



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:44 AM GMT

PDB ID : 2VX2
Title : CRYSTAL STRUCTURE OF HUMAN ENOYL COENZYME A HYDRATASE DOMAIN-CONTAINING PROTEIN 3 (ECHDC3)
Authors : Yue, W.W.; Guo, K.; Kochan, G.; Pilka, E.; Murray, J.W.; Salah, E.; Cocking, R.; Sun, Z.; Roos, A.K.; Pike, A.C.W.; Filippakopoulos, P.; Arrowsmith, C.; Wikstrom, M.; Edwards, A.; Bountra, C.; Oppermann, U.
Deposited on : 2008-06-30
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

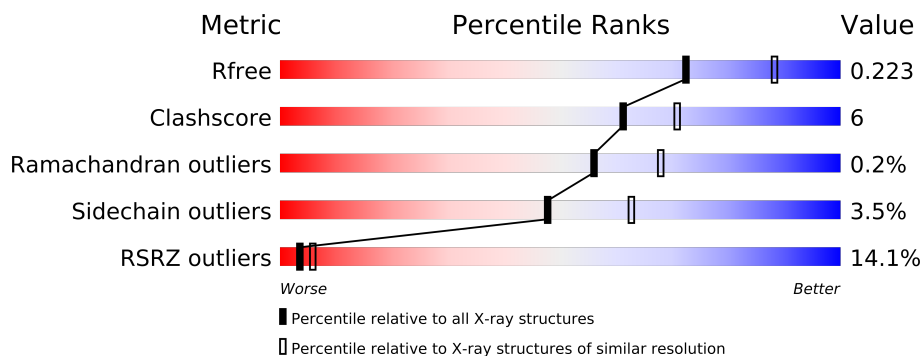
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	287	
1	B	287	
1	C	287	
1	D	287	
1	E	287	
1	F	287	
1	G	287	
1	H	287	
1	I	287	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17539 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	2	0
			1951	1228	345	367	11			
1	B	255	Total	C	N	O	S	0	1	0
			1904	1200	329	364	11			
1	C	256	Total	C	N	O	S	0	0	0
			1932	1215	341	365	11			
1	D	256	Total	C	N	O	S	0	1	0
			1936	1217	343	365	11			
1	E	255	Total	C	N	O	S	0	0	0
			1901	1199	329	362	11			
1	F	254	Total	C	N	O	S	0	0	0
			1879	1184	326	358	11			
1	G	253	Total	C	N	O	S	0	1	0
			1795	1129	313	342	11			
1	H	254	Total	C	N	O	S	0	1	0
			1850	1165	324	350	11			
1	I	254	Total	C	N	O	S	0	0	0
			1818	1144	315	348	11			

There are 225 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	EXPRESSION TAG	UNP Q96DC8
A	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	21	SER	-	EXPRESSION TAG	UNP Q96DC8
A	22	SER	-	EXPRESSION TAG	UNP Q96DC8
A	23	GLY	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
A	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
A	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
A	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
A	28	THR	-	EXPRESSION TAG	UNP Q96DC8
A	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
A	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
A	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
A	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
A	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
A	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
A	35	SER	-	EXPRESSION TAG	UNP Q96DC8
A	36	MET	-	EXPRESSION TAG	UNP Q96DC8
A	69	THR	ALA	CONFLICT	UNP Q96DC8
A	151	THR	ALA	CONFLICT	UNP Q96DC8
B	14	MET	-	EXPRESSION TAG	UNP Q96DC8
B	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	21	SER	-	EXPRESSION TAG	UNP Q96DC8
B	22	SER	-	EXPRESSION TAG	UNP Q96DC8
B	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
B	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
B	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
B	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
B	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
B	28	THR	-	EXPRESSION TAG	UNP Q96DC8
B	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
B	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
B	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
B	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
B	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
B	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
B	35	SER	-	EXPRESSION TAG	UNP Q96DC8
B	36	MET	-	EXPRESSION TAG	UNP Q96DC8
B	69	THR	ALA	CONFLICT	UNP Q96DC8
B	151	THR	ALA	CONFLICT	UNP Q96DC8
C	14	MET	-	EXPRESSION TAG	UNP Q96DC8
C	15	HIS	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	21	SER	-	EXPRESSION TAG	UNP Q96DC8
C	22	SER	-	EXPRESSION TAG	UNP Q96DC8
C	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
C	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
C	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
C	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
C	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
C	28	THR	-	EXPRESSION TAG	UNP Q96DC8
C	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
C	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
C	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
C	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
C	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
C	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
C	35	SER	-	EXPRESSION TAG	UNP Q96DC8
C	36	MET	-	EXPRESSION TAG	UNP Q96DC8
C	69	THR	ALA	CONFLICT	UNP Q96DC8
C	151	THR	ALA	CONFLICT	UNP Q96DC8
D	14	MET	-	EXPRESSION TAG	UNP Q96DC8
D	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	21	SER	-	EXPRESSION TAG	UNP Q96DC8
D	22	SER	-	EXPRESSION TAG	UNP Q96DC8
D	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
D	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
D	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
D	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
D	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
D	28	THR	-	EXPRESSION TAG	UNP Q96DC8
D	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
D	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
D	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
D	32	TYR	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
D	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
D	35	SER	-	EXPRESSION TAG	UNP Q96DC8
D	36	MET	-	EXPRESSION TAG	UNP Q96DC8
D	69	THR	ALA	CONFLICT	UNP Q96DC8
D	151	THR	ALA	CONFLICT	UNP Q96DC8
E	14	MET	-	EXPRESSION TAG	UNP Q96DC8
E	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	21	SER	-	EXPRESSION TAG	UNP Q96DC8
E	22	SER	-	EXPRESSION TAG	UNP Q96DC8
E	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
E	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
E	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
E	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
E	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
E	28	THR	-	EXPRESSION TAG	UNP Q96DC8
E	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
E	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
E	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
E	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
E	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
E	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
E	35	SER	-	EXPRESSION TAG	UNP Q96DC8
E	36	MET	-	EXPRESSION TAG	UNP Q96DC8
E	69	THR	ALA	CONFLICT	UNP Q96DC8
E	151	THR	ALA	CONFLICT	UNP Q96DC8
F	14	MET	-	EXPRESSION TAG	UNP Q96DC8
F	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	21	SER	-	EXPRESSION TAG	UNP Q96DC8
F	22	SER	-	EXPRESSION TAG	UNP Q96DC8
F	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
F	24	VAL	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
F	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
F	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
F	28	THR	-	EXPRESSION TAG	UNP Q96DC8
F	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
F	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
F	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
F	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
F	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
F	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
F	35	SER	-	EXPRESSION TAG	UNP Q96DC8
F	36	MET	-	EXPRESSION TAG	UNP Q96DC8
F	69	THR	ALA	CONFLICT	UNP Q96DC8
F	151	THR	ALA	CONFLICT	UNP Q96DC8
G	14	MET	-	EXPRESSION TAG	UNP Q96DC8
G	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	21	SER	-	EXPRESSION TAG	UNP Q96DC8
G	22	SER	-	EXPRESSION TAG	UNP Q96DC8
G	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
G	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
G	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
G	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
G	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
G	28	THR	-	EXPRESSION TAG	UNP Q96DC8
G	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
G	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
G	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
G	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
G	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
G	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
G	35	SER	-	EXPRESSION TAG	UNP Q96DC8
G	36	MET	-	EXPRESSION TAG	UNP Q96DC8
G	69	THR	ALA	CONFLICT	UNP Q96DC8
G	151	THR	ALA	CONFLICT	UNP Q96DC8
H	14	MET	-	EXPRESSION TAG	UNP Q96DC8
H	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	16	HIS	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	21	SER	-	EXPRESSION TAG	UNP Q96DC8
H	22	SER	-	EXPRESSION TAG	UNP Q96DC8
H	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
H	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
H	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
H	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
H	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
H	28	THR	-	EXPRESSION TAG	UNP Q96DC8
H	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
H	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
H	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
H	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
H	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
H	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
H	35	SER	-	EXPRESSION TAG	UNP Q96DC8
H	36	MET	-	EXPRESSION TAG	UNP Q96DC8
H	69	THR	ALA	CONFLICT	UNP Q96DC8
H	151	THR	ALA	CONFLICT	UNP Q96DC8
I	14	MET	-	EXPRESSION TAG	UNP Q96DC8
I	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	21	SER	-	EXPRESSION TAG	UNP Q96DC8
I	22	SER	-	EXPRESSION TAG	UNP Q96DC8
I	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
I	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
I	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
I	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
I	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
I	28	THR	-	EXPRESSION TAG	UNP Q96DC8
I	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
I	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
I	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
I	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
I	33	PHE	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
I	35	SER	-	EXPRESSION TAG	UNP Q96DC8
I	36	MET	-	EXPRESSION TAG	UNP Q96DC8
I	69	THR	ALA	CONFLICT	UNP Q96DC8
I	151	THR	ALA	CONFLICT	UNP Q96DC8

- Molecule 2 is water.

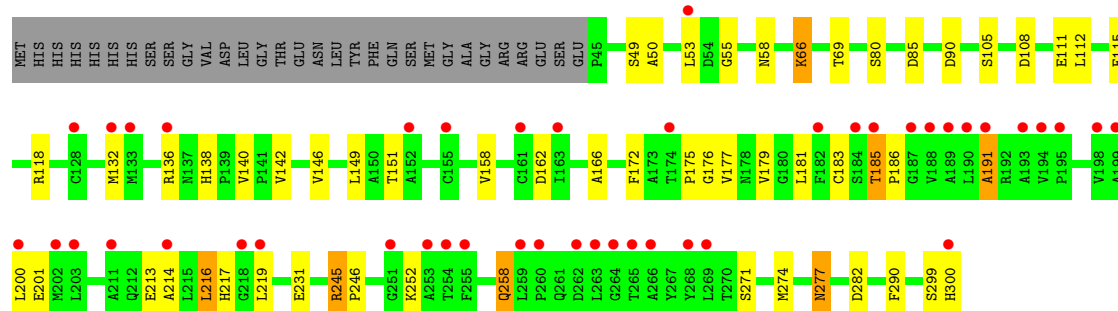
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	148	Total O 148 148	0	0
2	B	61	Total O 61 61	0	0
2	C	124	Total O 124 124	0	0
2	D	80	Total O 80 80	0	0
2	E	67	Total O 67 67	0	0
2	F	55	Total O 55 55	0	0
2	G	13	Total O 13 13	0	0
2	H	13	Total O 13 13	0	0
2	I	12	Total O 12 12	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

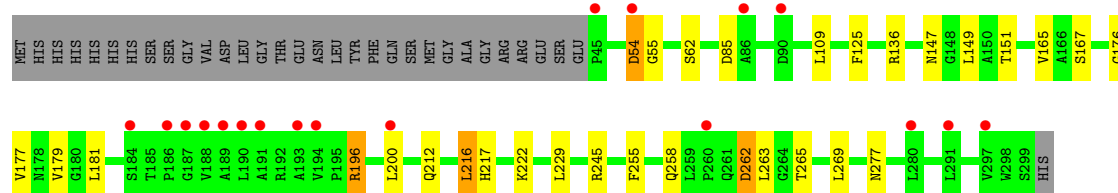
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain A: 



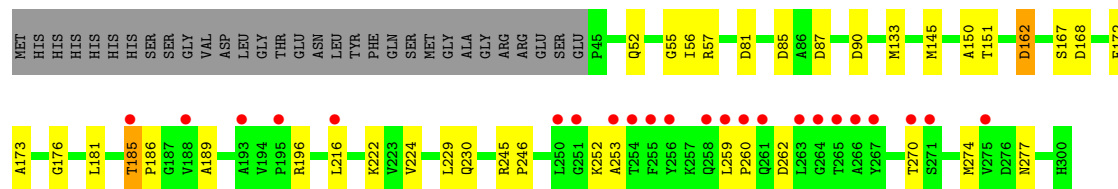
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain B: 



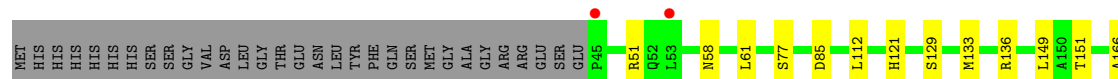
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

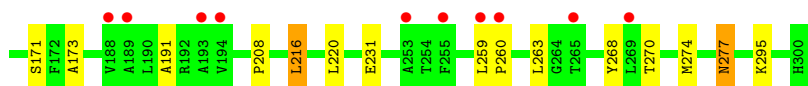
Chain C: 



• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

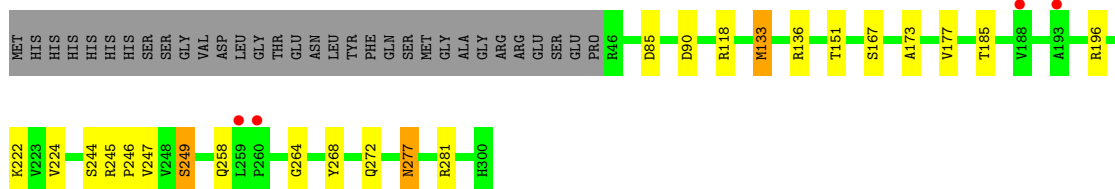
Chain D: 





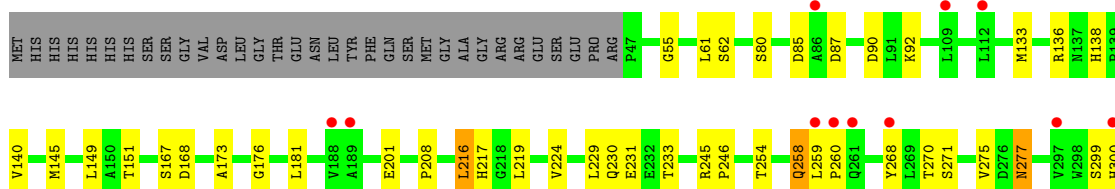
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain E:



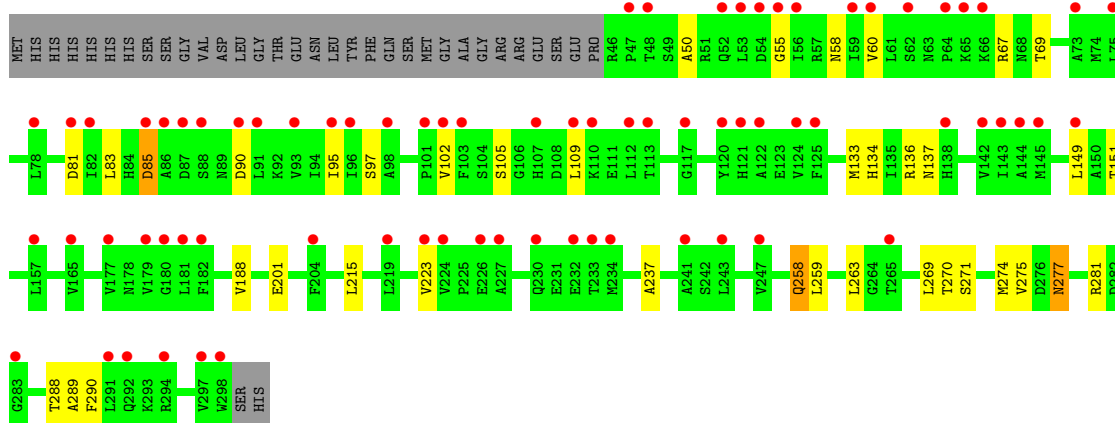
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain F:



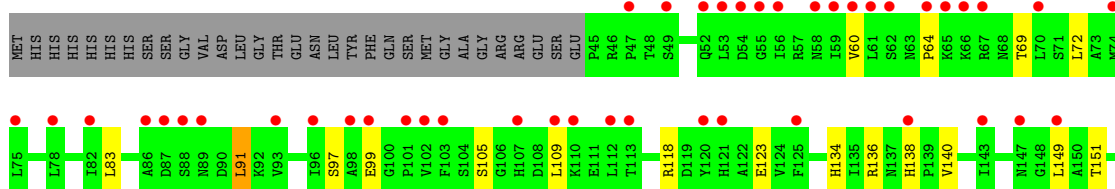
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

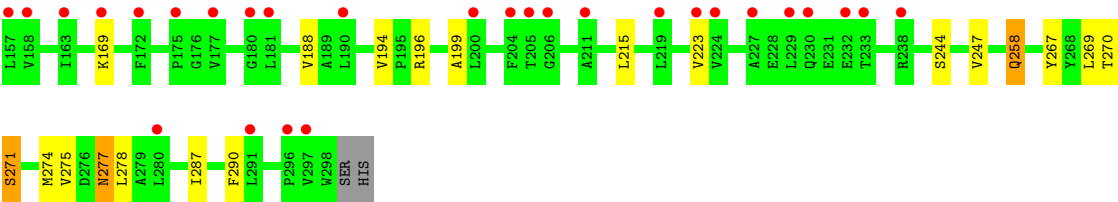
Chain G:



• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

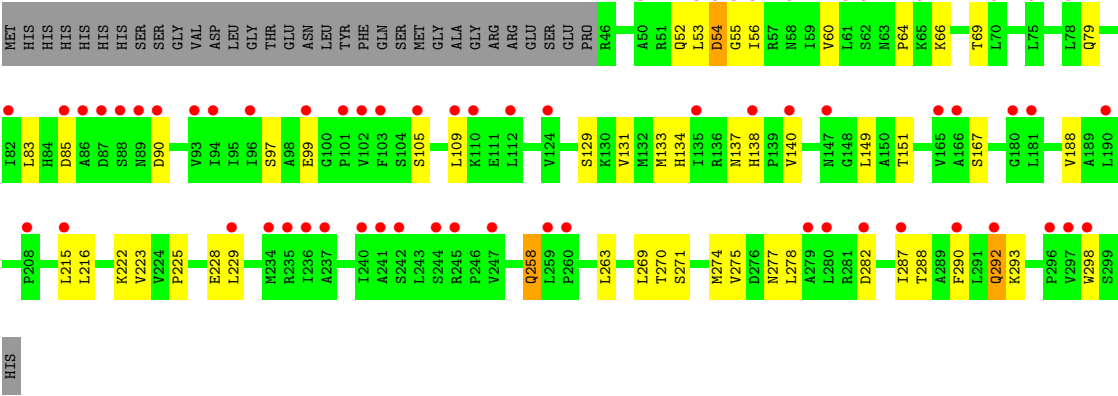
Chain H:





● Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.76Å 135.30Å 83.87Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	117.04 – 2.30 52.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (117.04-2.30) 99.4 (52.41-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.170 , 0.220 0.176 , 0.223	Depositor DCC
R_{free} test set	5767 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 8.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 114561 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17539	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	1.31	11/1985 (0.6%)	1.07	8/2688 (0.3%)
1	B	0.90	0/1939	0.86	2/2634 (0.1%)
1	C	1.09	3/1964 (0.2%)	0.97	5/2664 (0.2%)
1	D	0.93	1/1971 (0.1%)	0.85	1/2674 (0.0%)
1	E	0.89	0/1933	0.86	3/2626 (0.1%)
1	F	0.84	1/1911 (0.1%)	0.82	1/2599 (0.0%)
1	G	0.62	0/1828	0.61	0/2499
1	H	0.65	0/1884	0.63	1/2566 (0.0%)
1	I	0.62	0/1849	0.62	0/2523
All	All	0.90	16/17264 (0.1%)	0.83	21/23473 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ALA	CA-CB	8.88	1.71	1.52
1	A	158	VAL	CB-CG1	-7.10	1.38	1.52
1	D	231	GLU	CG-CD	6.87	1.62	1.51
1	A	179	VAL	CB-CG1	6.82	1.67	1.52
1	A	115	GLU	CD-OE1	6.49	1.32	1.25
1	A	231	GLU	CG-CD	5.88	1.60	1.51
1	A	115	GLU	CG-CD	5.86	1.60	1.51
1	C	253	ALA	CA-CB	5.62	1.64	1.52
1	A	172	PHE	CE2-CZ	-5.50	1.26	1.37
1	C	162	ASP	CB-CG	5.49	1.63	1.51
1	A	213	GLU	CG-CD	5.46	1.60	1.51
1	A	258	GLN	CG-CD	-5.35	1.38	1.51
1	A	142	VAL	CB-CG2	5.31	1.64	1.52
1	C	189	ALA	CA-CB	5.22	1.63	1.52
1	F	231	GLU	CG-CD	5.19	1.59	1.51
1	A	115	GLU	CD-OE2	5.09	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	118	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	245	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	53	LEU	CB-CG-CD2	-6.36	100.18	111.00
1	A	274	MET	CG-SD-CE	6.06	109.89	100.20
1	A	282	ASP	CB-CG-OD1	6.03	123.73	118.30
1	C	262	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	168	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	87	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	90	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	H	91	LEU	CB-CG-CD2	5.44	120.25	111.00
1	A	245	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	57	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	E	196	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	196	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	118	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	F	168	ASP	CB-CG-OD1	5.27	123.04	118.30
1	D	136	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	200	LEU	CB-CG-CD2	5.12	119.71	111.00
1	A	108	ASP	CB-CG-OD1	5.11	122.89	118.30
1	C	81	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1951	0	1997	30	0
1	B	1904	0	1918	25	0
1	C	1932	0	1961	26	0
1	D	1936	0	1963	15	0
1	E	1901	0	1905	13	0
1	F	1879	0	1873	34	0
1	G	1795	0	1715	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1850	0	1815	22	0
1	I	1818	0	1750	29	0
2	A	148	0	0	1	0
2	B	61	0	0	1	0
2	C	124	0	0	0	0
2	D	80	0	0	0	0
2	E	67	0	0	0	0
2	F	55	0	0	1	0
2	G	13	0	0	3	0
2	H	13	0	0	0	0
2	I	12	0	0	1	0
All	All	17539	0	16897	196	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (196) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69[A]:THR:HG22	1:A:105:SER:OG	1.57	1.03
1:A:111:GLU:CA	1:A:112:LEU:N	2.22	1.02
1:A:111:GLU:O	1:A:112:LEU:N	1.97	0.98
1:A:111:GLU:O	1:A:111:GLU:CA	2.22	0.88
1:C:185:THR:OG1	1:C:186:PRO:HD3	1.76	0.84
1:C:216:LEU:O	1:C:216:LEU:HD23	1.81	0.81
1:F:151:THR:HG22	1:F:173:ALA:HB3	1.61	0.81
1:G:83:LEU:HD21	1:G:134:HIS:CD2	2.16	0.80
1:H:83:LEU:HD21	1:H:134:HIS:CD2	2.17	0.79
1:A:214:ALA:HB1	1:A:219:LEU:HB3	1.64	0.78
1:A:69[A]:THR:CG2	1:A:105:SER:OG	2.34	0.76
1:B:216:LEU:HD22	1:B:217:HIS:CE1	2.20	0.76
1:D:263:LEU:HD23	1:E:133:MET:HE3	1.69	0.75
1:B:149:LEU:HG	1:B:151:THR:HG23	1.70	0.73
1:I:64:PRO:HG3	1:I:99:GLU:HB3	1.75	0.69
1:I:83:LEU:HD21	1:I:134:HIS:CD2	2.28	0.69
1:A:69[A]:THR:HG22	1:A:105:SER:HG	1.57	0.67
1:D:263:LEU:HD23	1:E:133:MET:CE	2.25	0.66
1:A:185:THR:OG1	1:A:186:PRO:HD3	1.95	0.65
1:B:216:LEU:O	1:B:216:LEU:HD23	1.97	0.65
1:I:53:LEU:O	1:I:54:ASP:HB2	1.97	0.64
1:C:185:THR:OG1	1:C:186:PRO:CD	2.44	0.63
1:B:216:LEU:C	1:B:216:LEU:HD23	2.18	0.63
1:E:268:TYR:CZ	1:E:272:GLN:OE1	2.51	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:151:THR:HG22	1:E:173:ALA:HB3	1.80	0.63
1:A:149:LEU:HG	1:A:151:THR:HG23	1.81	0.62
1:G:188:VAL:HG22	1:I:258:GLN:HG3	1.81	0.62
1:A:271:SER:HB2	1:B:125:PHE:HB3	1.81	0.60
1:C:216:LEU:C	1:C:216:LEU:HD23	2.22	0.60
1:D:191:ALA:HB1	1:F:259:LEU:CD1	2.32	0.60
1:F:145:MET:CE	1:F:230:GLN:HA	2.32	0.60
1:I:69:THR:HG22	1:I:105:SER:OG	2.01	0.59
1:B:263:LEU:HD23	1:C:133:MET:SD	2.42	0.59
1:H:271:SER:O	1:H:275:VAL:HG23	2.01	0.59
1:G:281:ARG:CB	2:G:2013:HOH:O	2.50	0.59
1:D:149:LEU:HD11	1:D:151:THR:CG2	2.31	0.59
1:C:176:GLY:HA3	1:C:181:LEU:O	2.03	0.58
1:H:69:THR:HG22	1:H:105:SER:OG	2.03	0.58
1:B:147:ASN:HA	1:B:167:SER:OG	2.03	0.58
1:F:145:MET:HE1	1:F:230:GLN:HA	1.86	0.56
1:F:216:LEU:HD13	1:F:217:HIS:CE1	2.40	0.56
1:F:149:LEU:HD11	1:F:151:THR:HG23	1.86	0.56
1:A:136[B]:ARG:NH2	2:A:2058:HOH:O	2.39	0.55
1:B:167:SER:HB3	1:B:229:LEU:HD22	1.87	0.55
1:G:271:SER:O	1:G:275:VAL:HG23	2.07	0.55
1:G:69:THR:HG22	1:G:105:SER:OG	2.06	0.55
1:F:92:LYS:HE3	1:F:300:HIS:CE1	2.42	0.55
1:G:136:ARG:NH1	1:I:263:LEU:HD22	2.21	0.55
1:I:271:SER:O	1:I:275:VAL:HG23	2.07	0.54
1:I:149:LEU:HG	1:I:151:THR:HG23	1.90	0.54
1:G:201:GLU:OE2	1:I:222:LYS:NZ	2.40	0.53
1:F:55:GLY:HA2	1:F:90:ASP:O	2.08	0.53
1:G:270:THR:O	1:G:274:MET:HG2	2.08	0.53
1:C:259:LEU:HB3	1:C:260:PRO:HD3	1.91	0.52
1:F:136:ARG:NH2	2:F:2014:HOH:O	2.43	0.52
1:F:271:SER:O	1:F:275:VAL:HG23	2.10	0.52
1:H:60:VAL:HG22	1:H:97:SER:OG	2.09	0.52
1:F:268:TYR:C	1:F:268:TYR:CD2	2.83	0.51
1:D:216:LEU:HD11	1:F:216:LEU:HD23	1.93	0.51
1:D:268:TYR:C	1:D:268:TYR:CD2	2.83	0.51
1:A:185:THR:CB	1:A:186:PRO:HD3	2.40	0.51
1:C:145:MET:CE	1:C:229:LEU:HG	2.41	0.51
1:F:216:LEU:HD22	1:F:216:LEU:O	2.11	0.51
1:I:60:VAL:HG22	1:I:97:SER:OG	2.10	0.51
1:G:263:LEU:HD22	1:H:136:ARG:NH1	2.26	0.51
1:G:83:LEU:HD21	1:G:134:HIS:HD2	1.73	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:GLY:HA3	1:A:181:LEU:O	2.11	0.50
1:A:245:ARG:HB3	1:A:246:PRO:HD3	1.93	0.50
1:G:149:LEU:HG	1:G:151:THR:HG23	1.93	0.50
1:G:215:LEU:HD22	1:G:223:VAL:HB	1.93	0.50
1:H:149:LEU:HG	1:H:151:THR:HG23	1.94	0.49
1:A:149:LEU:HG	1:A:151:THR:CG2	2.41	0.49
1:F:138:HIS:ND1	1:F:140:VAL:HG22	2.27	0.49
1:G:81:ASP:OD1	2:G:2001:HOH:O	2.18	0.49
1:E:277:ASN:C	1:E:277:ASN:HD22	2.15	0.49
1:F:259:LEU:HB3	1:F:260:PRO:HD3	1.94	0.49
1:B:255:PHE:O	1:B:258:GLN:HG3	2.13	0.49
1:A:191:ALA:HB1	1:C:259:LEU:CD1	2.42	0.49
1:I:79:GLN:HB2	1:I:131:VAL:HG22	1.94	0.49
1:I:215:LEU:HD22	1:I:223:VAL:HB	1.94	0.48
1:H:194:VAL:HG23	1:H:199:ALA:HB2	1.94	0.48
1:D:277:ASN:C	1:D:277:ASN:HD22	2.17	0.48
1:I:225:PRO:HD2	1:I:228:GLU:OE1	2.13	0.48
1:A:290:PHE:CD2	1:B:109:LEU:HD12	2.49	0.48
1:G:50:ALA:HA	1:G:58:ASN:O	2.14	0.48
1:A:136[B]:ARG:HH12	1:B:196:ARG:HH12	1.61	0.47
1:H:258:GLN:HG3	1:I:188:VAL:HG22	1.96	0.47
1:B:262:ASP:OD2	1:B:265:THR:OG1	2.30	0.47
1:D:270:THR:O	1:D:274:MET:HG2	2.14	0.47
1:E:264:GLY:HA2	1:F:133:MET:CE	2.44	0.47
1:A:111:GLU:N	1:A:112:LEU:N	2.61	0.47
1:F:149:LEU:CD1	1:F:151:THR:HG23	2.45	0.47
1:C:270:THR:O	1:C:274:MET:HG2	2.15	0.47
1:A:55:GLY:HA2	1:A:90:ASP:O	2.15	0.47
1:F:254:THR:HG22	1:F:270:THR:HG22	1.97	0.47
1:D:166:ALA:HB3	1:D:220:LEU:HD13	1.97	0.47
1:H:277:ASN:C	1:H:277:ASN:HD22	2.18	0.46
1:A:146:VAL:O	1:A:166:ALA:HA	2.15	0.46
1:C:151:THR:HG22	1:C:173:ALA:HB3	1.97	0.46
1:I:66:LYS:O	1:I:69:THR:HG23	2.16	0.46
1:D:149:LEU:HD11	1:D:151:THR:HG22	1.96	0.46
1:I:52:GLN:HA	1:I:56:ILE:O	2.15	0.46
1:G:258:GLN:HG3	1:H:188:VAL:HG22	1.96	0.46
1:F:277:ASN:HD22	1:F:277:ASN:C	2.19	0.46
1:H:278:LEU:CD2	1:H:287:ILE:HD11	2.46	0.46
1:B:179:VAL:HG23	1:B:179:VAL:O	2.16	0.46
1:H:215:LEU:HD22	1:H:223:VAL:HB	1.96	0.46
1:F:259:LEU:HB3	1:F:260:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:167:SER:HA	1:F:224:VAL:O	2.16	0.46
1:B:216:LEU:C	1:B:216:LEU:CD2	2.84	0.46
1:C:55:GLY:HA2	1:C:90:ASP:O	2.15	0.46
1:C:245:ARG:HB3	1:C:246:PRO:HD3	1.98	0.46
1:D:259:LEU:HB3	1:D:260:PRO:HD3	1.97	0.46
1:F:176:GLY:HA3	1:F:181:LEU:O	2.17	0.46
1:A:216:LEU:HD23	1:A:217:HIS:CE1	2.51	0.45
1:F:254:THR:CG2	1:F:270:THR:HG22	2.46	0.45
1:H:72:LEU:HD21	1:H:123:GLU:OE2	2.15	0.45
1:G:290:PHE:CD2	1:H:109:LEU:HD12	2.51	0.45
1:C:216:LEU:C	1:C:216:LEU:CD2	2.85	0.45
1:G:95:ILE:HD11	1:G:237:ALA:HB2	1.98	0.45
1:C:185:THR:HG1	1:C:186:PRO:HD3	1.81	0.45
1:G:109:LEU:HD12	1:I:290:PHE:CD2	2.52	0.45
1:E:245:ARG:HB3	1:E:246:PRO:HD3	1.98	0.45
1:H:244:SER:OG	1:H:247:VAL:HG23	2.16	0.45
1:A:219:LEU:O	1:A:219:LEU:HD12	2.17	0.45
1:C:145:MET:CE	1:C:230:GLN:HA	2.47	0.45
1:F:258:GLN:HG2	1:F:259:LEU:N	2.31	0.45
1:I:278:LEU:CD2	1:I:287:ILE:HD11	2.47	0.45
1:B:165:VAL:HG13	1:B:222:LYS:HB2	1.99	0.45
1:F:145:MET:HE2	1:F:233:THR:OG1	2.17	0.44
1:C:176:GLY:CA	1:C:181:LEU:O	2.65	0.44
1:H:138:HIS:CE1	1:H:140:VAL:HG22	2.52	0.44
1:D:149:LEU:HG	1:D:151:THR:HG23	1.98	0.44
1:B:216:LEU:HD22	1:B:217:HIS:ND1	2.31	0.44
1:B:54:ASP:N	1:B:54:ASP:OD1	2.48	0.44
1:A:138:HIS:ND1	1:A:140:VAL:HG22	2.33	0.44
1:B:212:GLN:HG3	2:B:2043:HOH:O	2.17	0.44
1:G:275:VAL:HG12	1:H:118:ARG:NH2	2.32	0.44
1:G:67:ARG:HD2	1:G:102:VAL:HG21	1.99	0.44
1:A:277:ASN:HD22	1:A:277:ASN:C	2.20	0.44
1:H:267:TYR:O	1:H:271:SER:OG	2.32	0.44
1:A:191:ALA:HB1	1:C:259:LEU:HD11	1.99	0.44
1:A:201:GLU:OE2	1:C:222:LYS:HE2	2.18	0.44
1:I:129:SER:O	1:I:133:MET:HG2	2.18	0.43
1:A:66:LYS:O	1:A:69[A]:THR:HG23	2.18	0.43
1:F:145:MET:HE2	1:F:229:LEU:HG	1.99	0.43
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.89	0.43
1:C:167:SER:HA	1:C:224:VAL:O	2.18	0.43
1:E:264:GLY:HA2	1:F:133:MET:HE1	1.99	0.43
1:H:270:THR:O	1:H:274:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:95:ILE:HD11	1:G:237:ALA:CB	2.49	0.43
1:G:277:ASN:HD22	1:G:277:ASN:C	2.22	0.43
1:C:176:GLY:C	1:C:181:LEU:O	2.57	0.43
1:C:150:ALA:O	1:C:172:PHE:HA	2.19	0.43
1:E:245:ARG:O	1:E:249:SER:HB2	2.18	0.43
1:A:50:ALA:HA	1:A:58:ASN:O	2.19	0.43
1:I:270:THR:O	1:I:274:MET:HG2	2.19	0.43
1:B:176:GLY:HA3	1:B:181:LEU:O	2.19	0.43
1:F:92:LYS:CE	1:F:300:HIS:CE1	3.02	0.42
1:E:167:SER:HA	1:E:224:VAL:O	2.19	0.42
1:I:288:THR:HG22	1:I:292:GLN:OE1	2.19	0.42
1:F:245:ARG:HB3	1:F:246:PRO:HD3	2.01	0.42
1:A:162:ASP:OD1	1:A:252:LYS:NZ	2.37	0.42
1:E:281:ARG:HB2	1:E:281:ARG:HE	1.63	0.42
1:G:50:ALA:HB3	2:G:2001:HOH:O	2.18	0.42
1:F:219:LEU:O	1:F:219:LEU:HD12	2.20	0.42
1:I:138:HIS:CE1	1:I:140:VAL:HG22	2.55	0.42
1:I:282:ASP:O	1:I:298:TRP:HZ3	2.01	0.42
1:C:52:GLN:HA	1:C:56:ILE:O	2.20	0.42
1:E:244:SER:OG	1:E:247:VAL:HG23	2.20	0.42
1:G:259:LEU:HD21	1:H:196:ARG:NE	2.34	0.42
1:C:162:ASP:OD1	1:C:252:LYS:NZ	2.45	0.42
1:F:173:ALA:HB2	1:F:208:PRO:HB3	2.02	0.42
1:I:167:SER:HB3	1:I:229:LEU:HD22	2.02	0.42
1:D:129:SER:O	1:D:133:MET:HG2	2.20	0.42
1:B:216:LEU:CD2	1:B:217:HIS:CE1	2.96	0.42
1:G:60:VAL:HG22	1:G:97:SER:OG	2.20	0.41
1:E:222:LYS:HE2	1:F:201:GLU:OE1	2.20	0.41
1:B:149:LEU:HD11	1:B:151:THR:HG22	2.02	0.41
1:B:136:ARG:HH12	1:C:196:ARG:HH12	1.69	0.41
1:D:112:LEU:HA	1:D:121:HIS:CD2	2.55	0.41
1:G:55:GLY:HA2	1:G:90:ASP:O	2.20	0.41
1:H:64:PRO:HG3	1:H:99:GLU:HB3	2.02	0.41
1:C:145:MET:HE3	1:C:230:GLN:HA	2.02	0.41
1:D:173:ALA:HB2	1:D:208:PRO:HB3	2.02	0.41
1:I:66:LYS:CB	2:I:2002:HOH:O	2.69	0.41
1:G:133:MET:O	1:G:137:ASN:ND2	2.52	0.41
1:B:149:LEU:CG	1:B:151:THR:HG23	2.46	0.41
1:I:133:MET:O	1:I:137:ASN:ND2	2.53	0.41
1:I:55:GLY:HA2	1:I:90:ASP:O	2.21	0.41
1:F:299:SER:O	1:F:300:HIS:HB2	2.21	0.40
1:H:290:PHE:CD2	1:I:109:LEU:HD12	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:138:HIS:CE1	1:F:140:VAL:HG22	2.56	0.40
1:I:216:LEU:HD12	1:I:216:LEU:HA	1.96	0.40
1:G:288:THR:HG22	1:G:289:ALA:N	2.36	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	254/287 (88%)	246 (97%)	7 (3%)	1 (0%)	43	52
1	B	254/287 (88%)	248 (98%)	6 (2%)	0	100	100
1	C	254/287 (88%)	245 (96%)	9 (4%)	0	100	100
1	D	255/287 (89%)	248 (97%)	7 (3%)	0	100	100
1	E	253/287 (88%)	248 (98%)	5 (2%)	0	100	100
1	F	252/287 (88%)	244 (97%)	8 (3%)	0	100	100
1	G	252/287 (88%)	239 (95%)	12 (5%)	1 (0%)	43	52
1	H	253/287 (88%)	243 (96%)	10 (4%)	0	100	100
1	I	252/287 (88%)	240 (95%)	9 (4%)	3 (1%)	19	19
All	All	2279/2583 (88%)	2201 (97%)	73 (3%)	5 (0%)	56	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	85	ASP
1	I	54	ASP
1	I	293	LYS
1	A	183	CYS
1	I	85	ASP

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	214/240 (89%)	201 (94%)	13 (6%)	26	34
1	B	206/240 (86%)	198 (96%)	8 (4%)	43	57
1	C	210/240 (88%)	207 (99%)	3 (1%)	78	90
1	D	210/240 (88%)	200 (95%)	10 (5%)	35	46
1	E	203/240 (85%)	195 (96%)	8 (4%)	43	57
1	F	200/240 (83%)	192 (96%)	8 (4%)	42	56
1	G	178/240 (74%)	174 (98%)	4 (2%)	64	81
1	H	190/240 (79%)	184 (97%)	6 (3%)	51	67
1	I	183/240 (76%)	179 (98%)	4 (2%)	64	81
All	All	1794/2160 (83%)	1730 (96%)	64 (4%)	48	61

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	66	LYS
1	A	80	SER
1	A	85	ASP
1	A	132	MET
1	A	175	PRO
1	A	177	VAL
1	A	185	THR
1	A	216	LEU
1	A	258	GLN
1	A	277	ASN
1	A	299	SER
1	A	300	HIS
1	B	54	ASP
1	B	62	SER
1	B	85	ASP
1	B	177	VAL
1	B	216	LEU
1	B	262	ASP

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Mol	Chain	Res	Type
1	B	269	LEU
1	B	277	ASN
1	C	85	ASP
1	C	185	THR
1	C	277	ASN
1	D	51[A]	ARG
1	D	51[B]	ARG
1	D	58	ASN
1	D	61	LEU
1	D	77	SER
1	D	85	ASP
1	D	171	SER
1	D	216	LEU
1	D	277	ASN
1	D	295	LYS
1	E	85	ASP
1	E	133	MET
1	E	136	ARG
1	E	177	VAL
1	E	185	THR
1	E	249	SER
1	E	258	GLN
1	E	277	ASN
1	F	61	LEU
1	F	62	SER
1	F	80	SER
1	F	85	ASP
1	F	87	ASP
1	F	216	LEU
1	F	258	GLN
1	F	277	ASN
1	G	85	ASP
1	G	258	GLN
1	G	269	LEU
1	G	277	ASN
1	H	91	LEU
1	H	169	LYS
1	H	258	GLN
1	H	269	LEU
1	H	271	SER
1	H	277	ASN
1	I	258	GLN

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Mol	Chain	Res	Type
1	I	269	LEU
1	I	277	ASN
1	I	292	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	63	ASN
1	C	261	GLN
1	I	134	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/287 (89%)	0.99	44 (17%) 2 4	11, 18, 25, 40	0
1	B	255/287 (88%)	0.71	18 (7%) 16 23	12, 18, 25, 56	0
1	C	256/287 (89%)	0.73	23 (8%) 10 16	10, 17, 26, 39	0
1	D	256/287 (89%)	0.55	12 (4%) 30 40	12, 18, 26, 41	0
1	E	255/287 (88%)	0.47	4 (1%) 68 77	13, 18, 26, 37	0
1	F	254/287 (88%)	0.57	11 (4%) 34 44	12, 18, 25, 39	1 (0%)
1	G	253/287 (88%)	1.47	75 (29%) 1 1	21, 25, 50, 74	1 (0%)
1	H	254/287 (88%)	1.36	72 (28%) 1 1	21, 25, 31, 51	0
1	I	254/287 (88%)	1.23	64 (25%) 1 2	21, 25, 61, 71	0
All	All	2293/2583 (88%)	0.89	323 (14%) 3 6	10, 20, 28, 74	2 (0%)

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	112	LEU	7.7
1	I	297	VAL	6.9
1	H	109	LEU	5.6
1	G	53	LEU	5.5
1	H	102	VAL	5.2
1	H	78	LEU	5.1
1	G	96	ILE	5.1
1	I	287	ILE	5.0
1	H	103	PHE	5.0
1	H	54	ASP	4.9
1	I	78	LEU	4.9
1	G	62	SER	4.8
1	I	240	ILE	4.8
1	I	53	LEU	4.6
1	I	237	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	86	ALA	4.6
1	H	112	LEU	4.6
1	I	75	LEU	4.5
1	I	56	ILE	4.5
1	G	88	SER	4.5
1	G	223	VAL	4.5
1	G	56	ILE	4.4
1	G	93	VAL	4.4
1	I	62	SER	4.3
1	H	149	LEU	4.2
1	G	297	VAL	4.2
1	H	229	LEU	4.1
1	G	291	LEU	4.1
1	I	86	ALA	4.1
1	G	86	ALA	4.1
1	B	45	PRO	4.0
1	G	233	THR	3.9
1	I	109	LEU	3.9
1	H	291	LEU	3.9
1	I	296	PRO	3.9
1	H	55	GLY	3.9
1	G	165	VAL	3.8
1	H	56	ILE	3.8
1	H	143	ILE	3.8
1	G	85	ASP	3.8
1	H	204	PHE	3.8
1	H	86	ALA	3.8
1	G	102	VAL	3.8
1	H	224	VAL	3.7
1	H	59	ILE	3.7
1	G	109	LEU	3.6
1	G	117	GLY	3.6
1	I	55	GLY	3.5
1	I	112	LEU	3.5
1	G	101	PRO	3.5
1	H	47	PRO	3.5
1	H	110	LYS	3.5
1	A	188	VAL	3.5
1	B	280	LEU	3.5
1	I	82	ILE	3.5
1	G	78	LEU	3.4
1	H	158	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	3.4
1	G	241	ALA	3.4
1	G	73	ALA	3.4
1	H	96	ILE	3.4
1	C	263	LEU	3.4
1	I	229	LEU	3.4
1	G	66	LYS	3.3
1	B	188	VAL	3.3
1	I	140	VAL	3.3
1	I	50	ALA	3.3
1	G	181	LEU	3.3
1	G	145	MET	3.3
1	H	98	ALA	3.3
1	G	243	LEU	3.2
1	H	82	ILE	3.2
1	C	270	THR	3.2
1	G	48	THR	3.2
1	G	298	TRP	3.2
1	G	177	VAL	3.2
1	F	188	VAL	3.2
1	H	60	VAL	3.2
1	E	259	LEU	3.1
1	C	267	TYR	3.1
1	G	230	GLN	3.1
1	H	75	LEU	3.1
1	G	98	ALA	3.1
1	A	255	PHE	3.1
1	G	90	ASP	3.1
1	F	259	LEU	3.1
1	I	101	PRO	3.1
1	I	103	PHE	3.1
1	A	264	GLY	3.1
1	C	264	GLY	3.1
1	I	54	ASP	3.0
1	I	87	ASP	3.0
1	I	61	LEU	3.0
1	H	223	VAL	3.0
1	C	259	LEU	3.0
1	D	194	VAL	3.0
1	G	91	LEU	3.0
1	G	121	HIS	3.0
1	G	283	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	208	PRO	3.0
1	B	297	VAL	3.0
1	H	227	ALA	2.9
1	I	241	ALA	2.9
1	H	88	SER	2.9
1	G	149	LEU	2.9
1	H	157	LEU	2.9
1	H	65	LYS	2.9
1	D	53	LEU	2.9
1	G	143	ILE	2.9
1	I	279	ALA	2.9
1	G	82	ILE	2.9
1	B	260	PRO	2.9
1	H	66	LYS	2.9
1	I	234	MET	2.9
1	H	175	PRO	2.9
1	H	205	THR	2.9
1	I	105	SER	2.9
1	A	265	THR	2.8
1	H	238	ARG	2.8
1	G	75	LEU	2.8
1	I	260	PRO	2.8
1	A	185	THR	2.8
1	G	52	GLN	2.8
1	A	199	ALA	2.8
1	A	191	ALA	2.8
1	H	101	PRO	2.8
1	H	113	THR	2.8
1	A	155	CYS	2.8
1	E	260	PRO	2.8
1	H	280	LEU	2.8
1	C	254	THR	2.8
1	H	121	HIS	2.8
1	A	161	CYS	2.8
1	H	61	LEU	2.8
1	C	195	PRO	2.7
1	H	172	PHE	2.7
1	I	282	ASP	2.7
1	A	189	ALA	2.7
1	H	58	ASN	2.7
1	C	265	THR	2.7
1	G	81	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	135	ILE	2.7
1	B	191	ALA	2.7
1	I	235	ARG	2.7
1	I	110	LYS	2.7
1	H	70	LEU	2.7
1	C	255	PHE	2.7
1	H	125	PHE	2.7
1	A	214	ALA	2.7
1	I	124	VAL	2.7
1	I	247	VAL	2.7
1	A	253	ALA	2.7
1	H	147	ASN	2.7
1	F	300	HIS	2.7
1	A	198	VAL	2.7
1	D	188	VAL	2.7
1	G	125	PHE	2.7
1	G	182	PHE	2.7
1	D	265	THR	2.6
1	B	90[A]	ASP	2.6
1	G	292	GLN	2.6
1	A	190	LEU	2.6
1	I	96	ILE	2.6
1	C	266	ALA	2.6
1	A	194	VAL	2.6
1	G	110	LYS	2.6
1	B	189	ALA	2.6
1	H	177	VAL	2.6
1	G	95	ILE	2.6
1	A	218	GLY	2.6
1	G	87	ASP	2.6
1	H	233	THR	2.6
1	I	94	ILE	2.6
1	C	188	VAL	2.6
1	G	124	VAL	2.6
1	G	59	ILE	2.5
1	A	266	ALA	2.5
1	I	242	SER	2.5
1	B	190	LEU	2.5
1	I	236	ILE	2.5
1	H	62	SER	2.5
1	A	254	THR	2.5
1	A	203	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	219	LEU	2.5
1	H	99	GLU	2.5
1	I	90	ASP	2.5
1	B	194	VAL	2.5
1	A	193	ALA	2.5
1	D	193	ALA	2.5
1	C	261	GLN	2.5
1	G	54	ASP	2.5
1	G	120	TYR	2.5
1	C	260	PRO	2.5
1	A	300	HIS	2.5
1	A	195	PRO	2.5
1	D	259	LEU	2.5
1	G	247	VAL	2.5
1	C	271	SER	2.4
1	G	179	VAL	2.4
1	I	180	GLY	2.4
1	A	136[A]	ARG	2.4
1	B	193	ALA	2.4
1	H	296	PRO	2.4
1	I	290	PHE	2.4
1	I	88	SER	2.4
1	G	219	LEU	2.4
1	H	53	LEU	2.4
1	H	232	GLU	2.4
1	A	182	PHE	2.4
1	G	138	HIS	2.4
1	A	200	LEU	2.4
1	H	200	LEU	2.4
1	G	142	VAL	2.4
1	A	133	MET	2.4
1	G	234	MET	2.4
1	I	65	LYS	2.4
1	A	268	TYR	2.4
1	H	181	LEU	2.4
1	F	189	ALA	2.4
1	H	190	LEU	2.3
1	E	188	VAL	2.3
1	I	245	ARG	2.3
1	G	103	PHE	2.3
1	A	263	LEU	2.3
1	B	291	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	109	LEU	2.3
1	I	215	LEU	2.3
1	D	189	ALA	2.3
1	I	138	HIS	2.3
1	A	260	PRO	2.3
1	H	64	PRO	2.3
1	A	184	SER	2.3
1	H	163	ILE	2.3
1	I	70	LEU	2.3
1	I	259	LEU	2.3
1	G	122	ALA	2.3
1	G	144	ALA	2.3
1	A	132	MET	2.3
1	C	185	THR	2.3
1	D	45	PRO	2.3
1	G	47	PRO	2.3
1	G	224	VAL	2.3
1	H	138	HIS	2.3
1	A	202	MET	2.3
1	I	58	ASN	2.3
1	G	232	GLU	2.3
1	D	260	PRO	2.3
1	F	86	ALA	2.3
1	A	163	ILE	2.2
1	C	258	GLN	2.2
1	G	294	ARG	2.2
1	A	219	LEU	2.2
1	I	166	ALA	2.2
1	I	280	LEU	2.2
1	H	180	GLY	2.2
1	H	169	LYS	2.2
1	H	107	HIS	2.2
1	A	262	ASP	2.2
1	H	89	ASN	2.2
1	D	269	LEU	2.2
1	G	157	LEU	2.2
1	I	190	LEU	2.2
1	I	93	VAL	2.2
1	H	67	ARG	2.2
1	G	265	THR	2.2
1	C	256	TYR	2.2
1	H	87	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	120	TYR	2.2
1	F	261	GLN	2.2
1	H	52	GLN	2.2
1	G	60	VAL	2.2
1	I	89	ASN	2.2
1	G	55	GLY	2.2
1	G	204	PHE	2.2
1	H	206	GLY	2.2
1	E	193	ALA	2.2
1	C	216	LEU	2.2
1	G	226	GLU	2.1
1	I	99	GLU	2.1
1	G	180	GLY	2.1
1	A	53	LEU	2.1
1	I	147	ASN	2.1
1	H	93	VAL	2.1
1	G	64	PRO	2.1
1	A	211	ALA	2.1
1	H	211	ALA	2.1
1	A	269	LEU	2.1
1	B	200	LEU	2.1
1	I	181	LEU	2.1
1	I	165	VAL	2.1
1	F	268	TYR	2.1
1	C	193	ALA	2.1
1	C	253	ALA	2.1
1	I	244	SER	2.1
1	B	187	GLY	2.1
1	B	186	PRO	2.1
1	A	128	CYS	2.1
1	D	255	PHE	2.1
1	B	54	ASP	2.1
1	H	297	VAL	2.1
1	G	107	HIS	2.1
1	B	184	SER	2.1
1	G	227	ALA	2.1
1	C	250	LEU	2.1
1	G	113	THR	2.1
1	A	251	GLY	2.0
1	C	251	GLY	2.0
1	H	74	MET	2.0
1	C	275	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	260	PRO	2.0
1	F	297	VAL	2.0
1	G	65	LYS	2.0
1	I	102	VAL	2.0
1	I	85	ASP	2.0
1	A	174	THR	2.0
1	A	152	ALA	2.0
1	D	253	ALA	2.0
1	H	49	SER	2.0
1	A	187	GLY	2.0
1	F	112	LEU	2.0
1	H	230	GLN	2.0
1	I	292	GLN	2.0
1	I	298	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.