36	0.41
1:C:194:ILE:N	1:C:195:PRO:HD2	2.35	0.41
1:E:240:LEU:CD2	1:F:243:ILE:HG23	2.50	0.41
1:A:105:SER:N	1:A:106:PRO:HD2	2.35	0.41
1:D:139:GLY:HA2	1:D:142:VAL:HG22	2.03	0.41
1:E:244:LEU:HD11	1:F:243:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:VAL:HG23	1:F:47:MET:SD	2.61	0.41
1:F:142:VAL:HG12	1:F:155:VAL:HG22	2.03	0.41
1:A:61:ASN:HA	1:A:62:PRO:HD3	1.99	0.41
1:E:139:GLY:HA2	1:E:142:VAL:HG22	2.03	0.41
1:A:147:ASP:HA	1:A:148:GLU:HA	1.85	0.40
1:D:152:LEU:HA	1:D:155:VAL:HG12	2.03	0.40
1:A:13:LEU:HB2	1:A:14:PRO:HD3	2.03	0.40
1:B:142:VAL:HG12	1:B:155:VAL:HG22	2.04	0.40
1:E:55:LEU:HD13	1:E:69:LEU:HD13	2.04	0.40
1:E:194:ILE:N	1:E:195:PRO:HD2	2.36	0.40
1:A:13:LEU:N	1:A:14:PRO:CD	2.85	0.40
1:C:60:LEU:HD23	1:E:60:LEU:HD21	2.02	0.40
1:E:142:VAL:HG12	1:E:155:VAL:HG22	2.04	0.40
1:F:139:GLY:HA2	1:F:142:VAL:HG22	2.02	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	273/303 (90%)	252 (92%)	19 (7%)	2 (1%)	18	49
1	B	273/303 (90%)	252 (92%)	19 (7%)	2 (1%)	18	49
1	C	273/303 (90%)	251 (92%)	20 (7%)	2 (1%)	18	49
1	D	273/303 (90%)	252 (92%)	19 (7%)	2 (1%)	18	49
1	E	273/303 (90%)	251 (92%)	20 (7%)	2 (1%)	18	49
1	F	273/303 (90%)	252 (92%)	19 (7%)	2 (1%)	18	49
All	All	1638/1818 (90%)	1510 (92%)	116 (7%)	12 (1%)	18	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	69	LEU
1	A	69	LEU
1	B	69	LEU
1	C	69	LEU
1	D	69	LEU
1	E	69	LEU
1	B	200	PRO
1	C	200	PRO
1	E	200	PRO
1	A	200	PRO
1	D	200	PRO
1	F	200	PRO

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	199/227 (88%)	195 (98%)	4 (2%)	48	68
1	B	199/227 (88%)	195 (98%)	4 (2%)	48	68
1	C	199/227 (88%)	195 (98%)	4 (2%)	48	68
1	D	199/227 (88%)	194 (98%)	5 (2%)	42	64
1	E	199/227 (88%)	194 (98%)	5 (2%)	42	64
1	F	199/227 (88%)	194 (98%)	5 (2%)	42	64
All	All	1194/1362 (88%)	1167 (98%)	27 (2%)	44	66

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	124	LEU
1	A	145	SER
1	A	223	GLU
1	B	3	LEU
1	B	124	LEU
1	B	145	SER

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Mol	Chain	Res	Type
1	B	223	GLU
1	C	3	LEU
1	C	124	LEU
1	C	145	SER
1	C	223	GLU
1	D	3	LEU
1	D	50	ASN
1	D	124	LEU
1	D	145	SER
1	D	223	GLU
1	E	3	LEU
1	E	60	LEU
1	E	124	LEU
1	E	145	SER
1	E	223	GLU
1	F	3	LEU
1	F	50	ASN
1	F	124	LEU
1	F	145	SER
1	F	223	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	246	GLN
1	B	51	ASN
1	B	246	GLN
1	C	51	ASN
1	C	246	GLN
1	D	51	ASN
1	D	246	GLN
1	E	51	ASN
1	E	246	GLN
1	F	51	ASN
1	F	246	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](#)

There are no ligands in this entry.

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	275/303 (90%)	0.63	38 (13%) 6 5	33, 67, 112, 135	0
1	B	275/303 (90%)	1.04	54 (19%) 3 3	26, 61, 111, 140	0
1	C	275/303 (90%)	0.65	39 (14%) 6 5	37, 69, 128, 161	0
1	D	275/303 (90%)	0.77	37 (13%) 7 6	38, 70, 110, 145	0
1	E	275/303 (90%)	1.34	72 (26%) 1 1	44, 83, 139, 191	0
1	F	275/303 (90%)	1.11	59 (21%) 2 2	41, 72, 127, 169	0
All	All	1650/1818 (90%)	0.92	299 (18%) 3 3	26, 70, 122, 191	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	ILE	11.1
1	C	72	GLY	10.5
1	B	229	ALA	10.4
1	F	71	VAL	9.1
1	F	66	LYS	8.4
1	B	274	VAL	8.2
1	B	275	ASP	8.2
1	F	73	ALA	8.1
1	B	231	ALA	7.9
1	E	63	ARG	7.7
1	D	223	GLU	7.3
1	E	121	LEU	7.3
1	A	107	LEU	7.1
1	F	223	GLU	7.0
1	B	121	LEU	7.0
1	E	72	GLY	6.2
1	E	122	HIS	6.1
1	B	117	HIS	5.9
1	E	43	ARG	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	71	VAL	5.7
1	F	74	VAL	5.7
1	B	233	VAL	5.6
1	A	229	ALA	5.6
1	A	66	LYS	5.5
1	E	3	LEU	5.5
1	C	223	GLU	5.4
1	E	71	VAL	5.4
1	C	259	ASN	5.4
1	F	67	ARG	5.3
1	B	276	MET	5.3
1	E	128	HIS	5.3
1	C	73	ALA	5.1
1	A	122	HIS	5.0
1	F	72	GLY	5.0
1	F	162	LEU	5.0
1	D	66	LYS	4.9
1	D	106	PRO	4.9
1	E	8	HIS	4.9
1	F	163	TYR	4.9
1	E	213	ALA	4.9
1	B	84	ALA	4.8
1	B	80	TRP	4.8
1	B	10	ILE	4.7
1	A	274	VAL	4.7
1	B	272	ILE	4.7
1	B	29	LEU	4.7
1	D	258	PHE	4.6
1	B	27	PHE	4.6
1	D	72	GLY	4.5
1	F	70	VAL	4.5
1	D	197	LEU	4.5
1	F	194	ILE	4.5
1	A	121	LEU	4.4
1	D	107	LEU	4.4
1	F	277	LEU	4.4
1	D	148	GLU	4.4
1	B	3	LEU	4.4
1	E	198	LEU	4.4
1	D	73	ALA	4.3
1	C	256	GLU	4.3
1	F	120	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	69	LEU	4.3
1	B	223	GLU	4.3
1	E	239	ALA	4.3
1	B	269	GLY	4.3
1	E	69	LEU	4.3
1	F	148	GLU	4.3
1	A	124	LEU	4.2
1	C	253	ARG	4.2
1	D	225	TYR	4.2
1	B	49	TYR	4.1
1	E	64	THR	4.1
1	E	127	LEU	4.1
1	E	107	LEU	4.1
1	A	255	LYS	4.1
1	B	270	ALA	4.1
1	D	255	LYS	4.1
1	D	71	VAL	4.0
1	E	98	ASN	4.0
1	E	4	VAL	4.0
1	E	62	PRO	4.0
1	A	104	LEU	4.0
1	A	259	ASN	3.9
1	E	70	VAL	3.9
1	E	269	GLY	3.9
1	C	8	HIS	3.9
1	B	43	ARG	3.9
1	E	148	GLU	3.8
1	F	225	TYR	3.8
1	A	3	LEU	3.8
1	F	59	ARG	3.7
1	F	217	LEU	3.7
1	A	148	GLU	3.7
1	D	124	LEU	3.7
1	C	3	LEU	3.7
1	F	191	LEU	3.7
1	A	106	PRO	3.6
1	E	143	ALA	3.6
1	C	74	VAL	3.6
1	C	47	MET	3.6
1	D	162	LEU	3.6
1	C	68	PRO	3.6
1	C	257	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	194	ILE	3.5
1	D	26	PRO	3.5
1	C	128	HIS	3.5
1	F	8	HIS	3.5
1	F	193	SER	3.5
1	E	73	ALA	3.5
1	D	265	PRO	3.5
1	E	262	LEU	3.5
1	E	56	ASP	3.4
1	E	124	LEU	3.4
1	C	151	SER	3.4
1	D	227	LEU	3.4
1	D	105	SER	3.3
1	C	77	ARG	3.3
1	E	50	ASN	3.3
1	C	251	LEU	3.3
1	F	64	THR	3.3
1	A	223	GLU	3.2
1	A	193	SER	3.2
1	E	182	ASP	3.2
1	F	168	SER	3.2
1	A	219	ILE	3.2
1	B	83	VAL	3.2
1	B	273	ILE	3.2
1	C	24	ARG	3.2
1	E	169	LEU	3.1
1	E	238	THR	3.1
1	F	127	LEU	3.1
1	F	258	PHE	3.1
1	A	111	ILE	3.1
1	F	220	ALA	3.1
1	F	221	GLY	3.1
1	F	210	MET	3.1
1	D	139	GLY	3.1
1	A	91	PHE	3.1
1	A	105	SER	3.0
1	B	135	SER	3.0
1	D	75	SER	3.0
1	A	131	ILE	3.0
1	A	163	TYR	3.0
1	A	162	LEU	3.0
1	B	5	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	3.0
1	F	9	THR	3.0
1	D	226	GLY	3.0
1	E	273	ILE	3.0
1	D	243	ILE	3.0
1	B	227	LEU	3.0
1	F	255	LYS	3.0
1	E	74	VAL	3.0
1	C	260	LEU	2.9
1	E	223	GLU	2.9
1	B	184	ASP	2.9
1	B	271	GLY	2.9
1	C	255	LYS	2.9
1	F	25	TYR	2.9
1	C	224	ALA	2.9
1	F	145	SER	2.9
1	F	150	SER	2.9
1	A	198	LEU	2.9
1	C	5	ARG	2.9
1	C	43	ARG	2.9
1	B	98	ASN	2.9
1	F	51	ASN	2.9
1	B	234	SER	2.9
1	E	117	HIS	2.9
1	E	131	ILE	2.9
1	B	148	GLU	2.9
1	F	63	ARG	2.9
1	B	193	SER	2.8
1	B	11	PHE	2.8
1	E	147	ASP	2.8
1	E	29	LEU	2.8
1	D	178	TYR	2.8
1	E	260	LEU	2.8
1	F	169	LEU	2.8
1	A	110	ALA	2.8
1	E	125	PRO	2.8
1	F	147	ASP	2.7
1	B	8	HIS	2.7
1	B	32	ALA	2.7
1	D	8	HIS	2.7
1	E	144	ALA	2.7
1	E	197	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	75	SER	2.7
1	D	122	HIS	2.7
1	E	92	ALA	2.7
1	A	103	LEU	2.7
1	F	160	PRO	2.7
1	A	102	LEU	2.7
1	E	274	VAL	2.7
1	F	161	TRP	2.7
1	F	149	ALA	2.7
1	E	77	ARG	2.6
1	C	60	LEU	2.6
1	D	219	ILE	2.6
1	B	232	THR	2.6
1	C	211	HIS	2.6
1	B	228	GLY	2.6
1	B	13	LEU	2.6
1	E	9	THR	2.6
1	E	152	LEU	2.6
1	C	245	VAL	2.6
1	F	213	ALA	2.6
1	E	123	PRO	2.6
1	E	114	THR	2.6
1	E	111	ILE	2.6
1	F	29	LEU	2.6
1	D	238	THR	2.6
1	F	22	LEU	2.5
1	F	124	LEU	2.5
1	B	132	VAL	2.5
1	C	148	GLU	2.5
1	D	220	ALA	2.5
1	F	229	ALA	2.5
1	E	47	MET	2.5
1	D	247	ALA	2.5
1	B	120	ARG	2.5
1	B	147	ASP	2.5
1	E	57	ILE	2.5
1	C	55	LEU	2.5
1	E	272	ILE	2.5
1	B	133	LEU	2.5
1	B	6	ILE	2.4
1	D	131	ILE	2.4
1	D	267	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	255	LYS	2.4
1	B	194	ILE	2.4
1	E	151	SER	2.4
1	E	60	LEU	2.4
1	B	122	HIS	2.4
1	C	247	ALA	2.4
1	E	94	ALA	2.4
1	A	127	LEU	2.4
1	B	21	LEU	2.4
1	D	145	SER	2.4
1	D	194	ILE	2.4
1	B	235	THR	2.3
1	C	9	THR	2.3
1	A	147	ASP	2.3
1	B	171	VAL	2.3
1	A	64	THR	2.3
1	C	237	LEU	2.3
1	F	76	LEU	2.3
1	A	75	SER	2.3
1	F	75	SER	2.3
1	E	244	LEU	2.3
1	B	33	ILE	2.3
1	E	189	HIS	2.3
1	E	168	SER	2.3
1	B	17	TYR	2.3
1	C	202	GLY	2.2
1	F	65	ALA	2.2
1	B	42	LEU	2.2
1	C	201	LYS	2.2
1	F	12	SER	2.2
1	F	100	TYR	2.2
1	B	108	VAL	2.2
1	C	67	ARG	2.2
1	E	90	TYR	2.2
1	D	119	LYS	2.2
1	E	120	ARG	2.2
1	E	243	ILE	2.2
1	C	65	ALA	2.2
1	E	181	MET	2.2
1	A	197	LEU	2.2
1	C	121	LEU	2.2
1	F	58	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	68	PRO	2.1
1	F	26	PRO	2.1
1	F	130	GLY	2.1
1	E	66	LYS	2.1
1	A	77	ARG	2.1
1	D	253	ARG	2.1
1	F	53	ALA	2.1
1	F	224	ALA	2.1
1	D	135	SER	2.1
1	D	51	ASN	2.1
1	F	240	LEU	2.1
1	C	59	ARG	2.1
1	E	199	GLY	2.1
1	A	201	LYS	2.1
1	E	119	LYS	2.1
1	E	201	LYS	2.1
1	F	117	HIS	2.1
1	F	17	TYR	2.1
1	E	129	LEU	2.1
1	A	275	ASP	2.1
1	B	9	THR	2.0
1	E	146	GLY	2.0
1	B	179	SER	2.0
1	C	6	ILE	2.0
1	E	193	SER	2.0
1	F	276	MET	2.0
1	E	165	ALA	2.0
1	A	186	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.