



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 08:21 AM EDT

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:

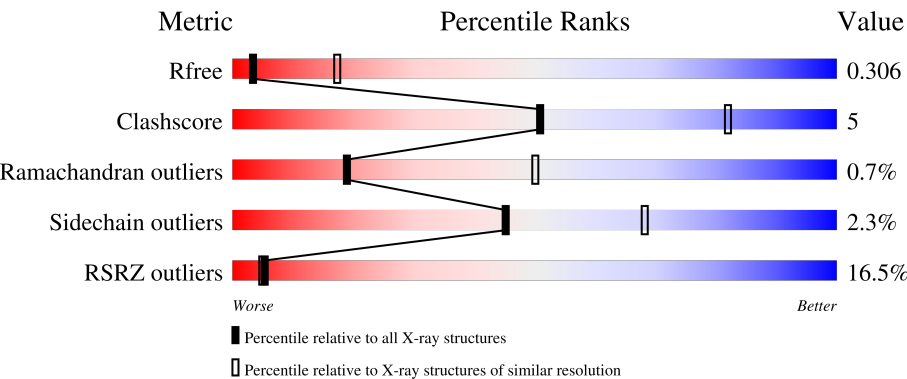
MolProbity : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

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 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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (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	<div><div>11%</div><div><div></div><div>80%</div><div>11%</div><div>•</div><div>9%</div></div></div>
1	B	303	<div><div>17%</div><div><div></div><div>80%</div><div>10%</div><div>•</div><div>9%</div></div></div>
1	C	303	<div><div>12%</div><div><div></div><div>80%</div><div>10%</div><div>•</div><div>9%</div></div></div>
1	D	303	<div><div>12%</div><div><div></div><div>81%</div><div>10%</div><div>•</div><div>9%</div></div></div>
1	E	303	<div><div>21%</div><div><div></div><div>80%</div><div>10%</div><div>•</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	303	<div><div></div><div>17%</div><div>79%</div><div>11%</div><div>•</div><div>9%</div></div>

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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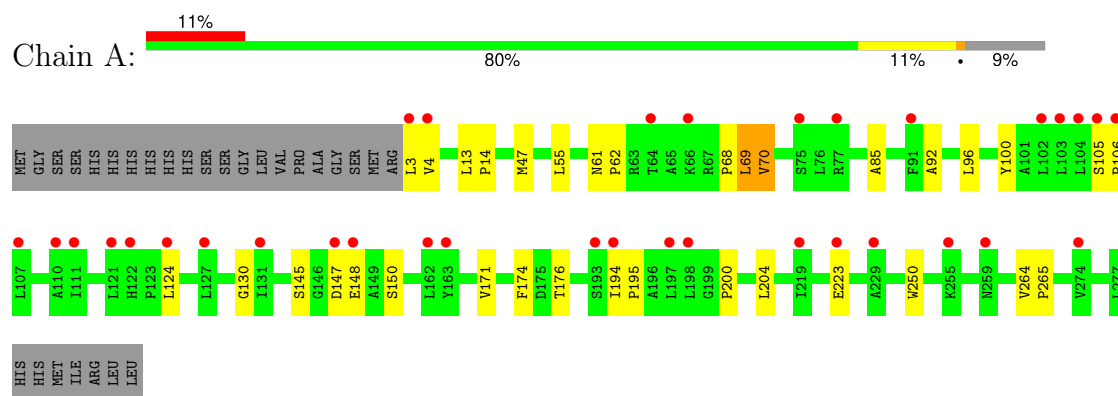
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	HIS	-	expression tag	UNP Q9YBM8
F	-11	HIS	-	expression tag	UNP Q9YBM8
F	-10	HIS	-	expression tag	UNP Q9YBM8
F	-9	HIS	-	expression tag	UNP Q9YBM8
F	-8	SER	-	expression tag	UNP Q9YBM8
F	-7	SER	-	expression 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

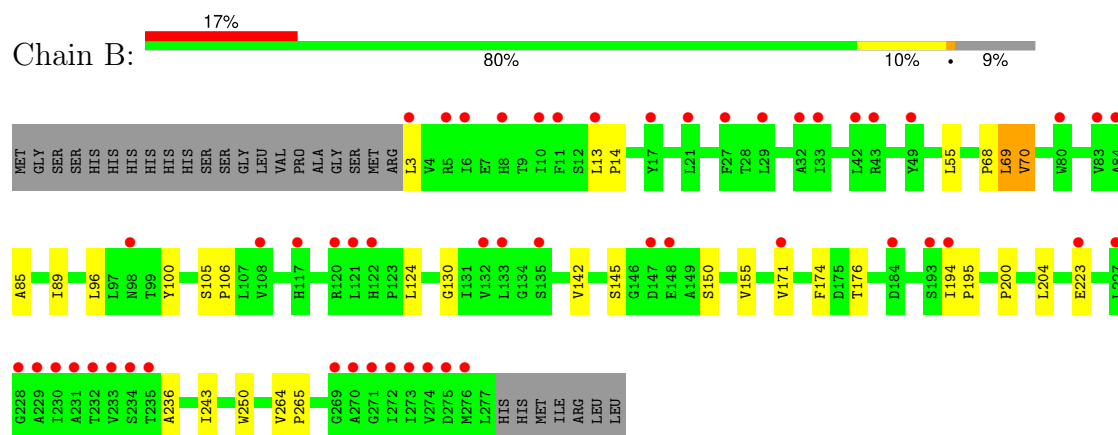
3 Residue-property plots

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.

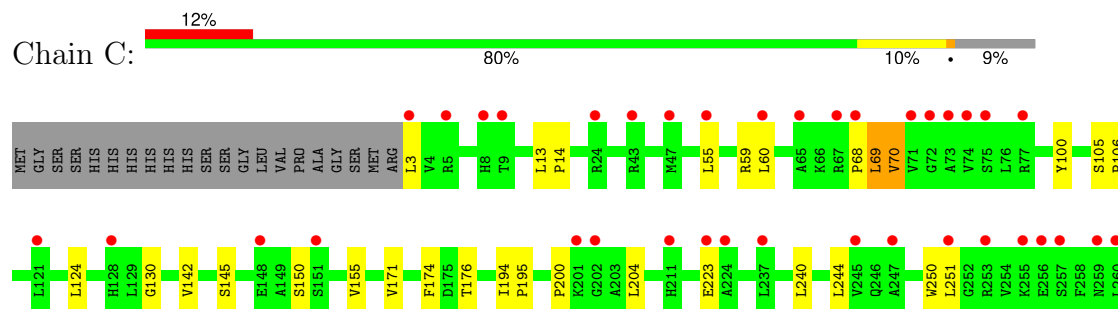
- Molecule 1: 4-hydroxybenzoate octaprenyltransferase

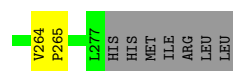


- Molecule 1: 4-hydroxybenzoate octaprenyltransferase

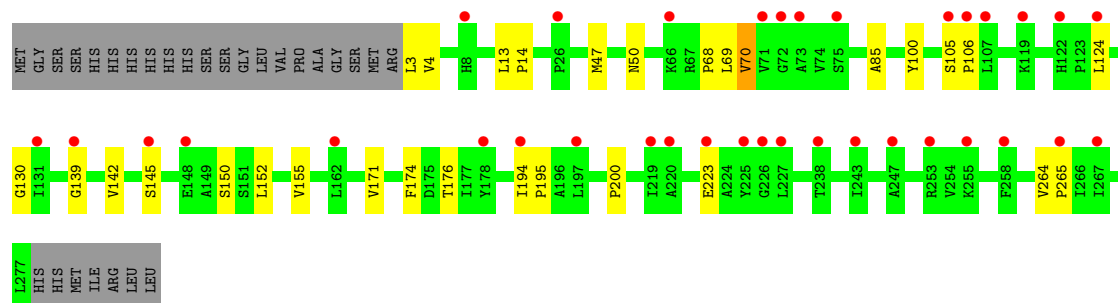
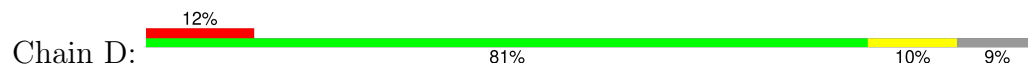


- Molecule 1: 4-hydroxybenzoate octaprenyltransferase

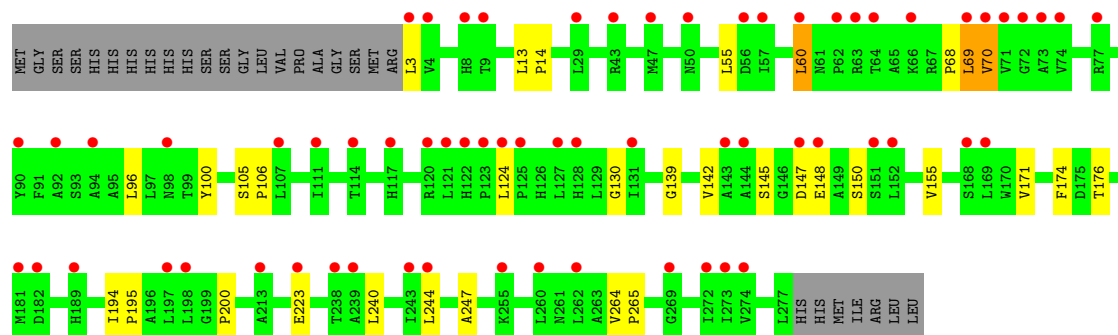




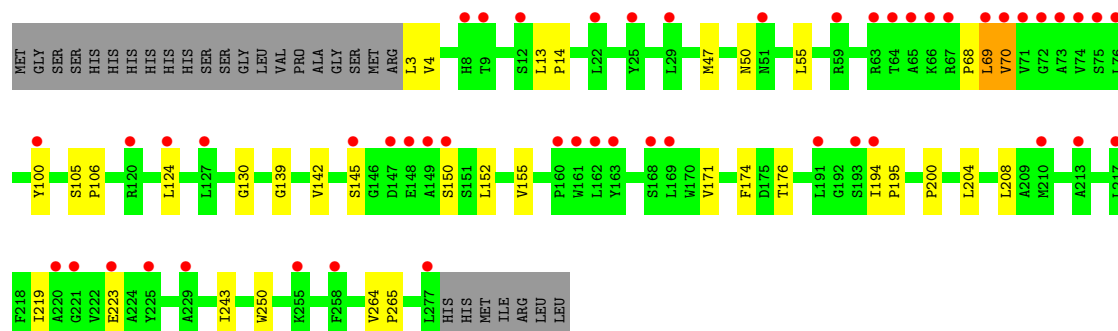
• Molecule 1: 4-hydroxybenzoate octaprenyltransferase



• 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 (5.05%)	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%)	19	50
1	B	273/303 (90%)	252 (92%)	19 (7%)	2 (1%)	19	50
1	C	273/303 (90%)	251 (92%)	20 (7%)	2 (1%)	19	50
1	D	273/303 (90%)	252 (92%)	19 (7%)	2 (1%)	19	50
1	E	273/303 (90%)	251 (92%)	20 (7%)	2 (1%)	19	50
1	F	273/303 (90%)	252 (92%)	19 (7%)	2 (1%)	19	50
All	All	1638/1818 (90%)	1510 (92%)	116 (7%)	12 (1%)	19	50

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%)	50	71
1	B	199/227 (88%)	195 (98%)	4 (2%)	50	71
1	C	199/227 (88%)	195 (98%)	4 (2%)	50	71
1	D	199/227 (88%)	194 (98%)	5 (2%)	42	67
1	E	199/227 (88%)	194 (98%)	5 (2%)	42	67
1	F	199/227 (88%)	194 (98%)	5 (2%)	42	67
All	All	1194/1362 (88%)	1167 (98%)	27 (2%)	45	68

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%)	0.48	34 (12%)	9 9	33, 67, 112, 135	0
1	B	275/303 (90%)	0.90	52 (18%)	4 3	26, 61, 111, 140	0
1	C	275/303 (90%)	0.51	37 (13%)	8 8	37, 69, 128, 161	0
1	D	275/303 (90%)	0.63	35 (12%)	9 9	38, 70, 110, 145	0
1	E	275/303 (90%)	1.20	65 (23%)	2 2	44, 83, 139, 191	0
1	F	275/303 (90%)	0.96	50 (18%)	4 4	41, 72, 127, 169	0
All	All	1650/1818 (90%)	0.78	273 (16%)	5 5	26, 70, 122, 191	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	ILE	10.9
1	B	229	ALA	10.3
1	C	72	GLY	10.2
1	F	71	VAL	8.9
1	F	66	LYS	8.3
1	B	274	VAL	8.0
1	B	275	ASP	8.0
1	F	73	ALA	7.9
1	B	231	ALA	7.7
1	E	63	ARG	7.6
1	D	223	GLU	7.3
1	E	121	LEU	7.2
1	A	107	LEU	6.9
1	F	223	GLU	6.9
1	B	121	LEU	6.8
1	E	72	GLY	6.0
1	E	122	HIS	5.9
1	B	117	HIS	5.8
1	E	43	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	71	VAL	5.6
1	F	74	VAL	5.5
1	B	233	VAL	5.5
1	A	229	ALA	5.4
1	A	66	LYS	5.4
1	C	223	GLU	5.4
1	E	3	LEU	5.3
1	E	71	VAL	5.3
1	F	67	ARG	5.3
1	C	259	ASN	5.2
1	E	128	HIS	5.1
1	B	276	MET	5.1
1	C	73	ALA	4.9
1	D	66	LYS	4.8
1	F	162	LEU	4.8
1	A	122	HIS	4.8
1	F	72	GLY	4.8
1	E	8	HIS	4.8
1	D	106	PRO	4.7
1	E	213	ALA	4.7
1	F	163	TYR	4.7
1	B	84	ALA	4.7
1	B	10	ILE	4.6
1	A	274	VAL	4.6
1	B	272	ILE	4.6
1	B	29	LEU	4.5
1	B	80	TRP	4.5
1	D	258	PHE	4.4
1	B	27	PHE	4.4
1	F	70	VAL	4.4
1	D	197	LEU	4.4
1	F	194	ILE	4.4
1	D	72	GLY	4.4
1	D	148	GLU	4.3
1	A	121	LEU	4.3
1	D	107	LEU	4.3
1	F	277	LEU	4.3
1	B	3	LEU	4.3
1	F	120	ARG	4.2
1	C	256	GLU	4.2
1	E	198	LEU	4.2
1	B	223	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	73	ALA	4.2
1	F	69	LEU	4.2
1	E	239	ALA	4.2
1	F	148	GLU	4.2
1	B	269	GLY	4.1
1	E	69	LEU	4.1
1	C	253	ARG	4.1
1	A	124	LEU	4.1
1	D	225	TYR	4.0
1	A	255	LYS	4.0
1	D	255	LYS	4.0
1	E	127	LEU	4.0
1	E	64	THR	4.0
1	B	49	TYR	3.9
1	B	270	ALA	3.9
1	E	107	LEU	3.9
1	E	98	ASN	3.9
1	D	71	VAL	3.9
1	E	4	VAL	3.8
1	A	104	LEU	3.8
1	E	62	PRO	3.8
1	B	43	ARG	3.8
1	A	259	ASN	3.8
1	E	70	VAL	3.8
1	E	148	GLU	3.7
1	E	269	GLY	3.7
1	C	8	HIS	3.7
1	F	59	ARG	3.6
1	A	148	GLU	3.6
1	F	225	TYR	3.6
1	A	3	LEU	3.6
1	F	217	LEU	3.6
1	D	124	LEU	3.5
1	C	3	LEU	3.5
1	E	143	ALA	3.5
1	F	191	LEU	3.5
1	A	106	PRO	3.5
1	C	74	VAL	3.5
1	D	162	LEU	3.4
1	C	47	MET	3.4
1	C	68	PRO	3.4
1	A	194	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	257	SER	3.4
1	E	73	ALA	3.3
1	D	26	PRO	3.3
1	E	262	LEU	3.3
1	C	128	HIS	3.3
1	F	8	HIS	3.3
1	F	193	SER	3.3
1	D	265	PRO	3.3
1	E	124	LEU	3.2
1	E	56	ASP	3.2
1	D	227	LEU	3.2
1	C	77	ARG	3.2
1	C	151	SER	3.2
1	D	105	SER	3.2
1	E	50	ASN	3.2
1	C	251	LEU	3.1
1	F	64	THR	3.1
1	A	223	GLU	3.1
1	C	24	ARG	3.1
1	A	219	ILE	3.0
1	E	182	ASP	3.0
1	A	193	SER	3.0
1	B	83	VAL	3.0
1	B	273	ILE	3.0
1	F	168	SER	3.0
1	E	169	LEU	3.0
1	E	238	THR	3.0
1	F	127	LEU	3.0
1	A	111	ILE	3.0
1	F	220	ALA	3.0
1	F	221	GLY	2.9
1	F	258	PHE	2.9
1	B	5	ARG	2.9
1	D	139	GLY	2.9
1	F	210	MET	2.9
1	A	91	PHE	2.9
1	A	131	ILE	2.9
1	A	162	LEU	2.9
1	A	4	VAL	2.9
1	F	9	THR	2.9
1	A	105	SER	2.9
1	B	135	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	75	SER	2.9
1	F	255	LYS	2.9
1	A	163	TYR	2.9
1	E	273	ILE	2.9
1	D	226	GLY	2.8
1	D	243	ILE	2.8
1	E	223	GLU	2.8
1	B	227	LEU	2.8
1	C	255	LYS	2.8
1	E	74	VAL	2.8
1	C	260	LEU	2.8
1	C	5	ARG	2.8
1	C	43	ARG	2.8
1	B	271	GLY	2.8
1	B	184	ASP	2.8
1	C	224	ALA	2.8
1	F	63	ARG	2.7
1	F	25	TYR	2.7
1	A	198	LEU	2.7
1	B	98	ASN	2.7
1	F	51	ASN	2.7
1	B	148	GLU	2.7
1	E	131	ILE	2.7
1	F	145	SER	2.7
1	F	150	SER	2.7
1	E	117	HIS	2.7
1	B	234	SER	2.7
1	B	193	SER	2.7
1	E	29	LEU	2.6
1	B	11	PHE	2.6
1	E	147	ASP	2.6
1	E	260	LEU	2.6
1	F	169	LEU	2.6
1	A	110	ALA	2.6
1	D	178	TYR	2.6
1	B	32	ALA	2.6
1	E	125	PRO	2.6
1	E	144	ALA	2.6
1	F	147	ASP	2.6
1	B	8	HIS	2.6
1	E	197	LEU	2.6
1	E	92	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	8	HIS	2.6
1	A	103	LEU	2.5
1	E	77	ARG	2.5
1	E	274	VAL	2.5
1	C	75	SER	2.5
1	D	122	HIS	2.5
1	A	102	LEU	2.5
1	F	149	ALA	2.5
1	F	160	PRO	2.5
1	D	219	ILE	2.5
1	C	60	LEU	2.5
1	B	232	THR	2.5
1	F	213	ALA	2.5
1	C	245	VAL	2.5
1	B	13	LEU	2.4
1	E	152	LEU	2.4
1	C	211	HIS	2.4
1	E	9	THR	2.4
1	B	228	GLY	2.4
1	F	161	TRP	2.4
1	E	111	ILE	2.4
1	E	114	THR	2.4
1	E	123	PRO	2.4
1	F	29	LEU	2.4
1	C	148	GLU	2.4
1	D	238	THR	2.4
1	D	220	ALA	2.4
1	F	229	ALA	2.4
1	B	132	VAL	2.4
1	B	120	ARG	2.4
1	F	22	LEU	2.4
1	F	124	LEU	2.4
1	D	247	ALA	2.4
1	E	47	MET	2.4
1	E	57	ILE	2.3
1	C	55	LEU	2.3
1	E	255	LYS	2.3
1	E	272	ILE	2.3
1	B	147	ASP	2.3
1	B	133	LEU	2.3
1	B	6	ILE	2.3
1	D	131	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	267	ILE	2.3
1	B	194	ILE	2.3
1	C	247	ALA	2.3
1	E	60	LEU	2.3
1	E	94	ALA	2.3
1	E	151	SER	2.3
1	B	122	HIS	2.2
1	A	127	LEU	2.2
1	B	21	LEU	2.2
1	D	194	ILE	2.2
1	D	145	SER	2.2
1	B	235	THR	2.2
1	C	9	THR	2.2
1	B	171	VAL	2.2
1	A	147	ASP	2.2
1	A	64	THR	2.2
1	C	237	LEU	2.2
1	F	76	LEU	2.2
1	E	244	LEU	2.2
1	A	75	SER	2.1
1	F	75	SER	2.1
1	B	33	ILE	2.1
1	C	201	LYS	2.1
1	F	65	ALA	2.1
1	C	67	ARG	2.1
1	E	189	HIS	2.1
1	B	42	LEU	2.1
1	B	108	VAL	2.1
1	E	168	SER	2.1
1	B	17	TYR	2.1
1	C	202	GLY	2.1
1	D	119	LYS	2.1
1	E	120	ARG	2.1
1	F	12	SER	2.1
1	F	100	TYR	2.1
1	C	65	ALA	2.0
1	E	243	ILE	2.0
1	E	90	TYR	2.0
1	A	197	LEU	2.0
1	C	121	LEU	2.0
1	E	181	MET	2.0
1	A	77	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	253	ARG	2.0
1	E	66	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.