



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:57 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

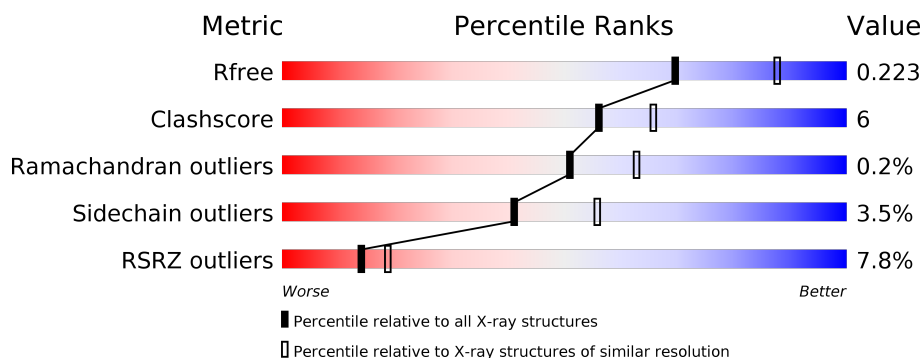
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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. 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	287	<div> <div>70%</div> <div>17%</div> <div>•</div> <div>11%</div> </div>
1	B	287	<div> <div>78%</div> <div>9%</div> <div>•</div> <div>11%</div> </div>
1	C	287	<div> <div>76%</div> <div>13%</div> <div>•</div> <div>11%</div> </div>
1	D	287	<div> <div>79%</div> <div>9%</div> <div>•</div> <div>11%</div> </div>
1	E	287	<div> <div>80%</div> <div>7%</div> <div>•</div> <div>11%</div> </div>
1	F	287	<div> <div>74%</div> <div>14%</div> <div>•</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	287	<div><div></div><div>21%</div><div></div><div>75%</div><div></div><div>13%</div><div></div><div>•</div><div>12%</div></div>
1	H	287	<div><div></div><div>15%</div><div></div><div>75%</div><div></div><div>12%</div><div></div><div>•</div><div>11%</div></div>
1	I	287	<div><div></div><div>15%</div><div></div><div>71%</div><div></div><div>17%</div><div></div><div>•</div><div>11%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17539 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 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

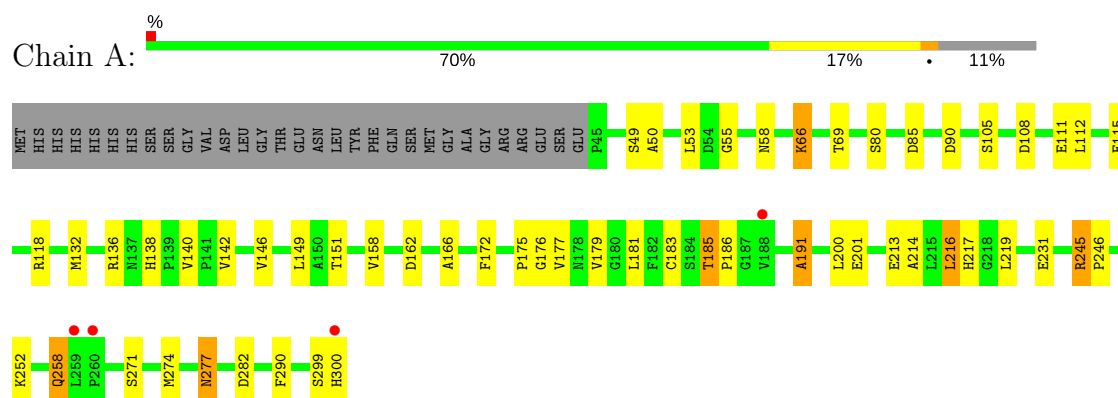
- Molecule 2 is water.

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

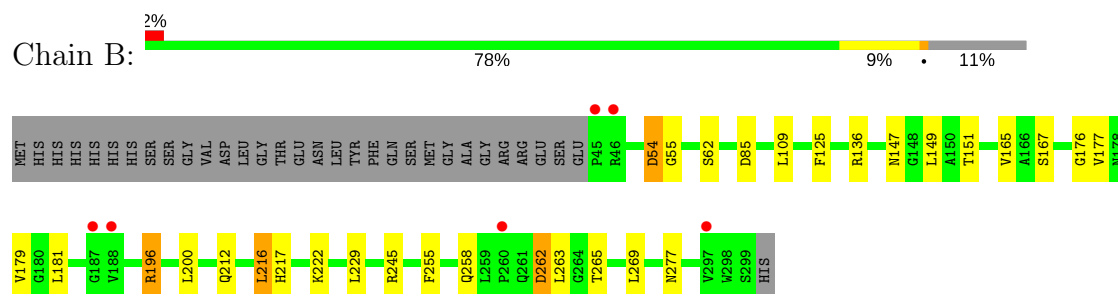
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

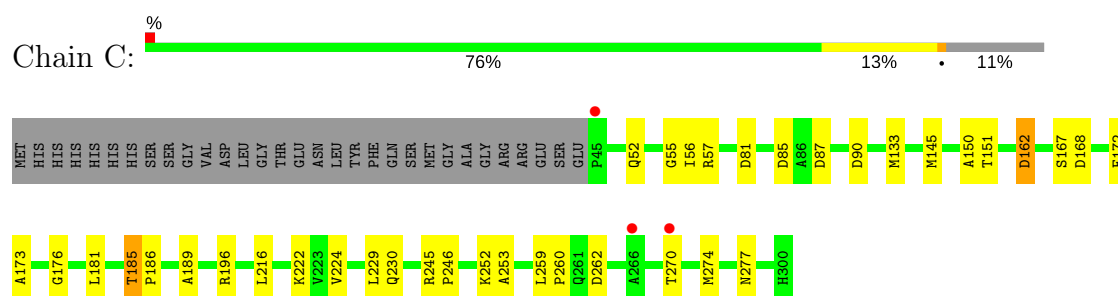
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3



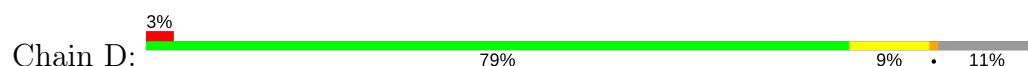
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

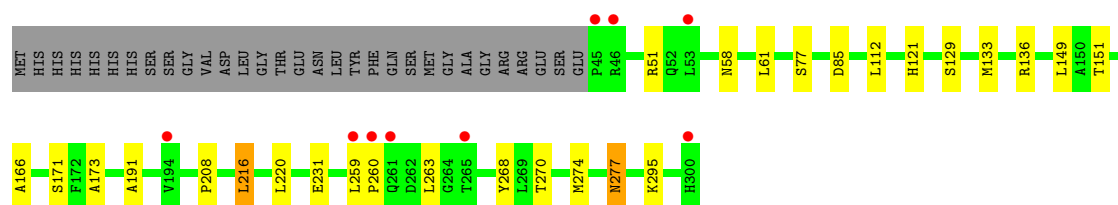


• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

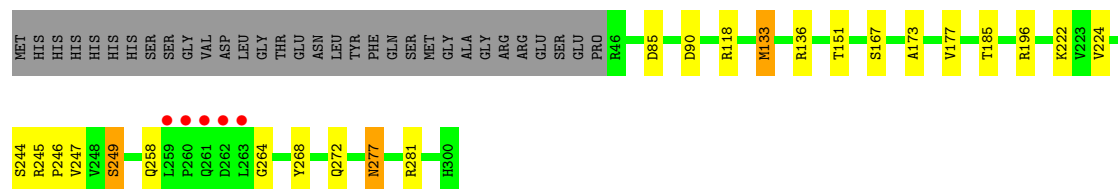
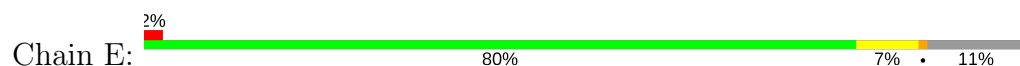


• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

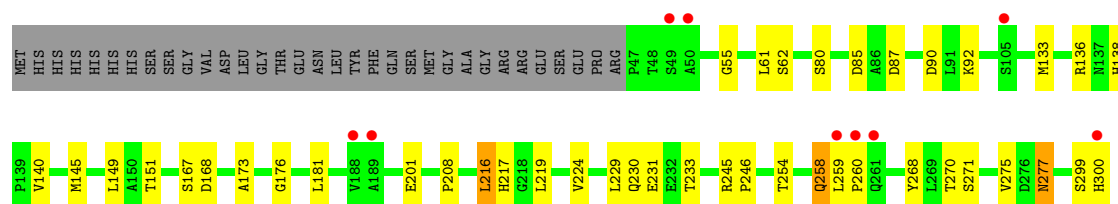




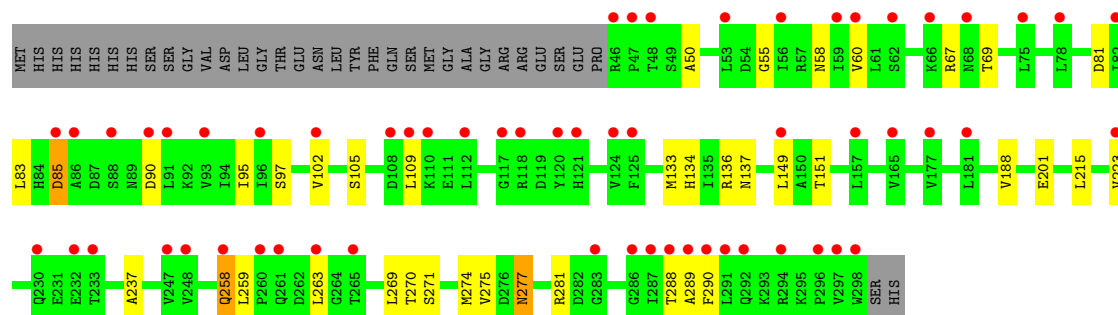
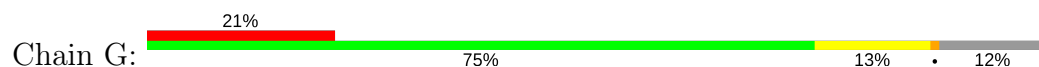
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3



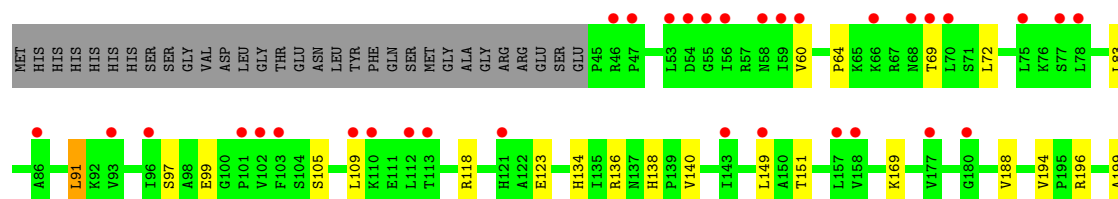
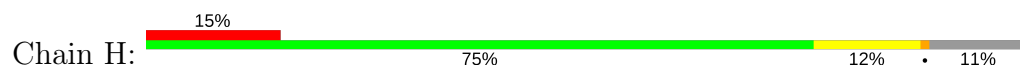
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

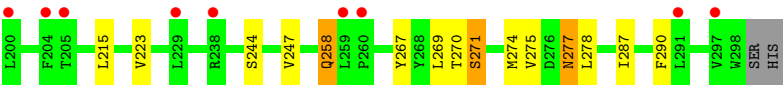


• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

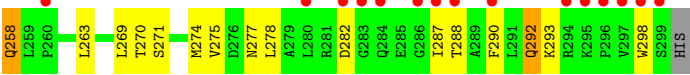
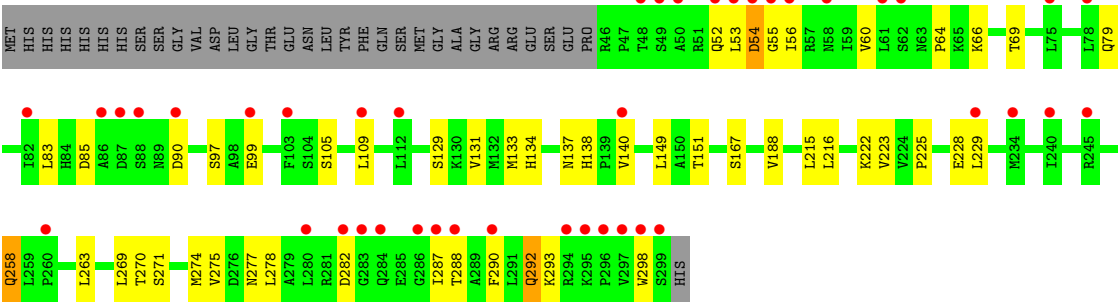


• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3





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



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)	0.32 , 47.8	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	0.95	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.

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	1.31	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 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	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
1	H	1850	0	1815	22	0
1	I	1818	0	1750	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 6.

All (196) 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: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	Interatomic distance (Å)	Clash overlap (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:B:147:ASN:HA	1:B:167:SER:OG	2.03	0.58
1:H:69:THR:HG22	1:H:105: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:F:92:LYS:HE3	1:F:300:HIS:CE1	2.42	0.55
1:G:69:THR:HG22	1:G:105:SER:OG	2.06	0.55
1:G:136:ARG:NH1	1:I:263:LEU:HD22	2.21	0.55
1:I:149:LEU:HG	1:I:151:THR:HG23	1.90	0.54
1:I:271:SER:O	1:I:275:VAL:HG23	2.07	0.54
1:F:55:GLY:HA2	1:F:90:ASP:O	2.08	0.53
1:G:201:GLU:OE2	1:I:222:LYS:NZ	2.40	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:268:TYR:C	1:D:268:TYR:CD2	2.83	0.51
1:D:216:LEU:HD11	1:F:216:LEU:HD23	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLY:HA3	1:A:181:LEU:O	2.11	0.50
1:G:83:LEU:HD21	1:G:134:HIS:HD2	1.73	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:E:277:ASN:C	1:E:277:ASN:HD22	2.15	0.49
1:G:81:ASP:OD1	2:G:2001:HOH:O	2.18	0.49
1:B:255:PHE:O	1:B:258:GLN:HG3	2.13	0.49
1:F:259:LEU:HB3	1:F:260:PRO:HD3	1.94	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:B:262:ASP:OD2	1:B:265:THR:OG1	2.30	0.47
1:H:258:GLN:HG3	1:I:188:VAL:HG22	1.96	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:A:55:GLY:HA2	1:A:90:ASP:O	2.15	0.47
1:C:270:THR:O	1:C:274:MET:HG2	2.15	0.47
1:D:166:ALA:HB3	1:D:220:LEU:HD13	1.97	0.47
1:F:149:LEU:CD1	1:F:151:THR:HG23	2.45	0.47
1:F:254:THR:HG22	1:F:270:THR:HG22	1.97	0.47
1:A:146:VAL:O	1:A:166:ALA:HA	2.15	0.46
1:H:277:ASN:C	1:H:277:ASN:HD22	2.18	0.46
1:C:151:THR:HG22	1:C:173:ALA:HB3	1.97	0.46
1:D:149:LEU:HD11	1:D:151:THR:HG22	1.96	0.46
1:G:258:GLN:HG3	1:H:188:VAL:HG22	1.96	0.46
1:I:52:GLN:HA	1:I:56:ILE:O	2.15	0.46
1:I:66:LYS:O	1:I:69:THR:HG23	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:LEU:HD22	1:H:223:VAL:HB	1.96	0.46
1:F:167:SER:HA	1:F:224:VAL:O	2.16	0.46
1:F:259:LEU:HB3	1:F:260:PRO:CD	2.45	0.46
1:B:216:LEU:C	1:B:216:LEU:CD2	2.84	0.46
1:C:245:ARG:HB3	1:C:246:PRO:HD3	1.98	0.46
1:C:55:GLY:HA2	1:C:90:ASP:O	2.15	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:G:290:PHE:CD2	1:H:109:LEU:HD12	2.51	0.45
1:H:72:LEU:HD21	1:H:123:GLU:OE2	2.15	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: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:G:109:LEU:HD12	1:I:290:PHE:CD2	2.52	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:B:165:VAL:HG13	1:B:222:LYS:HB2	1.99	0.45
1:I:278:LEU:CD2	1:I:287:ILE:HD11	2.47	0.45
1:C:176:GLY:CA	1:C:181:LEU:O	2.65	0.44
1:F:145:MET:HE2	1:F:233:THR:OG1	2.17	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: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:H:267:TYR:O	1:H:271:SER:OG	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:150:ALA:O	1:C:172:PHE:HA	2.19	0.43
1:C:176:GLY:C	1:C:181:LEU:O	2.57	0.43
1:A:50:ALA:HA	1:A:58:ASN:O	2.19	0.43
1:B:176:GLY:HA3	1:B:181:LEU:O	2.19	0.43
1:E:245:ARG:O	1:E:249:SER:HB2	2.18	0.43
1:I:270:THR:O	1:I:274:MET:HG2	2.19	0.43
1:F:92:LYS:CE	1:F:300:HIS:CE1	3.02	0.42
1:A:162:ASP:OD1	1:A:252:LYS:NZ	2.37	0.42
1:E:167:SER:HA	1:E:224:VAL:O	2.19	0.42
1:F:245:ARG:HB3	1:F:246:PRO:HD3	2.01	0.42
1:I:288:THR:HG22	1:I:292:GLN:OE1	2.19	0.42
1:E:281:ARG:HB2	1:E:281:ARG:HE	1.63	0.42
1:F:219:LEU:O	1:F:219:LEU:HD12	2.20	0.42
1:G:50:ALA:HB3	2:G:2001:HOH:O	2.18	0.42
1:I:138:HIS:CE1	1:I:140:VAL:HG22	2.55	0.42
1:C:52:GLN:HA	1:C:56:ILE:O	2.20	0.42
1:I:282:ASP:O	1:I:298:TRP:HZ3	2.01	0.42
1:C:162:ASP:OD1	1:C:252:LYS:NZ	2.45	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:F:173:ALA:HB2	1:F:208:PRO:HB3	2.02	0.42
1:D:129:SER:O	1:D:133:MET:HG2	2.20	0.42
1:I:167:SER:HB3	1:I:229:LEU:HD22	2.02	0.42
1:B:216:LEU:CD2	1:B:217:HIS:CE1	2.96	0.42
1:E:222:LYS:HE2	1:F:201:GLU:OE1	2.20	0.41
1:G:60:VAL:HG22	1:G:97:SER:OG	2.20	0.41
1:B:136:ARG:HH12	1:C:196:ARG:HH12	1.69	0.41
1:B:149:LEU:HD11	1:B:151:THR:HG22	2.02	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:G:133:MET:O	1:G:137:ASN:ND2	2.52	0.41
1:I:66:LYS:CB	2:I:2002:HOH:O	2.69	0.41
1:I:133:MET:O	1:I:137:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:GLY:HA2	1:I:90:ASP:O	2.21	0.41
1:B:149:LEU:CG	1:B:151:THR:HG23	2.46	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
1:F:138:HIS:CE1	1:F:140:VAL:HG22	2.56	0.40
1:G:288:THR:HG22	1:G:289:ALA:N	2.36	0.40
1:I:216:LEU:HD12	1:I:216:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/287 (88%)	246 (97%)	7 (3%)	1 (0%)	38	47
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%)	38	47
1	H	253/287 (88%)	243 (96%)	10 (4%)	0	100	100
1	I	252/287 (88%)	240 (95%)	9 (4%)	3 (1%)	15	16
All	All	2279/2583 (88%)	2201 (97%)	73 (3%)	5 (0%)	51	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	85	ASP

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Mol	Chain	Res	Type
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%)	22	29
1	B	206/240 (86%)	198 (96%)	8 (4%)	37	51
1	C	210/240 (88%)	207 (99%)	3 (1%)	71	85
1	D	210/240 (88%)	200 (95%)	10 (5%)	30	40
1	E	203/240 (85%)	195 (96%)	8 (4%)	37	51
1	F	200/240 (83%)	192 (96%)	8 (4%)	36	50
1	G	178/240 (74%)	174 (98%)	4 (2%)	57	74
1	H	190/240 (79%)	184 (97%)	6 (3%)	44	60
1	I	183/240 (76%)	179 (98%)	4 (2%)	57	74
All	All	1794/2160 (83%)	1730 (96%)	64 (4%)	41	55

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [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 carbohydrates 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	256/287 (89%)	0.37	4 (1%) 72 77	11, 18, 25, 40	0
1	B	255/287 (88%)	0.31	6 (2%) 59 66	12, 18, 25, 56	0
1	C	256/287 (89%)	0.26	3 (1%) 79 82	10, 17, 26, 39	0
1	D	256/287 (89%)	0.30	9 (3%) 44 51	12, 18, 26, 41	0
1	E	255/287 (88%)	0.25	5 (1%) 65 72	13, 18, 26, 37	0
1	F	254/287 (88%)	0.39	9 (3%) 44 51	12, 18, 25, 39	1 (0%)
1	G	253/287 (88%)	1.16	59 (23%) 1 1	21, 25, 50, 74	1 (0%)
1	H	254/287 (88%)	0.97	42 (16%) 2 3	21, 25, 31, 51	0
1	I	254/287 (88%)	0.97	42 (16%) 2 3	21, 25, 61, 71	0
All	All	2293/2583 (88%)	0.55	179 (7%) 14 19	10, 20, 28, 74	2 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	297	VAL	7.7
1	G	112	LEU	6.4
1	H	109	LEU	5.3
1	H	102	VAL	5.0
1	G	53	LEU	4.5
1	G	289	ALA	4.5
1	G	297	VAL	4.4
1	I	50	ALA	4.2
1	I	53	LEU	4.2
1	I	56	ILE	4.1
1	G	291	LEU	4.1
1	H	103	PHE	4.1
1	I	112	LEU	4.0
1	H	149	LEU	4.0
1	B	45	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	233	THR	3.9
1	I	287	ILE	3.9
1	G	298	TRP	3.8
1	G	93	VAL	3.8
1	G	96	ILE	3.8
1	G	287	ILE	3.7
1	H	112	LEU	3.7
1	G	62	SER	3.7
1	G	86	ALA	3.7
1	H	110	LYS	3.6
1	H	78	LEU	3.6
1	I	260	PRO	3.6
1	I	296	PRO	3.6
1	H	47	PRO	3.5
1	I	75	LEU	3.5
1	H	56	ILE	3.5
1	I	298	TRP	3.5
1	I	282	ASP	3.4
1	F	259	LEU	3.4
1	F	300	HIS	3.4
1	G	265	THR	3.4
1	H	66	LYS	3.3
1	I	78	LEU	3.3
1	I	62	SER	3.3
1	I	295	LYS	3.3
1	G	290	PHE	3.3
1	H	55	GLY	3.2
1	G	102	VAL	3.2
1	I	82	ILE	3.2
1	I	290	PHE	3.2
1	G	56	ILE	3.1
1	G	247	VAL	3.1
1	C	45	PRO	3.1
1	G	117	GLY	3.1
1	G	294	ARG	3.1
1	H	204	PHE	3.1
1	H	58	ASN	3.0
1	G	283	GLY	3.0
1	I	288	THR	3.0
1	I	54	ASP	3.0
1	G	223	VAL	3.0
1	E	260	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	288	THR	3.0
1	G	124	VAL	2.9
1	I	109	LEU	2.9
1	G	78	LEU	2.9
1	G	109	LEU	2.9
1	H	157	LEU	2.9
1	H	229	LEU	2.9
1	D	259	LEU	2.9
1	I	283	GLY	2.9
1	I	86	ALA	2.9
1	A	300	HIS	2.8
1	F	260	PRO	2.8
1	G	88	SER	2.8
1	H	259	LEU	2.8
1	I	55	GLY	2.8
1	H	59	ILE	2.8
1	G	59	ILE	2.8
1	G	121	HIS	2.8
1	I	49	SER	2.7
1	H	200	LEU	2.7
1	F	50	ALA	2.7
1	G	48	THR	2.7
1	G	110	LYS	2.7
1	D	260	PRO	2.7
1	I	286	GLY	2.7
1	G	82	ILE	2.7
1	I	48	THR	2.7
1	G	66	LYS	2.7
1	G	91	LEU	2.7
1	B	297	VAL	2.6
1	H	291	LEU	2.6
1	H	143	ILE	2.6
1	G	118	ARG	2.6
1	H	53	LEU	2.6
1	H	70	LEU	2.6
1	I	280	LEU	2.6
1	G	149	LEU	2.5
1	G	248	VAL	2.5
1	G	292	GLN	2.5
1	H	260	PRO	2.5
1	I	284	GLN	2.5
1	G	47	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	96	ILE	2.5
1	D	265	THR	2.5
1	D	46	ARG	2.5
1	I	245	ARG	2.5
1	E	259	LEU	2.5
1	I	229	LEU	2.5
1	F	49	SER	2.4
1	G	60	VAL	2.4
1	I	58	ASN	2.4
1	H	68	ASN	2.4
1	A	259	LEU	2.4
1	G	68	ASN	2.4
1	I	240	ILE	2.4
1	G	232	GLU	2.4
1	E	261	GLN	2.4
1	D	45	PRO	2.4
1	G	165	VAL	2.4
1	H	158	VAL	2.4
1	I	103	PHE	2.4
1	H	177	VAL	2.4
1	I	234	MET	2.3
1	H	77	SER	2.3
1	G	120	TYR	2.3
1	H	121	HIS	2.3
1	G	230	GLN	2.3
1	B	260	PRO	2.3
1	G	125	PHE	2.3
1	I	90	ASP	2.3
1	H	46	ARG	2.3
1	F	188	VAL	2.3
1	H	93	VAL	2.3
1	I	88	SER	2.3
1	C	270	THR	2.2
1	G	286	GLY	2.2
1	G	75	LEU	2.2
1	F	261	GLN	2.2
1	I	140	VAL	2.2
1	C	266	ALA	2.2
1	I	294	ARG	2.2
1	H	180	GLY	2.2
1	H	54	ASP	2.2
1	I	99	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	260	PRO	2.2
1	H	101	PRO	2.2
1	E	263	LEU	2.2
1	F	189	ALA	2.2
1	D	53	LEU	2.2
1	G	85	ASP	2.2
1	D	300	HIS	2.1
1	I	87	ASP	2.1
1	G	261	GLN	2.1
1	G	177	VAL	2.1
1	I	61	LEU	2.1
1	D	194	VAL	2.1
1	H	297	VAL	2.1
1	G	46	ARG	2.1
1	B	187	GLY	2.1
1	G	260	PRO	2.1
1	G	263	LEU	2.1
1	H	205	THR	2.1
1	H	238	ARG	2.1
1	G	296	PRO	2.1
1	I	299	SER	2.1
1	G	90	ASP	2.1
1	B	188	VAL	2.1
1	H	60	VAL	2.1
1	E	262	ASP	2.1
1	I	52	GLN	2.1
1	H	69	THR	2.1
1	G	157	LEU	2.0
1	H	113	THR	2.0
1	F	105	SER	2.0
1	G	108	ASP	2.0
1	B	46	ARG	2.0
1	H	75	LEU	2.0
1	A	188	VAL	2.0
1	G	181	LEU	2.0
1	D	261	GLN	2.0
1	G	258	GLN	2.0
1	H	86	ALA	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 [i](#)

There are no carbohydrates 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.