



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID : 2QQ2 / pdb_00002qq2
Title : Crystal structure of C-terminal domain of Human acyl-CoA thioesterase 7
Authors : Busam, R.; Lehtio, L.; Arrowsmith, C.H.; Berglund, H.; Collins, R.; Dahlgren, L.G.; Herman, M.D.; Edwards, A.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmberg-Schiavone, L.; Johansson, I.; Kallas, A.; Karlberg, T.; Kotenyova, T.; Moche, M.; Nordlund, P.; Nyman, T.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Thorsell, A.G.; Tresaugues, L.; van den Berg, S.; Weigelt, J.; Welin, M.; Persson, C.; Structural Genomics Consortium (SGC)
Deposited on : 2007-07-26
Resolution : 2.80 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)

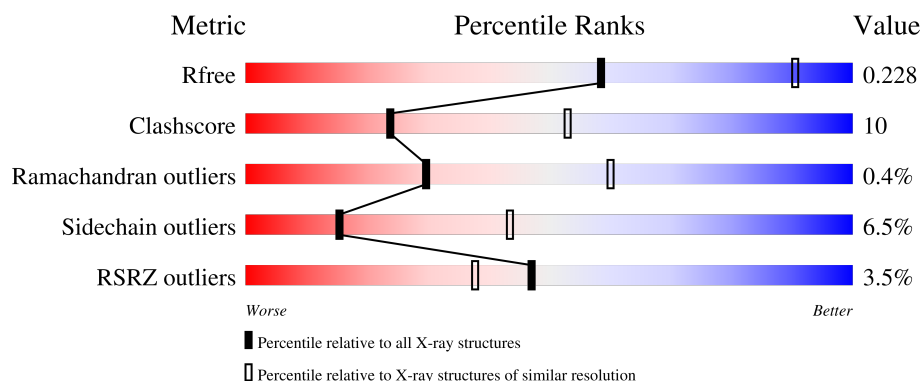
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	193	
1	B	193	
1	C	193	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	193	 % 60% 18% • 21%
1	E	193	 % 61% 14% • 22%
1	F	193	 3% 61% 13% •• 23%
1	G	193	 8% 61% 13% • 23%
1	H	193	 3% 62% 15% • 21%
1	I	193	 4% 64% 14% • 20%
1	J	193	 11% 61% 12% • 26%
1	K	193	 % 61% 18% • 19%
1	L	193	 % 62% 16% •• 20%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14037 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 Cytosolic acyl coenzyme A thioester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1188	745	210	225	8			
1	B	156	Total	C	N	O	S	0	0	0
			1199	749	212	230	8			
1	C	157	Total	C	N	O	S	0	0	0
			1199	751	214	226	8			
1	D	153	Total	C	N	O	S	0	0	0
			1169	733	203	225	8			
1	E	150	Total	C	N	O	S	0	0	0
			1147	718	202	219	8			
1	F	149	Total	C	N	O	S	0	0	0
			1143	717	201	217	8			
1	G	148	Total	C	N	O	S	0	0	0
			1128	709	196	215	8			
1	H	153	Total	C	N	O	S	0	0	0
			1175	736	208	223	8			
1	I	154	Total	C	N	O	S	0	0	0
			1187	743	208	228	8			
1	J	143	Total	C	N	O	S	0	0	0
			1102	692	193	209	8			
1	K	156	Total	C	N	O	S	0	0	0
			1207	754	214	231	8			
1	L	154	Total	C	N	O	S	0	0	0
			1193	745	214	226	8			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MET	-	expression tag	UNP O00154
A	177	HIS	-	expression tag	UNP O00154
A	178	HIS	-	expression tag	UNP O00154
A	179	HIS	-	expression tag	UNP O00154
A	180	HIS	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
A	181	HIS	-	expression tag	UNP O00154
A	182	HIS	-	expression tag	UNP O00154
A	183	SER	-	expression tag	UNP O00154
A	184	SER	-	expression tag	UNP O00154
A	185	GLY	-	expression tag	UNP O00154
A	186	VAL	-	expression tag	UNP O00154
A	187	ASP	-	expression tag	UNP O00154
A	188	LEU	-	expression tag	UNP O00154
A	189	GLY	-	expression tag	UNP O00154
A	190	THR	-	expression tag	UNP O00154
A	191	GLU	-	expression tag	UNP O00154
A	192	ASN	-	expression tag	UNP O00154
A	193	LEU	-	expression tag	UNP O00154
A	194	TYR	-	expression tag	UNP O00154
A	195	PHE	-	expression tag	UNP O00154
A	196	GLN	-	expression tag	UNP O00154
A	197	SER	-	expression tag	UNP O00154
A	198	MET	-	expression tag	UNP O00154
B	176	MET	-	expression tag	UNP O00154
B	177	HIS	-	expression tag	UNP O00154
B	178	HIS	-	expression tag	UNP O00154
B	179	HIS	-	expression tag	UNP O00154
B	180	HIS	-	expression tag	UNP O00154
B	181	HIS	-	expression tag	UNP O00154
B	182	HIS	-	expression tag	UNP O00154
B	183	SER	-	expression tag	UNP O00154
B	184	SER	-	expression tag	UNP O00154
B	185	GLY	-	expression tag	UNP O00154
B	186	VAL	-	expression tag	UNP O00154
B	187	ASP	-	expression tag	UNP O00154
B	188	LEU	-	expression tag	UNP O00154
B	189	GLY	-	expression tag	UNP O00154
B	190	THR	-	expression tag	UNP O00154
B	191	GLU	-	expression tag	UNP O00154
B	192	ASN	-	expression tag	UNP O00154
B	193	LEU	-	expression tag	UNP O00154
B	194	TYR	-	expression tag	UNP O00154
B	195	PHE	-	expression tag	UNP O00154
B	196	GLN	-	expression tag	UNP O00154
B	197	SER	-	expression tag	UNP O00154
B	198	MET	-	expression tag	UNP O00154
C	176	MET	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	HIS	-	expression tag	UNP O00154
C	178	HIS	-	expression tag	UNP O00154
C	179	HIS	-	expression tag	UNP O00154
C	180	HIS	-	expression tag	UNP O00154
C	181	HIS	-	expression tag	UNP O00154
C	182	HIS	-	expression tag	UNP O00154
C	183	SER	-	expression tag	UNP O00154
C	184	SER	-	expression tag	UNP O00154
C	185	GLY	-	expression tag	UNP O00154
C	186	VAL	-	expression tag	UNP O00154
C	187	ASP	-	expression tag	UNP O00154
C	188	LEU	-	expression tag	UNP O00154
C	189	GLY	-	expression tag	UNP O00154
C	190	THR	-	expression tag	UNP O00154
C	191	GLU	-	expression tag	UNP O00154
C	192	ASN	-	expression tag	UNP O00154
C	193	LEU	-	expression tag	UNP O00154
C	194	TYR	-	expression tag	UNP O00154
C	195	PHE	-	expression tag	UNP O00154
C	196	GLN	-	expression tag	UNP O00154
C	197	SER	-	expression tag	UNP O00154
C	198	MET	-	expression tag	UNP O00154
D	176	MET	-	expression tag	UNP O00154
D	177	HIS	-	expression tag	UNP O00154
D	178	HIS	-	expression tag	UNP O00154
D	179	HIS	-	expression tag	UNP O00154
D	180	HIS	-	expression tag	UNP O00154
D	181	HIS	-	expression tag	UNP O00154
D	182	HIS	-	expression tag	UNP O00154
D	183	SER	-	expression tag	UNP O00154
D	184	SER	-	expression tag	UNP O00154
D	185	GLY	-	expression tag	UNP O00154
D	186	VAL	-	expression tag	UNP O00154
D	187	ASP	-	expression tag	UNP O00154
D	188	LEU	-	expression tag	UNP O00154
D	189	GLY	-	expression tag	UNP O00154
D	190	THR	-	expression tag	UNP O00154
D	191	GLU	-	expression tag	UNP O00154
D	192	ASN	-	expression tag	UNP O00154
D	193	LEU	-	expression tag	UNP O00154
D	194	TYR	-	expression tag	UNP O00154
D	195	PHE	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
D	196	GLN	-	expression tag	UNP O00154
D	197	SER	-	expression tag	UNP O00154
D	198	MET	-	expression tag	UNP O00154
E	176	MET	-	expression tag	UNP O00154
E	177	HIS	-	expression tag	UNP O00154
E	178	HIS	-	expression tag	UNP O00154
E	179	HIS	-	expression tag	UNP O00154
E	180	HIS	-	expression tag	UNP O00154
E	181	HIS	-	expression tag	UNP O00154
E	182	HIS	-	expression tag	UNP O00154
E	183	SER	-	expression tag	UNP O00154
E	184	SER	-	expression tag	UNP O00154
E	185	GLY	-	expression tag	UNP O00154
E	186	VAL	-	expression tag	UNP O00154
E	187	ASP	-	expression tag	UNP O00154
E	188	LEU	-	expression tag	UNP O00154
E	189	GLY	-	expression tag	UNP O00154
E	190	THR	-	expression tag	UNP O00154
E	191	GLU	-	expression tag	UNP O00154
E	192	ASN	-	expression tag	UNP O00154
E	193	LEU	-	expression tag	UNP O00154
E	194	TYR	-	expression tag	UNP O00154
E	195	PHE	-	expression tag	UNP O00154
E	196	GLN	-	expression tag	UNP O00154
E	197	SER	-	expression tag	UNP O00154
E	198	MET	-	expression tag	UNP O00154
F	176	MET	-	expression tag	UNP O00154
F	177	HIS	-	expression tag	UNP O00154
F	178	HIS	-	expression tag	UNP O00154
F	179	HIS	-	expression tag	UNP O00154
F	180	HIS	-	expression tag	UNP O00154
F	181	HIS	-	expression tag	UNP O00154
F	182	HIS	-	expression tag	UNP O00154
F	183	SER	-	expression tag	UNP O00154
F	184	SER	-	expression tag	UNP O00154
F	185	GLY	-	expression tag	UNP O00154
F	186	VAL	-	expression tag	UNP O00154
F	187	ASP	-	expression tag	UNP O00154
F	188	LEU	-	expression tag	UNP O00154
F	189	GLY	-	expression tag	UNP O00154
F	190	THR	-	expression tag	UNP O00154
F	191	GLU	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
F	192	ASN	-	expression tag	UNP O00154
F	193	LEU	-	expression tag	UNP O00154
F	194	TYR	-	expression tag	UNP O00154
F	195	PHE	-	expression tag	UNP O00154
F	196	GLN	-	expression tag	UNP O00154
F	197	SER	-	expression tag	UNP O00154
F	198	MET	-	expression tag	UNP O00154
G	176	MET	-	expression tag	UNP O00154
G	177	HIS	-	expression tag	UNP O00154
G	178	HIS	-	expression tag	UNP O00154
G	179	HIS	-	expression tag	UNP O00154
G	180	HIS	-	expression tag	UNP O00154
G	181	HIS	-	expression tag	UNP O00154
G	182	HIS	-	expression tag	UNP O00154
G	183	SER	-	expression tag	UNP O00154
G	184	SER	-	expression tag	UNP O00154
G	185	GLY	-	expression tag	UNP O00154
G	186	VAL	-	expression tag	UNP O00154
G	187	ASP	-	expression tag	UNP O00154
G	188	LEU	-	expression tag	UNP O00154
G	189	GLY	-	expression tag	UNP O00154
G	190	THR	-	expression tag	UNP O00154
G	191	GLU	-	expression tag	UNP O00154
G	192	ASN	-	expression tag	UNP O00154
G	193	LEU	-	expression tag	UNP O00154
G	194	TYR	-	expression tag	UNP O00154
G	195	PHE	-	expression tag	UNP O00154
G	196	GLN	-	expression tag	UNP O00154
G	197	SER	-	expression tag	UNP O00154
G	198	MET	-	expression tag	UNP O00154
H	176	MET	-	expression tag	UNP O00154
H	177	HIS	-	expression tag	UNP O00154
H	178	HIS	-	expression tag	UNP O00154
H	179	HIS	-	expression tag	UNP O00154
H	180	HIS	-	expression tag	UNP O00154
H	181	HIS	-	expression tag	UNP O00154
H	182	HIS	-	expression tag	UNP O00154
H	183	SER	-	expression tag	UNP O00154
H	184	SER	-	expression tag	UNP O00154
H	185	GLY	-	expression tag	UNP O00154
H	186	VAL	-	expression tag	UNP O00154
H	187	ASP	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
H	188	LEU	-	expression tag	UNP O00154
H	189	GLY	-	expression tag	UNP O00154
H	190	THR	-	expression tag	UNP O00154
H	191	GLU	-	expression tag	UNP O00154
H	192	ASN	-	expression tag	UNP O00154
H	193	LEU	-	expression tag	UNP O00154
H	194	TYR	-	expression tag	UNP O00154
H	195	PHE	-	expression tag	UNP O00154
H	196	GLN	-	expression tag	UNP O00154
H	197	SER	-	expression tag	UNP O00154
H	198	MET	-	expression tag	UNP O00154
I	176	MET	-	expression tag	UNP O00154
I	177	HIS	-	expression tag	UNP O00154
I	178	HIS	-	expression tag	UNP O00154
I	179	HIS	-	expression tag	UNP O00154
I	180	HIS	-	expression tag	UNP O00154
I	181	HIS	-	expression tag	UNP O00154
I	182	HIS	-	expression tag	UNP O00154
I	183	SER	-	expression tag	UNP O00154
I	184	SER	-	expression tag	UNP O00154
I	185	GLY	-	expression tag	UNP O00154
I	186	VAL	-	expression tag	UNP O00154
I	187	ASP	-	expression tag	UNP O00154
I	188	LEU	-	expression tag	UNP O00154
I	189	GLY	-	expression tag	UNP O00154
I	190	THR	-	expression tag	UNP O00154
I	191	GLU	-	expression tag	UNP O00154
I	192	ASN	-	expression tag	UNP O00154
I	193	LEU	-	expression tag	UNP O00154
I	194	TYR	-	expression tag	UNP O00154
I	195	PHE	-	expression tag	UNP O00154
I	196	GLN	-	expression tag	UNP O00154
I	197	SER	-	expression tag	UNP O00154
I	198	MET	-	expression tag	UNP O00154
J	176	MET	-	expression tag	UNP O00154
J	177	HIS	-	expression tag	UNP O00154
J	178	HIS	-	expression tag	UNP O00154
J	179	HIS	-	expression tag	UNP O00154
J	180	HIS	-	expression tag	UNP O00154
J	181	HIS	-	expression tag	UNP O00154
J	182	HIS	-	expression tag	UNP O00154
J	183	SER	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
J	184	SER	-	expression tag	UNP O00154
J	185	GLY	-	expression tag	UNP O00154
J	186	VAL	-	expression tag	UNP O00154
J	187	ASP	-	expression tag	UNP O00154
J	188	LEU	-	expression tag	UNP O00154
J	189	GLY	-	expression tag	UNP O00154
J	190	THR	-	expression tag	UNP O00154
J	191	GLU	-	expression tag	UNP O00154
J	192	ASN	-	expression tag	UNP O00154
J	193	LEU	-	expression tag	UNP O00154
J	194	TYR	-	expression tag	UNP O00154
J	195	PHE	-	expression tag	UNP O00154
J	196	GLN	-	expression tag	UNP O00154
J	197	SER	-	expression tag	UNP O00154
J	198	MET	-	expression tag	UNP O00154
K	176	MET	-	expression tag	UNP O00154
K	177	HIS	-	expression tag	UNP O00154
K	178	HIS	-	expression tag	UNP O00154
K	179	HIS	-	expression tag	UNP O00154
K	180	HIS	-	expression tag	UNP O00154
K	181	HIS	-	expression tag	UNP O00154
K	182	HIS	-	expression tag	UNP O00154
K	183	SER	-	expression tag	UNP O00154
K	184	SER	-	expression tag	UNP O00154
K	185	GLY	-	expression tag	UNP O00154
K	186	VAL	-	expression tag	UNP O00154
K	187	ASP	-	expression tag	UNP O00154
K	188	LEU	-	expression tag	UNP O00154
K	189	GLY	-	expression tag	UNP O00154
K	190	THR	-	expression tag	UNP O00154
K	191	GLU	-	expression tag	UNP O00154
K	192	ASN	-	expression tag	UNP O00154
K	193	LEU	-	expression tag	UNP O00154
K	194	TYR	-	expression tag	UNP O00154
K	195	PHE	-	expression tag	UNP O00154
K	196	GLN	-	expression tag	UNP O00154
K	197	SER	-	expression tag	UNP O00154
K	198	MET	-	expression tag	UNP O00154
L	176	MET	-	expression tag	UNP O00154
L	177	HIS	-	expression tag	UNP O00154
L	178	HIS	-	expression tag	UNP O00154
L	179	HIS	-	expression tag	UNP O00154

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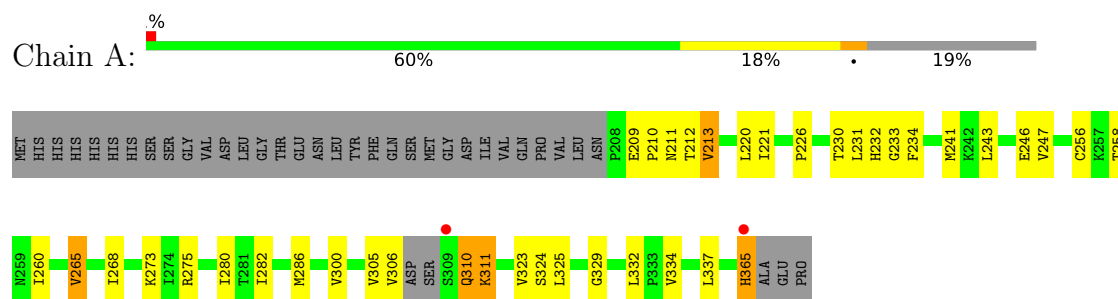
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Chain	Residue	Modelled	Actual	Comment	Reference
L	180	HIS	-	expression tag	UNP O00154
L	181	HIS	-	expression tag	UNP O00154
L	182	HIS	-	expression tag	UNP O00154
L	183	SER	-	expression tag	UNP O00154
L	184	SER	-	expression tag	UNP O00154
L	185	GLY	-	expression tag	UNP O00154
L	186	VAL	-	expression tag	UNP O00154
L	187	ASP	-	expression tag	UNP O00154
L	188	LEU	-	expression tag	UNP O00154
L	189	GLY	-	expression tag	UNP O00154
L	190	THR	-	expression tag	UNP O00154
L	191	GLU	-	expression tag	UNP O00154
L	192	ASN	-	expression tag	UNP O00154
L	193	LEU	-	expression tag	UNP O00154
L	194	TYR	-	expression tag	UNP O00154
L	195	PHE	-	expression tag	UNP O00154
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L	198	MET	-	expression tag	UNP O00154

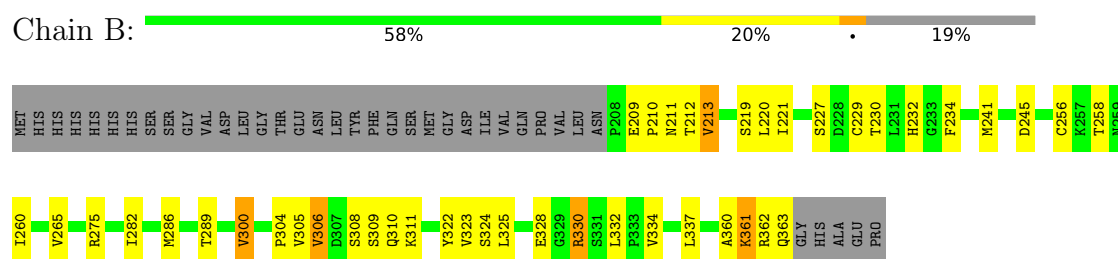
3 Residue-property plots

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.

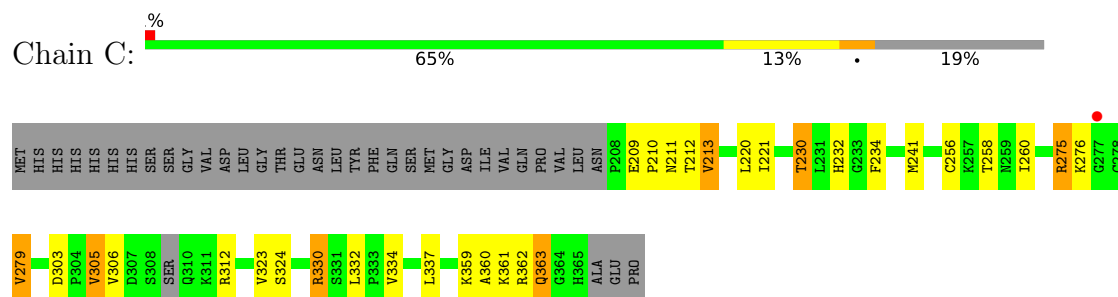
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



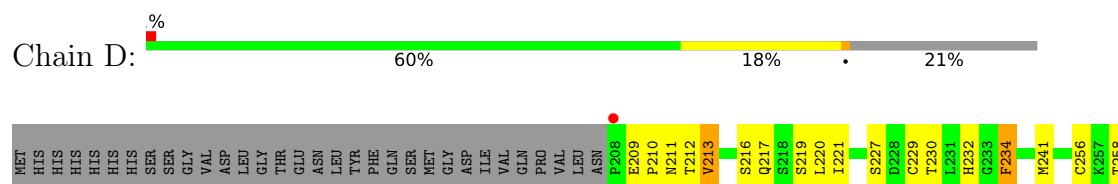
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

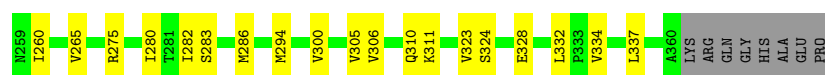


- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

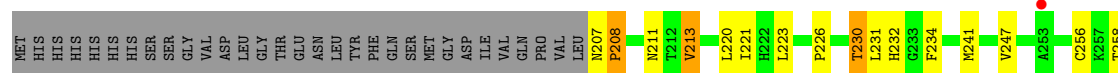


- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

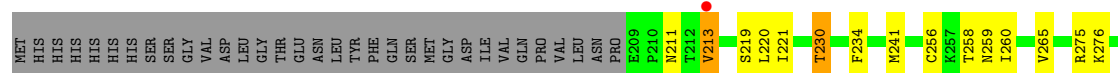




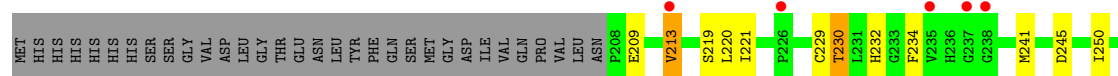
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



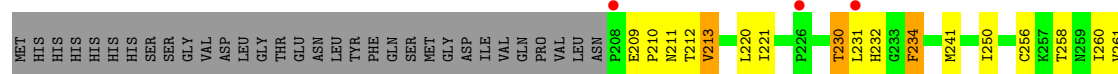
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

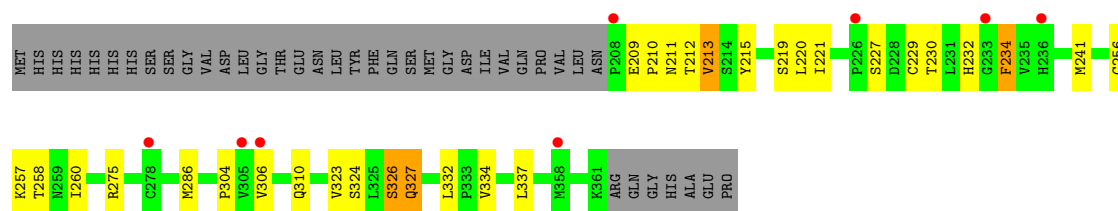


- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

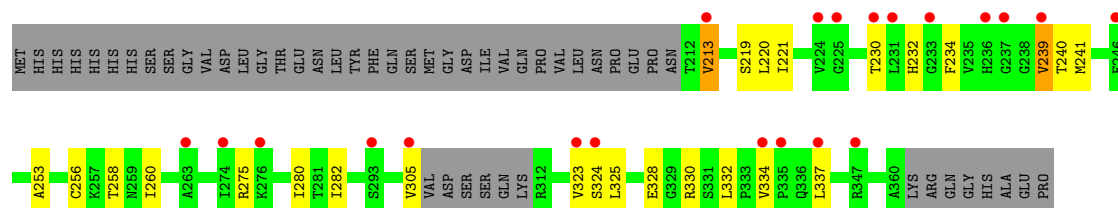


- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

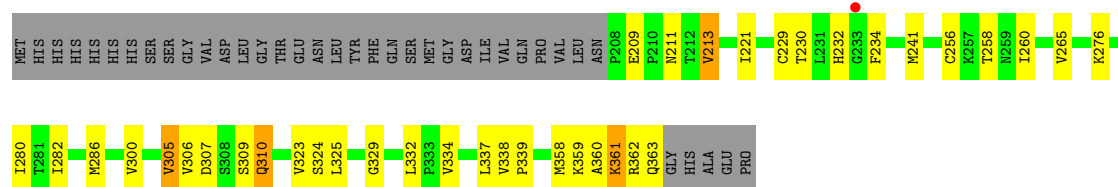




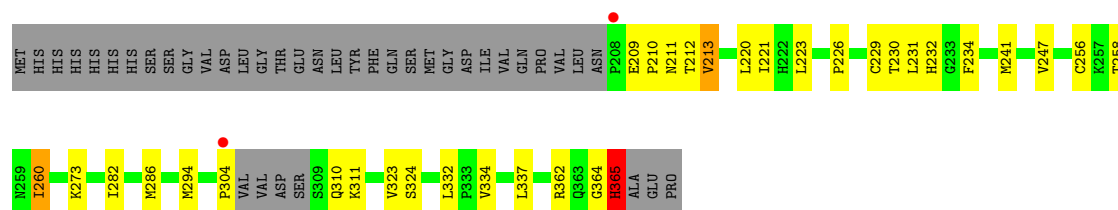
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.95Å 81.60Å 105.10Å 79.61° 89.70° 74.12°	Depositor
Resolution (Å)	19.87 – 2.80 19.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.87-2.80) 95.3 (19.87-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.3.0032	Depositor
R, R_{free}	0.216 , 0.239 0.207 , 0.228	Depositor DCC
R_{free} test set	2984 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	81.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 80.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14037	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.10	1/1208 (0.1%)	1.13	4/1628 (0.2%)
1	B	0.85	0/1220	1.01	2/1646 (0.1%)
1	C	0.88	0/1219	1.01	1/1642 (0.1%)
1	D	0.99	3/1190 (0.3%)	1.01	3/1607 (0.2%)
1	E	0.92	1/1167 (0.1%)	1.02	1/1576 (0.1%)
1	F	0.79	1/1162 (0.1%)	0.94	2/1568 (0.1%)
1	G	0.92	2/1148 (0.2%)	1.02	3/1550 (0.2%)
1	H	0.68	0/1195	0.90	1/1612 (0.1%)
1	I	0.70	0/1208	0.94	2/1629 (0.1%)
1	J	1.09	4/1120 (0.4%)	1.04	0/1509
1	K	0.96	0/1228	1.04	6/1655 (0.4%)
1	L	0.79	1/1214 (0.1%)	0.94	3/1633 (0.2%)
All	All	0.90	13/14279 (0.1%)	1.00	28/19255 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	HIS	C-O	20.43	1.64	1.23
1	D	328	GLU	CD-OE1	13.50	1.51	1.25
1	J	328	GLU	CD-OE1	12.85	1.49	1.25
1	J	328	GLU	CD-OE2	12.47	1.49	1.25
1	G	311	LYS	N-CA	12.35	1.69	1.46
1	J	330	ARG	CZ-NH1	11.49	1.48	1.32
1	L	365	HIS	C-O	10.31	1.44	1.23
1	D	328	GLU	CD-OE2	9.54	1.43	1.25
1	G	282	ILE	CA-CB	-6.33	1.46	1.53
1	E	298	VAL	CA-CB	-5.86	1.47	1.54
1	J	239	VAL	CA-CB	-5.74	1.48	1.54
1	D	283	SER	CA-C	-5.15	1.46	1.52
1	F	330	ARG	CZ-NH1	5.02	1.39	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	305	VAL	N-CA-C	-8.39	105.00	113.47
1	A	365	HIS	CA-C-O	-7.57	107.94	120.80
1	A	305	VAL	N-CA-C	-6.95	106.23	112.90
1	L	365	HIS	CA-C-O	-6.78	109.27	120.80
1	G	250	ILE	N-CA-C	-5.84	104.82	110.72
1	C	279	VAL	N-CA-C	-5.75	100.12	108.17
1	D	229	CYS	N-CA-C	5.74	119.07	109.95
1	K	211	ASN	N-CA-C	5.71	116.62	108.74
1	K	265	VAL	N-CA-C	-5.64	99.99	108.12
1	L	311	LYS	N-CA-C	5.62	119.08	110.20
1	A	265	VAL	N-CA-C	-5.60	100.06	108.12
1	A	243	LEU	N-CA-C	-5.41	105.46	111.36
1	F	265	VAL	N-CA-C	-5.41	100.69	108.48
1	B	229	CYS	N-CA-C	5.35	118.44	110.14
1	G	229	CYS	N-CA-C	5.34	118.44	109.95
1	G	282	ILE	CB-CA-C	-5.34	103.83	111.31
1	I	234	PHE	N-CA-C	5.33	118.42	109.95
1	D	234	PHE	N-CA-C	5.32	118.41	109.95
1	I	229	CYS	N-CA-C	5.31	118.21	109.72
1	H	234	PHE	N-CA-C	5.28	118.33	110.14
1	D	265	VAL	N-CA-C	-5.28	100.52	108.12
1	E	211	ASN	N-CA-C	5.19	116.70	108.96
1	K	229	CYS	N-CA-C	5.08	118.03	109.95
1	B	265	VAL	N-CA-C	-5.06	100.84	108.12
1	F	211	ASN	N-CA-C	5.05	116.75	109.07
1	K	209	GLU	CA-C-N	5.01	125.02	120.21
1	K	209	GLU	C-N-CA	5.01	125.02	120.21
1	L	229	CYS	N-CA-C	5.01	117.90	110.14

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	1188	0	1188	35	0
1	B	1199	0	1197	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1199	0	1201	26	0
1	D	1169	0	1167	24	0
1	E	1147	0	1132	32	0
1	F	1143	0	1142	30	0
1	G	1128	0	1122	25	0
1	H	1175	0	1171	29	0
1	I	1187	0	1193	25	0
1	J	1102	0	1108	17	0
1	K	1207	0	1214	29	0
1	L	1193	0	1196	23	0
All	All	14037	0	14031	282	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 10.

All (282) 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:G:311:LYS:N	1:G:311:LYS:CA	1.69	1.52
1:A:365:HIS:C	1:A:365:HIS:O	1.64	1.39
1:H:261:VAL:HG22	1:H:325:LEU:HD11	1.22	1.17
1:E:256:CYS:HB3	1:E:258:THR:HG22	1.24	1.16
1:G:256:CYS:HB3	1:G:258:THR:HG22	1.18	1.15
1:F:256:CYS:HB3	1:F:258:THR:HG22	1.19	1.14
1:H:256:CYS:HB3	1:H:258:THR:HG22	1.19	1.14
1:B:256:CYS:HB3	1:B:258:THR:HG22	1.22	1.14
1:L:256:CYS:HB3	1:L:258:THR:HG22	1.21	1.14
1:C:256:CYS:HB3	1:C:258:THR:HG22	1.18	1.12
1:K:256:CYS:HB3	1:K:258:THR:HG22	1.24	1.11
1:I:256:CYS:HB3	1:I:258:THR:HG22	1.20	1.10
1:J:256:CYS:HB3	1:J:258:THR:HG22	1.14	1.10
1:D:256:CYS:HB3	1:D:258:THR:HG22	1.18	1.09
1:A:256:CYS:HB3	1:A:258:THR:HG22	1.14	1.07
1:H:275:ARG:HG2	1:H:275:ARG:HH11	1.17	1.05
1:B:234:PHE:HE2	1:B:275:ARG:NH1	1.55	1.04
1:E:231:LEU:HD21	1:K:276:LYS:HB3	1.42	1.00
1:A:231:LEU:HD21	1:C:276:LYS:HB3	1.46	0.97
1:F:276:LYS:HB3	1:H:231:LEU:HD21	1.47	0.94
1:F:306:VAL:O	1:F:306:VAL:HG12	1.71	0.91
1:B:234:PHE:HE2	1:B:275:ARG:HH11	1.11	0.89
1:G:276:LYS:HB3	1:L:231:LEU:HD21	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:HA	1:C:330:ARG:HH21	1.39	0.87
1:H:241:MET:HE2	1:I:241:MET:HB3	1.57	0.87
1:B:304:PRO:HG2	1:B:310:GLN:HB3	1.57	0.86
1:H:275:ARG:HG2	1:H:275:ARG:NH1	1.82	0.86
1:A:256:CYS:CB	1:A:258:THR:HG22	2.05	0.85
1:I:304:PRO:HG2	1:I:310:GLN:HB2	1.58	0.85
1:F:256:CYS:CB	1:F:258:THR:HG22	2.07	0.83
1:H:256:CYS:CB	1:H:258:THR:HG22	2.08	0.83
1:F:256:CYS:HB3	1:F:258:THR:CG2	2.07	0.82
1:J:256:CYS:HB3	1:J:258:THR:CG2	2.05	0.82
1:H:256:CYS:HB3	1:H:258:THR:CG2	2.07	0.82
1:G:256:CYS:HB3	1:G:258:THR:CG2	2.07	0.81
1:H:209:GLU:O	1:H:212:THR:HG22	1.80	0.81
1:A:256:CYS:HB3	1:A:258:THR:CG2	2.05	0.81
1:L:256:CYS:CB	1:L:258:THR:HG22	2.08	0.80
1:K:256:CYS:CB	1:K:258:THR:HG22	2.10	0.80
1:A:241:MET:HE2	1:B:241:MET:HB3	1.62	0.80
1:B:308:SER:O	1:B:310:GLN:N	2.12	0.80
1:C:256:CYS:CB	1:C:258:THR:HG22	2.09	0.80
1:B:330:ARG:HB2	1:B:330:ARG:HH11	1.46	0.79
1:H:275:ARG:HH11	1:H:275:ARG:CG	1.96	0.79
1:G:256:CYS:CB	1:G:258:THR:HG22	2.08	0.79
1:F:306:VAL:O	1:F:306:VAL:CG1	2.32	0.76
1:E:256:CYS:CB	1:E:258:THR:HG22	2.12	0.76
1:C:330:ARG:HA	1:C:330:ARG:NH2	2.01	0.76
1:D:256:CYS:HB3	1:D:258:THR:CG2	2.08	0.76
1:H:363:GLN:HA	1:H:363:GLN:OE1	1.84	0.76
1:C:256:CYS:HB3	1:C:258:THR:CG2	2.09	0.76
1:I:256:CYS:HB3	1:I:258:THR:CG2	2.09	0.76
1:F:305:VAL:CG1	1:I:257:LYS:HA	2.16	0.75
1:J:241:MET:HB3	1:L:241:MET:HE2	1.68	0.75
1:G:305:VAL:HG21	1:J:253:ALA:HB1	1.69	0.75
1:B:234:PHE:CE2	1:B:275:ARG:NH1	2.48	0.74
1:L:209:GLU:O	1:L:212:THR:HG22	1.87	0.74
1:D:241:MET:HB3	1:E:241:MET:HE2	1.69	0.74
1:L:256:CYS:HB3	1:L:258:THR:CG2	2.10	0.73
1:L:258:THR:HG21	1:L:324:SER:OG	1.89	0.72
1:K:256:CYS:HB3	1:K:258:THR:CG2	2.12	0.72
1:E:256:CYS:HB3	1:E:258:THR:CG2	2.12	0.71
1:H:261:VAL:HG22	1:H:325:LEU:CD1	2.12	0.71
1:I:256:CYS:CB	1:I:258:THR:HG22	2.10	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLU:O	1:B:212:THR:HG22	1.91	0.70
1:F:305:VAL:HG13	1:I:257:LYS:HA	1.72	0.69
1:D:219:SER:O	1:K:221:ILE:HG13	1.91	0.69
1:B:256:CYS:CB	1:B:258:THR:HG22	2.13	0.69
1:C:305:VAL:O	1:C:305:VAL:CG1	2.40	0.69
1:D:256:CYS:CB	1:D:258:THR:HG22	2.10	0.69
1:B:256:CYS:HB3	1:B:258:THR:CG2	2.13	0.67
1:C:234:PHE:HE2	1:C:275:ARG:HD2	1.59	0.67
1:E:258:THR:HG21	1:E:324:SER:OG	1.94	0.67
1:L:362:ARG:O	1:L:362:ARG:HG3	1.94	0.67
1:F:241:MET:HE2	1:G:241:MET:HB3	1.76	0.66
1:I:209:GLU:O	1:I:212:THR:HG22	1.96	0.66
1:A:241:MET:HB3	1:B:241:MET:HE2	1.78	0.66
1:I:275:ARG:HH12	1:I:304:PRO:HB3	1.61	0.66
1:E:311:LYS:HG2	1:E:312:ARG:N	2.12	0.65
1:G:311:LYS:N	1:G:311:LYS:C	2.53	0.65
1:B:305:VAL:O	1:B:305:VAL:HG12	1.97	0.65
1:K:360:ALA:O	1:K:363:GLN:N	2.30	0.64
1:A:258:THR:HG21	1:A:324:SER:OG	1.97	0.63
1:F:219:SER:O	1:I:221:ILE:HG13	1.99	0.63
1:D:241:MET:HE2	1:E:241:MET:HB3	1.80	0.63
1:A:310:GLN:OE1	1:A:311:LYS:N	2.32	0.63
1:F:241:MET:HB3	1:G:241:MET:HE2	1.80	0.63
1:K:358:MET:O	1:K:362:ARG:HD3	1.96	0.63
1:H:258:THR:HG21	1:H:324:SER:OG	1.99	0.62
1:C:230:THR:HG22	1:C:234:PHE:H	1.65	0.62
1:F:221:ILE:HG13	1:I:219:SER:O	2.00	0.62
1:H:241:MET:HB3	1:I:241:MET:HE2	1.81	0.62
1:C:209:GLU:O	1:C:212:THR:HG22	2.00	0.61
1:B:308:SER:C	1:B:310:GLN:H	2.06	0.60
1:C:362:ARG:O	1:C:362:ARG:HG2	2.01	0.60
1:E:234:PHE:HE2	1:E:275:ARG:HD3	1.65	0.60
1:J:230:THR:HG22	1:J:234:PHE:H	1.67	0.59
1:C:234:PHE:CE2	1:C:275:ARG:HD2	2.37	0.59
1:C:241:MET:HE2	1:K:241:MET:HB3	1.84	0.59
1:B:209:GLU:HG3	1:F:292:LYS:NZ	2.19	0.58
1:G:220:LEU:HD23	1:G:221:ILE:N	2.18	0.58
1:J:258:THR:HG21	1:J:324:SER:OG	2.03	0.58
1:C:305:VAL:O	1:C:305:VAL:HG13	2.03	0.58
1:E:231:LEU:HD11	1:K:276:LYS:HG2	1.86	0.57
1:I:258:THR:HG21	1:I:324:SER:OG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:CE2	1:A:275:ARG:HD2	2.40	0.57
1:F:305:VAL:HG12	1:I:257:LYS:HA	1.86	0.57
1:B:258:THR:HG21	1:B:324:SER:OG	2.05	0.56
1:B:282:ILE:HG13	1:B:300:VAL:HG13	1.87	0.56
1:D:258:THR:HG21	1:D:324:SER:OG	2.05	0.56
1:H:305:VAL:HG23	1:H:306:VAL:HG23	1.86	0.56
1:I:210:PRO:HA	1:I:215:TYR:CD1	2.40	0.56
1:D:234:PHE:CD2	1:D:275:ARG:HG2	2.41	0.56
1:E:207:ASN:N	1:E:208:PRO:HD3	2.20	0.56
1:K:230:THR:HG22	1:K:234:PHE:H	1.69	0.56
1:B:360:ALA:O	1:B:362:ARG:N	2.39	0.56
1:B:230:THR:HG22	1:B:234:PHE:H	1.71	0.56
1:D:310:GLN:HG2	1:D:311:LYS:H	1.71	0.56
1:K:360:ALA:C	1:K:362:ARG:N	2.64	0.56
1:F:221:ILE:HD12	1:I:219:SER:H	1.70	0.55
1:E:230:THR:HG22	1:E:234:PHE:H	1.70	0.55
1:K:258:THR:HG21	1:K:324:SER:OG	2.07	0.55
1:J:220:LEU:HD23	1:J:221:ILE:N	2.22	0.55
1:D:234:PHE:CE2	1:D:275:ARG:HG2	2.42	0.55
1:C:241:MET:HB3	1:K:241:MET:HE2	1.88	0.54
1:G:230:THR:HG22	1:G:234:PHE:H	1.73	0.54
1:B:219:SER:O	1:C:221:ILE:HG13	2.07	0.54
1:H:209:GLU:O	1:H:212:THR:CG2	2.54	0.54
1:E:327:GLN:CD	1:E:327:GLN:H	2.15	0.53
1:F:305:VAL:HG12	1:I:257:LYS:C	2.34	0.53
1:C:258:THR:HG21	1:C:324:SER:OG	2.08	0.53
1:E:330:ARG:HB3	1:E:330:ARG:CZ	2.37	0.53
1:E:220:LEU:HD23	1:E:221:ILE:N	2.25	0.52
1:D:230:THR:HG22	1:D:234:PHE:H	1.74	0.52
1:F:213:VAL:HG12	1:F:337:LEU:HD11	1.91	0.52
1:B:230:THR:HG23	1:B:232:HIS:H	1.73	0.52
1:L:304:PRO:HD2	1:L:310:GLN:O	2.10	0.52
1:A:247:VAL:HG21	1:A:282:ILE:HG22	1.92	0.52
1:D:209:GLU:O	1:D:212:THR:HG22	2.09	0.52
1:D:210:PRO:O	1:D:211:ASN:HB2	2.10	0.52
1:L:256:CYS:SG	1:L:294:MET:SD	3.08	0.51
1:G:230:THR:HG23	1:G:232:HIS:H	1.76	0.51
1:A:220:LEU:HD23	1:A:221:ILE:N	2.26	0.51
1:B:275:ARG:HB2	1:B:275:ARG:CZ	2.40	0.51
1:F:230:THR:HG22	1:F:234:PHE:H	1.75	0.51
1:I:326:SER:OG	1:I:327:GLN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:VAL:HG12	1:D:337:LEU:HD11	1.93	0.51
1:I:230:THR:HG22	1:I:234:PHE:H	1.76	0.50
1:D:219:SER:H	1:K:221:ILE:HD12	1.75	0.50
1:A:233:GLY:HA3	1:A:275:ARG:NH2	2.26	0.50
1:B:210:PRO:O	1:B:211:ASN:HB2	2.10	0.50
1:G:221:ILE:HD12	1:J:219:SER:H	1.77	0.50
1:A:221:ILE:HB	1:E:220:LEU:HA	1.94	0.49
1:A:210:PRO:O	1:A:211:ASN:HB2	2.12	0.49
1:C:213:VAL:HG12	1:C:337:LEU:HD11	1.94	0.49
1:E:234:PHE:CE2	1:E:275:ARG:HD3	2.47	0.49
1:F:326:SER:OG	1:F:330:ARG:HG3	2.12	0.49
1:B:362:ARG:CZ	1:B:362:ARG:HB3	2.42	0.49
1:E:280:ILE:HG13	1:E:282:ILE:HD11	1.93	0.49
1:A:213:VAL:HG12	1:A:337:LEU:HD11	1.93	0.49
1:L:230:THR:HG22	1:L:234:PHE:H	1.77	0.48
1:A:209:GLU:O	1:A:212:THR:HG22	2.13	0.48
1:G:213:VAL:HG12	1:G:337:LEU:HD11	1.93	0.48
1:G:219:SER:O	1:J:221:ILE:HG13	2.13	0.48
1:B:360:ALA:O	1:B:361:LYS:C	2.54	0.48
1:G:359:LYS:HA	1:G:359:LYS:HD3	1.62	0.48
1:C:230:THR:HG23	1:C:232:HIS:H	1.79	0.48
1:K:306:VAL:HG12	1:K:307:ASP:N	2.29	0.48
1:D:230:THR:HG23	1:D:232:HIS:H	1.77	0.48
1:J:241:MET:HE2	1:L:241:MET:HB3	1.95	0.48
1:A:234:PHE:CD2	1:A:275:ARG:HD2	2.49	0.48
1:A:230:THR:HG23	1:A:232:HIS:H	1.79	0.47
1:C:210:PRO:O	1:C:211:ASN:HB2	2.14	0.47
1:H:213:VAL:HG12	1:H:337:LEU:HD11	1.95	0.47
1:I:213:VAL:HG12	1:I:337:LEU:HD11	1.95	0.47
1:E:213:VAL:HG12	1:E:337:LEU:HD11	1.97	0.47
1:H:362:ARG:O	1:H:363:GLN:C	2.57	0.47
1:B:227:SER:HB2	1:E:226:PRO:HG2	1.96	0.47
1:D:305:VAL:HG13	1:D:305:VAL:O	2.15	0.47
1:E:207:ASN:N	1:E:208:PRO:CD	2.77	0.47
1:G:221:ILE:HG13	1:J:219:SER:O	2.14	0.47
1:A:230:THR:HG22	1:A:234:PHE:H	1.79	0.47
1:H:282:ILE:HG13	1:H:300:VAL:HG13	1.96	0.47
1:B:213:VAL:HG12	1:B:337:LEU:HD11	1.96	0.47
1:B:362:ARG:O	1:B:363:GLN:C	2.58	0.47
1:J:213:VAL:HG12	1:J:337:LEU:HD11	1.97	0.47
1:D:310:GLN:HG2	1:D:311:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:GLU:O	1:G:335:PRO:HB3	2.15	0.47
1:J:230:THR:HG23	1:J:232:HIS:H	1.80	0.47
1:F:305:VAL:HG12	1:I:257:LYS:CA	2.45	0.46
1:J:325:LEU:HD11	1:L:273:LYS:CE	2.46	0.46
1:E:311:LYS:CG	1:E:312:ARG:N	2.78	0.46
1:H:261:VAL:CG2	1:H:325:LEU:HD11	2.16	0.46
1:A:226:PRO:HG2	1:D:227:SER:HB2	1.97	0.46
1:C:360:ALA:O	1:C:361:LYS:C	2.57	0.46
1:E:230:THR:HG23	1:E:232:HIS:H	1.80	0.46
1:H:230:THR:HG22	1:H:234:PHE:H	1.80	0.46
1:L:213:VAL:HG12	1:L:337:LEU:HD11	1.97	0.46
1:H:230:THR:HG23	1:H:232:HIS:H	1.81	0.46
1:K:282:ILE:HG13	1:K:300:VAL:HG13	1.98	0.45
1:A:247:VAL:HG21	1:A:282:ILE:CG2	2.46	0.45
1:K:360:ALA:O	1:K:362:ARG:N	2.49	0.45
1:A:365:HIS:O	1:A:365:HIS:CB	2.65	0.45
1:B:360:ALA:C	1:B:362:ARG:N	2.75	0.45
1:K:213:VAL:HG12	1:K:337:LEU:HD11	1.99	0.45
1:L:247:VAL:HG21	1:L:282:ILE:HG22	1.99	0.45
1:B:220:LEU:HD23	1:B:221:ILE:N	2.32	0.44
1:F:276:LYS:HG2	1:H:231:LEU:HD11	1.99	0.44
1:F:282:ILE:N	1:F:282:ILE:HD12	2.32	0.44
1:L:210:PRO:O	1:L:211:ASN:HB2	2.17	0.44
1:H:220:LEU:HD23	1:H:221:ILE:N	2.33	0.44
1:C:220:LEU:HD23	1:C:221:ILE:N	2.32	0.44
1:F:282:ILE:HG13	1:F:300:VAL:HG13	1.99	0.44
1:A:310:GLN:O	1:A:311:LYS:HB2	2.17	0.44
1:D:220:LEU:HD23	1:D:221:ILE:N	2.33	0.44
1:D:282:ILE:HG13	1:D:300:VAL:HG13	2.00	0.44
1:F:256:CYS:SG	1:F:294:MET:SD	3.15	0.44
1:B:286:MET:HE3	1:B:289:THR:CG2	2.48	0.43
1:G:245:ASP:OD1	1:G:322:TYR:OH	2.31	0.43
1:I:230:THR:HG23	1:I:232:HIS:H	1.83	0.43
1:L:364:GLY:C	1:L:365:HIS:CD2	2.96	0.43
1:L:230:THR:HG23	1:L:232:HIS:H	1.83	0.43
1:B:209:GLU:HG3	1:F:292:LYS:HZ2	1.81	0.43
1:B:245:ASP:OD1	1:B:322:TYR:OH	2.34	0.43
1:H:256:CYS:SG	1:H:294:MET:SD	3.16	0.43
1:K:325:LEU:HD22	1:K:329:GLY:O	2.18	0.43
1:F:286:MET:HE3	1:F:289:THR:HG22	2.01	0.43
1:H:325:LEU:N	1:H:325:LEU:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:210:PRO:O	1:I:211:ASN:HB2	2.18	0.43
1:E:311:LYS:HE2	1:E:311:LYS:HB3	1.59	0.43
1:K:280:ILE:HD13	1:K:280:ILE:HG21	1.71	0.43
1:A:265:VAL:HG11	1:A:268:ILE:HD11	2.00	0.43
1:C:303:ASP:OD1	1:C:312:ARG:HB2	2.18	0.43
1:A:325:LEU:HD22	1:A:329:GLY:O	2.19	0.43
1:H:359:LYS:O	1:H:362:ARG:O	2.36	0.43
1:A:231:LEU:HD11	1:C:276:LYS:HG2	2.01	0.43
1:E:231:LEU:HD11	1:K:276:LYS:CG	2.49	0.43
1:A:220:LEU:HA	1:E:221:ILE:HB	2.01	0.42
1:A:220:LEU:HD23	1:A:220:LEU:C	2.43	0.42
1:G:219:SER:H	1:J:221:ILE:HD12	1.84	0.42
1:H:210:PRO:O	1:H:211:ASN:HB2	2.19	0.42
1:B:286:MET:HE3	1:B:289:THR:HG22	2.00	0.42
1:D:216:SER:O	1:D:217:GLN:C	2.60	0.42
1:G:282:ILE:N	1:G:282:ILE:HD12	2.34	0.42
1:J:239:VAL:O	1:J:240:THR:C	2.60	0.42
1:K:230:THR:HG23	1:K:232:HIS:H	1.84	0.42
1:A:282:ILE:HG13	1:A:300:VAL:HG13	2.01	0.42
1:B:305:VAL:O	1:B:305:VAL:CG1	2.65	0.42
1:I:227:SER:HB2	1:L:226:PRO:HG2	2.02	0.42
1:K:359:LYS:HD3	1:K:359:LYS:HA	1.72	0.42
1:E:256:CYS:SG	1:E:294:MET:SD	3.18	0.42
1:F:259:ASN:HB2	1:G:232:HIS:CE1	2.55	0.42
1:H:250:ILE:HD11	1:L:223:LEU:HD13	2.02	0.42
1:E:247:VAL:HG21	1:E:282:ILE:HG22	2.02	0.41
1:D:256:CYS:SG	1:D:294:MET:SD	3.18	0.41
1:F:220:LEU:HD23	1:F:221:ILE:N	2.35	0.41
1:G:277:GLY:O	1:G:305:VAL:HG12	2.20	0.41
1:K:338:VAL:HA	1:K:339:PRO:HD3	1.90	0.41
1:K:361:LYS:HB3	1:K:361:LYS:HE2	1.74	0.41
1:C:359:LYS:O	1:C:363:GLN:HB2	2.21	0.41
1:K:280:ILE:HG13	1:K:282:ILE:HD11	2.01	0.41
1:A:246:GLU:HG2	1:E:223:LEU:CD2	2.50	0.41
1:G:327:GLN:HG2	1:G:328:GLU:N	2.34	0.41
1:I:220:LEU:HD23	1:I:221:ILE:N	2.35	0.41
1:E:247:VAL:HG21	1:E:282:ILE:CG2	2.51	0.41
1:J:280:ILE:HG13	1:J:282:ILE:HD11	2.02	0.41
1:A:234:PHE:HE2	1:A:275:ARG:HD2	1.85	0.41
1:A:273:LYS:HE2	1:B:325:LEU:HD11	2.03	0.41
1:B:209:GLU:HG3	1:F:292:LYS:HZ1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ILE:HD13	1:D:280:ILE:HG21	1.72	0.41
1:K:360:ALA:C	1:K:362:ARG:H	2.27	0.41
1:G:213:VAL:HG22	1:G:344:GLU:OE2	2.21	0.41
1:L:260:ILE:H	1:L:260:ILE:HG13	1.77	0.41
1:E:208:PRO:HG2	1:E:335:PRO:HG3	2.02	0.40
1:K:306:VAL:CG1	1:K:307:ASP:N	2.84	0.40
1:L:220:LEU:HD23	1:L:221:ILE:N	2.37	0.40
1:A:280:ILE:HG13	1:A:282:ILE:HD11	2.03	0.40
1:K:309:SER:O	1:K:310:GLN:HB2	2.20	0.40
1:A:246:GLU:HG2	1:E:223:LEU:HD23	2.03	0.40
1:C:279:VAL:HG23	1:C:305:VAL:HG21	2.02	0.40
1:F:280:ILE:HG21	1:F:280:ILE:HD13	1.77	0.40
1:L:247:VAL:HG21	1:L:282:ILE:CG2	2.51	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	152/193 (79%)	144 (95%)	7 (5%)	1 (1%)	18	47
1	B	154/193 (80%)	146 (95%)	5 (3%)	3 (2%)	6	22
1	C	153/193 (79%)	143 (94%)	10 (6%)	0	100	100
1	D	151/193 (78%)	141 (93%)	10 (7%)	0	100	100
1	E	146/193 (76%)	140 (96%)	5 (3%)	1 (1%)	18	47
1	F	145/193 (75%)	139 (96%)	6 (4%)	0	100	100
1	G	144/193 (75%)	138 (96%)	6 (4%)	0	100	100
1	H	149/193 (77%)	142 (95%)	7 (5%)	0	100	100
1	I	152/193 (79%)	142 (93%)	9 (6%)	1 (1%)	18	47
1	J	139/193 (72%)	134 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	154/193 (80%)	144 (94%)	8 (5%)	2 (1%)	9	31
1	L	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
All	All	1789/2316 (77%)	1696 (95%)	85 (5%)	8 (0%)	30	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	309	SER
1	B	361	LYS
1	K	361	LYS
1	A	311	LYS
1	B	306	VAL
1	K	310	GLN
1	I	306	VAL
1	E	208	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	131/168 (78%)	123 (94%)	8 (6%)	17	46
1	B	134/168 (80%)	124 (92%)	10 (8%)	12	37
1	C	132/168 (79%)	121 (92%)	11 (8%)	10	32
1	D	131/168 (78%)	124 (95%)	7 (5%)	20	52
1	E	126/168 (75%)	118 (94%)	8 (6%)	16	45
1	F	127/168 (76%)	116 (91%)	11 (9%)	9	30
1	G	125/168 (74%)	118 (94%)	7 (6%)	19	50
1	H	130/168 (77%)	119 (92%)	11 (8%)	10	31
1	I	134/168 (80%)	126 (94%)	8 (6%)	17	47
1	J	123/168 (73%)	116 (94%)	7 (6%)	18	49
1	K	136/168 (81%)	129 (95%)	7 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	133/168 (79%)	126 (95%)	7 (5%)	20	52
All	All	1562/2016 (78%)	1460 (94%)	102 (6%)	15	43

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	VAL
1	A	260	ILE
1	A	286	MET
1	A	306	VAL
1	A	310	GLN
1	A	323	VAL
1	A	332	LEU
1	A	334	VAL
1	B	213	VAL
1	B	260	ILE
1	B	300	VAL
1	B	306	VAL
1	B	311	LYS
1	B	323	VAL
1	B	328	GLU
1	B	330	ARG
1	B	332	LEU
1	B	334	VAL
1	C	213	VAL
1	C	230	THR
1	C	260	ILE
1	C	275	ARG
1	C	305	VAL
1	C	306	VAL
1	C	323	VAL
1	C	330	ARG
1	C	332	LEU
1	C	334	VAL
1	C	363	GLN
1	D	213	VAL
1	D	260	ILE
1	D	286	MET
1	D	306	VAL
1	D	323	VAL
1	D	332	LEU
1	D	334	VAL

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Mol	Chain	Res	Type
1	E	213	VAL
1	E	230	THR
1	E	260	ILE
1	E	275	ARG
1	E	323	VAL
1	E	330	ARG
1	E	332	LEU
1	E	334	VAL
1	F	213	VAL
1	F	230	THR
1	F	260	ILE
1	F	275	ARG
1	F	286	MET
1	F	300	VAL
1	F	310	GLN
1	F	323	VAL
1	F	330	ARG
1	F	332	LEU
1	F	334	VAL
1	G	213	VAL
1	G	230	THR
1	G	260	ILE
1	G	323	VAL
1	G	327	GLN
1	G	332	LEU
1	G	334	VAL
1	H	213	VAL
1	H	230	THR
1	H	260	ILE
1	H	275	ARG
1	H	286	MET
1	H	323	VAL
1	H	327	GLN
1	H	332	LEU
1	H	334	VAL
1	H	362	ARG
1	H	363	GLN
1	I	213	VAL
1	I	260	ILE
1	I	286	MET
1	I	323	VAL
1	I	326	SER

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Mol	Chain	Res	Type
1	I	327	GLN
1	I	332	LEU
1	I	334	VAL
1	J	213	VAL
1	J	260	ILE
1	J	275	ARG
1	J	305	VAL
1	J	323	VAL
1	J	332	LEU
1	J	334	VAL
1	K	213	VAL
1	K	260	ILE
1	K	286	MET
1	K	305	VAL
1	K	323	VAL
1	K	332	LEU
1	K	334	VAL
1	L	213	VAL
1	L	260	ILE
1	L	286	MET
1	L	323	VAL
1	L	332	LEU
1	L	334	VAL
1	L	365	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	B	232	HIS
1	B	327	GLN
1	G	327	GLN
1	H	327	GLN
1	I	327	GLN
1	J	236	HIS
1	K	259	ASN
1	L	269	ASN
1	L	365	HIS

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](#)

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	156/193 (80%)	0.20	2 (1%) 75 66	65, 83, 108, 122	0
1	B	156/193 (80%)	-0.03	0 100 100	65, 84, 110, 119	0
1	C	157/193 (81%)	0.10	1 (0%) 85 80	65, 83, 107, 122	0
1	D	153/193 (79%)	0.18	1 (0%) 84 77	65, 83, 110, 132	0
1	E	150/193 (77%)	0.07	1 (0%) 84 77	65, 83, 104, 111	0
1	F	149/193 (77%)	0.41	6 (4%) 42 33	65, 83, 102, 111	0
1	G	148/193 (76%)	0.80	15 (10%) 12 9	65, 83, 101, 111	0
1	H	153/193 (79%)	0.35	6 (3%) 43 34	65, 83, 104, 111	0
1	I	154/193 (79%)	0.59	8 (5%) 33 25	65, 83, 107, 111	0
1	J	143/193 (74%)	1.10	21 (14%) 6 4	65, 83, 102, 111	0
1	K	156/193 (80%)	-0.04	1 (0%) 85 80	65, 83, 108, 130	0
1	L	154/193 (79%)	0.19	2 (1%) 75 66	65, 83, 104, 111	0
All	All	1829/2316 (78%)	0.32	64 (3%) 47 38	65, 83, 107, 132	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	HIS	4.0
1	G	279	VAL	3.8
1	J	239	VAL	3.5
1	G	273	LYS	3.4
1	I	358	MET	3.4
1	J	334	VAL	3.4
1	J	337	LEU	3.2
1	J	236	HIS	3.2
1	J	237	GLY	3.2
1	I	208	PRO	3.0
1	J	305	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	277	GLY	2.8
1	J	231	LEU	2.7
1	I	233	GLY	2.7
1	F	334	VAL	2.7
1	J	233	GLY	2.6
1	F	213	VAL	2.6
1	H	325	LEU	2.6
1	J	263	ALA	2.6
1	H	276	LYS	2.5
1	G	274	ILE	2.5
1	J	246	GLU	2.5
1	I	306	VAL	2.5
1	J	213	VAL	2.5
1	J	276	LYS	2.5
1	J	225	GLY	2.5
1	F	301	ASP	2.5
1	G	226	PRO	2.4
1	J	335	PRO	2.4
1	D	208	PRO	2.4
1	J	347	ARG	2.4
1	J	324	SER	2.4
1	G	213	VAL	2.3
1	J	230	THR	2.3
1	J	323	VAL	2.3
1	G	272	ASP	2.3
1	I	226	PRO	2.3
1	G	276	LYS	2.3
1	F	306	VAL	2.3
1	G	238	GLY	2.3
1	I	236	HIS	2.2
1	G	289	THR	2.2
1	J	293	SER	2.2
1	L	208	PRO	2.2
1	G	360	ALA	2.2
1	F	325	LEU	2.2
1	H	231	LEU	2.2
1	G	235	VAL	2.2
1	J	274	ILE	2.1
1	I	305	VAL	2.1
1	J	224	VAL	2.1
1	E	253	ALA	2.1
1	H	208	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	325	LEU	2.1
1	I	278	CYS	2.1
1	G	237	GLY	2.1
1	H	307	ASP	2.1
1	K	233	GLY	2.1
1	H	226	PRO	2.1
1	L	304	PRO	2.1
1	A	309	SER	2.0
1	G	305	VAL	2.0
1	G	336	GLN	2.0
1	F	288	PHE	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.