Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2025 – 02:08 PM EDT

PDB ID	:	9D2T / pdb_00009d2t
Title	:	Crystal structure of S. aureus Threonine deaminase regulatory domain
Authors	:	Rock, C.O.; Yun, M.
Deposited on	:	2024-08-09
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:

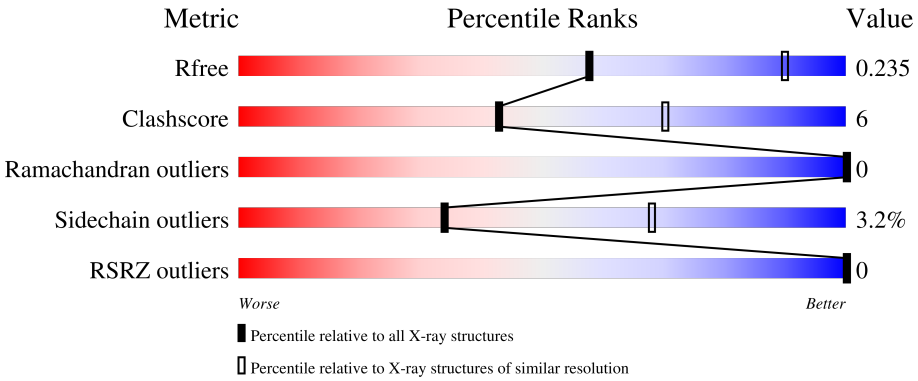
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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 <=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	107	70% 8% • 21%
1	B	107	59% 13% • 27%
1	C	107	66% 13% 21%
1	D	107	64% 12% • 23%
1	E	107	70% 9% 21%

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Mol	Chain	Length	Quality of chain
1	F	107	60% 15% 25%
1	G	107	60% 16% 24%
1	H	107	62% 14% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5429 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 L-threonine dehydratase biosynthetic IlvA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			695	447	118	128	2			
1	B	78	Total	C	N	O	S	0	0	0
			643	417	107	117	2			
1	C	85	Total	C	N	O	S	0	0	0
			688	445	116	126	1			
1	D	82	Total	C	N	O	S	0	0	0
			675	436	113	124	2			
1	E	85	Total	C	N	O	S	0	0	0
			688	444	116	127	1			
1	F	80	Total	C	N	O	S	0	0	0
			666	431	111	122	2			
1	H	83	Total	C	N	O	S	0	0	0
			683	443	115	123	2			
1	G	81	Total	C	N	O	S	0	0	0
			677	440	114	121	2			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	MET	-	initiating methionine	UNP Q2FF63
A	317	GLY	-	expression tag	UNP Q2FF63
A	318	SER	-	expression tag	UNP Q2FF63
A	319	SER	-	expression tag	UNP Q2FF63
A	320	HIS	-	expression tag	UNP Q2FF63
A	321	HIS	-	expression tag	UNP Q2FF63
A	322	HIS	-	expression tag	UNP Q2FF63
A	323	HIS	-	expression tag	UNP Q2FF63
A	324	HIS	-	expression tag	UNP Q2FF63
A	325	HIS	-	expression tag	UNP Q2FF63
A	326	SER	-	expression tag	UNP Q2FF63
A	327	SER	-	expression tag	UNP Q2FF63
A	328	GLY	-	expression tag	UNP Q2FF63

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Chain	Residue	Modelled	Actual	Comment	Reference
A	329	LEU	-	expression tag	UNP Q2FF63
A	330	VAL	-	expression tag	UNP Q2FF63
A	331	PRO	-	expression tag	UNP Q2FF63
A	332	ARG	-	expression tag	UNP Q2FF63
A	333	GLY	-	expression tag	UNP Q2FF63
A	334	SER	-	expression tag	UNP Q2FF63
A	335	HIS	-	expression tag	UNP Q2FF63
B	316	MET	-	initiating methionine	UNP Q2FF63
B	317	GLY	-	expression tag	UNP Q2FF63
B	318	SER	-	expression tag	UNP Q2FF63
B	319	SER	-	expression tag	UNP Q2FF63
B	320	HIS	-	expression tag	UNP Q2FF63
B	321	HIS	-	expression tag	UNP Q2FF63
B	322	HIS	-	expression tag	UNP Q2FF63
B	323	HIS	-	expression tag	UNP Q2FF63
B	324	HIS	-	expression tag	UNP Q2FF63
B	325	HIS	-	expression tag	UNP Q2FF63
B	326	SER	-	expression tag	UNP Q2FF63
B	327	SER	-	expression tag	UNP Q2FF63
B	328	GLY	-	expression tag	UNP Q2FF63
B	329	LEU	-	expression tag	UNP Q2FF63
B	330	VAL	-	expression tag	UNP Q2FF63
B	331	PRO	-	expression tag	UNP Q2FF63
B	332	ARG	-	expression tag	UNP Q2FF63
B	333	GLY	-	expression tag	UNP Q2FF63
B	334	SER	-	expression tag	UNP Q2FF63
B	335	HIS	-	expression tag	UNP Q2FF63
C	316	MET	-	initiating methionine	UNP Q2FF63
C	317	GLY	-	expression tag	UNP Q2FF63
C	318	SER	-	expression tag	UNP Q2FF63
C	319	SER	-	expression tag	UNP Q2FF63
C	320	HIS	-	expression tag	UNP Q2FF63
C	321	HIS	-	expression tag	UNP Q2FF63
C	322	HIS	-	expression tag	UNP Q2FF63
C	323	HIS	-	expression tag	UNP Q2FF63
C	324	HIS	-	expression tag	UNP Q2FF63
C	325	HIS	-	expression tag	UNP Q2FF63
C	326	SER	-	expression tag	UNP Q2FF63
C	327	SER	-	expression tag	UNP Q2FF63
C	328	GLY	-	expression tag	UNP Q2FF63
C	329	LEU	-	expression tag	UNP Q2FF63
C	330	VAL	-	expression tag	UNP Q2FF63

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Chain	Residue	Modelled	Actual	Comment	Reference
C	331	PRO	-	expression tag	UNP Q2FF63
C	332	ARG	-	expression tag	UNP Q2FF63
C	333	GLY	-	expression tag	UNP Q2FF63
C	334	SER	-	expression tag	UNP Q2FF63
C	335	HIS	-	expression tag	UNP Q2FF63
D	316	MET	-	initiating methionine	UNP Q2FF63
D	317	GLY	-	expression tag	UNP Q2FF63
D	318	SER	-	expression tag	UNP Q2FF63
D	319	SER	-	expression tag	UNP Q2FF63
D	320	HIS	-	expression tag	UNP Q2FF63
D	321	HIS	-	expression tag	UNP Q2FF63
D	322	HIS	-	expression tag	UNP Q2FF63
D	323	HIS	-	expression tag	UNP Q2FF63
D	324	HIS	-	expression tag	UNP Q2FF63
D	325	HIS	-	expression tag	UNP Q2FF63
D	326	SER	-	expression tag	UNP Q2FF63
D	327	SER	-	expression tag	UNP Q2FF63
D	328	GLY	-	expression tag	UNP Q2FF63
D	329	LEU	-	expression tag	UNP Q2FF63
D	330	VAL	-	expression tag	UNP Q2FF63
D	331	PRO	-	expression tag	UNP Q2FF63
D	332	ARG	-	expression tag	UNP Q2FF63
D	333	GLY	-	expression tag	UNP Q2FF63
D	334	SER	-	expression tag	UNP Q2FF63
D	335	HIS	-	expression tag	UNP Q2FF63
E	316	MET	-	initiating methionine	UNP Q2FF63
E	317	GLY	-	expression tag	UNP Q2FF63
E	318	SER	-	expression tag	UNP Q2FF63
E	319	SER	-	expression tag	UNP Q2FF63
E	320	HIS	-	expression tag	UNP Q2FF63
E	321	HIS	-	expression tag	UNP Q2FF63
E	322	HIS	-	expression tag	UNP Q2FF63
E	323	HIS	-	expression tag	UNP Q2FF63
E	324	HIS	-	expression tag	UNP Q2FF63
E	325	HIS	-	expression tag	UNP Q2FF63
E	326	SER	-	expression tag	UNP Q2FF63
E	327	SER	-	expression tag	UNP Q2FF63
E	328	GLY	-	expression tag	UNP Q2FF63
E	329	LEU	-	expression tag	UNP Q2FF63
E	330	VAL	-	expression tag	UNP Q2FF63
E	331	PRO	-	expression tag	UNP Q2FF63
E	332	ARG	-	expression tag	UNP Q2FF63

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Chain	Residue	Modelled	Actual	Comment	Reference
E	333	GLY	-	expression tag	UNP Q2FF63
E	334	SER	-	expression tag	UNP Q2FF63
E	335	HIS	-	expression tag	UNP Q2FF63
F	316	MET	-	initiating methionine	UNP Q2FF63
F	317	GLY	-	expression tag	UNP Q2FF63
F	318	SER	-	expression tag	UNP Q2FF63
F	319	SER	-	expression tag	UNP Q2FF63
F	320	HIS	-	expression tag	UNP Q2FF63
F	321	HIS	-	expression tag	UNP Q2FF63
F	322	HIS	-	expression tag	UNP Q2FF63
F	323	HIS	-	expression tag	UNP Q2FF63
F	324	HIS	-	expression tag	UNP Q2FF63
F	325	HIS	-	expression tag	UNP Q2FF63
F	326	SER	-	expression tag	UNP Q2FF63
F	327	SER	-	expression tag	UNP Q2FF63
F	328	GLY	-	expression tag	UNP Q2FF63
F	329	LEU	-	expression tag	UNP Q2FF63
F	330	VAL	-	expression tag	UNP Q2FF63
F	331	PRO	-	expression tag	UNP Q2FF63
F	332	ARG	-	expression tag	UNP Q2FF63
F	333	GLY	-	expression tag	UNP Q2FF63
F	334	SER	-	expression tag	UNP Q2FF63
F	335	HIS	-	expression tag	UNP Q2FF63
H	316	MET	-	initiating methionine	UNP Q2FF63
H	317	GLY	-	expression tag	UNP Q2FF63
H	318	SER	-	expression tag	UNP Q2FF63
H	319	SER	-	expression tag	UNP Q2FF63
H	320	HIS	-	expression tag	UNP Q2FF63
H	321	HIS	-	expression tag	UNP Q2FF63
H	322	HIS	-	expression tag	UNP Q2FF63
H	323	HIS	-	expression tag	UNP Q2FF63
H	324	HIS	-	expression tag	UNP Q2FF63
H	325	HIS	-	expression tag	UNP Q2FF63
H	326	SER	-	expression tag	UNP Q2FF63
H	327	SER	-	expression tag	UNP Q2FF63
H	328	GLY	-	expression tag	UNP Q2FF63
H	329	LEU	-	expression tag	UNP Q2FF63
H	330	VAL	-	expression tag	UNP Q2FF63
H	331	PRO	-	expression tag	UNP Q2FF63
H	332	ARG	-	expression tag	UNP Q2FF63
H	333	GLY	-	expression tag	UNP Q2FF63
H	334	SER	-	expression tag	UNP Q2FF63

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Chain	Residue	Modelled	Actual	Comment	Reference
H	335	HIS	-	expression tag	UNP Q2FF63
G	316	MET	-	initiating methionine	UNP Q2FF63
G	317	GLY	-	expression tag	UNP Q2FF63
G	318	SER	-	expression tag	UNP Q2FF63
G	319	SER	-	expression tag	UNP Q2FF63
G	320	HIS	-	expression tag	UNP Q2FF63
G	321	HIS	-	expression tag	UNP Q2FF63
G	322	HIS	-	expression tag	UNP Q2FF63
G	323	HIS	-	expression tag	UNP Q2FF63
G	324	HIS	-	expression tag	UNP Q2FF63
G	325	HIS	-	expression tag	UNP Q2FF63
G	326	SER	-	expression tag	UNP Q2FF63
G	327	SER	-	expression tag	UNP Q2FF63
G	328	GLY	-	expression tag	UNP Q2FF63
G	329	LEU	-	expression tag	UNP Q2FF63
G	330	VAL	-	expression tag	UNP Q2FF63
G	331	PRO	-	expression tag	UNP Q2FF63
G	332	ARG	-	expression tag	UNP Q2FF63
G	333	GLY	-	expression tag	UNP Q2FF63
G	334	SER	-	expression tag	UNP Q2FF63
G	335	HIS	-	expression tag	UNP Q2FF63

- Molecule 2 is water.

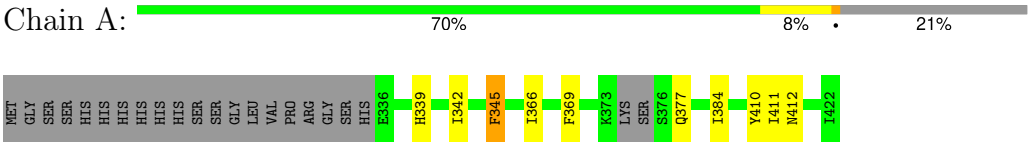
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	C	3	Total O 3 3	0	0
2	D	4	Total O 4 4	0	0
2	E	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0
2	H	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

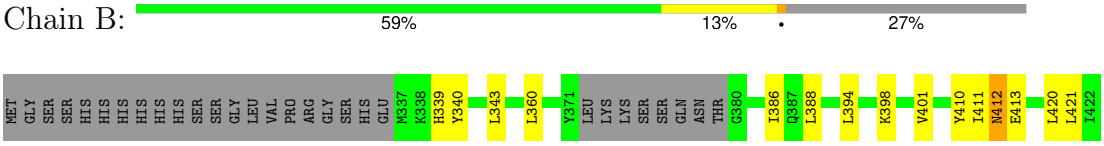
• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain A:



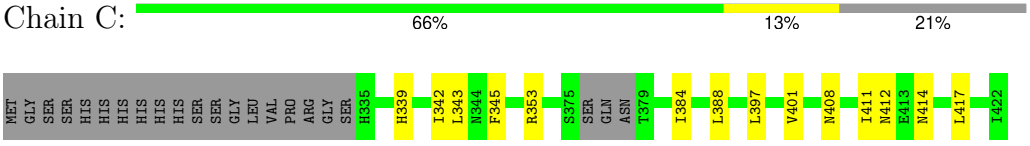
• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain B:



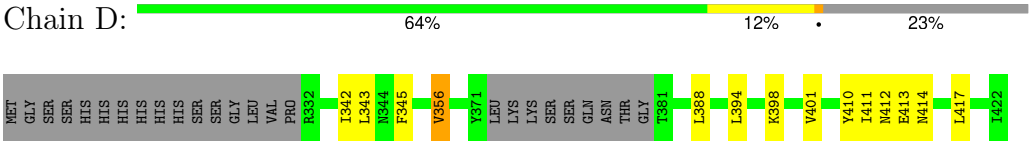
• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain C:



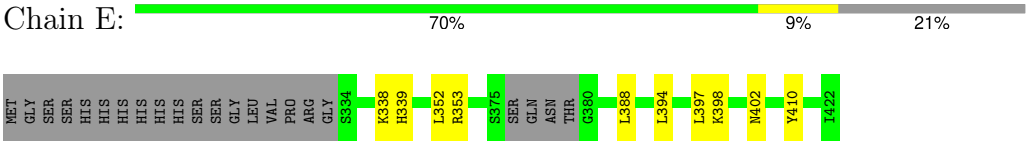
• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain D:



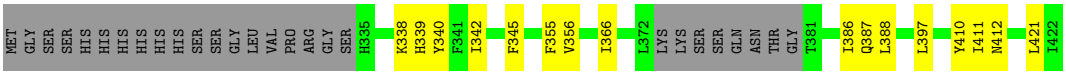
• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain E:



• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain F:

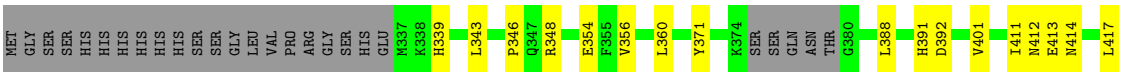


• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain H:

• Molecule 1: L-threonine dehydratase biosynthetic IlvA

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	88.92Å 88.92Å 213.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.46 – 2.80 44.46 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.46-2.80) 97.8 (44.46-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.192 , 0.239 0.190 , 0.235	Depositor DCC
R_{free} test set	18776 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	82.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 121.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.304 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5429	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/709	0.39	0/957
1	B	0.25	0/657	0.40	0/887
1	C	0.25	0/702	0.39	0/949
1	D	0.25	0/689	0.39	0/929
1	E	0.25	0/702	0.39	0/948
1	F	0.24	0/680	0.38	0/917
1	G	0.24	0/691	0.39	0/929
1	H	0.25	0/697	0.38	0/939
All	All	0.25	0/5527	0.39	0/7455

There are no bond length outliers.

There are no bond angle outliers.

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	695	0	676	5	0
1	B	643	0	630	10	0
1	C	688	0	668	8	0
1	D	675	0	659	7	0
1	E	688	0	669	8	0
1	F	666	0	654	10	0
1	G	677	0	684	9	0
1	H	683	0	677	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
All	All	5429	0	5317	65	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 (65) 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:F:388:LEU:HD21	1:F:397:LEU:HD22	1.69	0.74
1:B:360:LEU:HD21	1:B:386:ILE:HD13	1.72	0.71
1:E:388:LEU:HD11	1:E:397:LEU:HD22	1.79	0.65
1:F:342:ILE:HD11	1:F:421:LEU:HD21	1.79	0.64
1:G:346:PRO:HB2	1:G:348:ARG:HG2	1.81	0.62
1:A:342:ILE:HG13	1:A:411:ILE:HD11	1.82	0.61
1:G:343:LEU:HD21	1:G:401:VAL:HG13	1.83	0.60
1:H:360:LEU:HD21	1:H:386:ILE:HD13	1.84	0.58
1:D:410:TYR:CZ	1:D:412:ASN:HB2	2.40	0.56
1:D:343:LEU:HD21	1:D:401:VAL:HG13	1.88	0.56
1:G:348:ARG:NH1	1:G:354:GLU:OE1	2.38	0.56
1:C:388:LEU:HD21	1:C:397:LEU:HD22	1.87	0.55
1:E:398:LYS:O	1:E:402:ASN:ND2	2.37	0.55
1:B:413:GLU:OE1	1:H:398:LYS:NZ	2.33	0.55
1:G:414:ASN:HD22	1:G:417:LEU:HG	1.72	0.54
1:C:343:LEU:HD13	1:C:384:ILE:HD12	1.88	0.54
1:C:342:ILE:HG13	1:C:411:ILE:HD11	1.91	0.53
1:B:343:LEU:HD21	1:B:401:VAL:HG13	1.90	0.52
1:A:345:PHE:HE1	1:A:384:ILE:HD11	1.73	0.52
1:E:339:HIS:HD2	1:E:388:LEU:HD13	1.75	0.52
1:H:348:ARG:NH1	1:H:354:GLU:OE1	2.43	0.52
1:C:343:LEU:HD21	1:C:401:VAL:HG13	1.91	0.52
1:H:342:ILE:HG13	1:H:411:ILE:HD11	1.91	0.51
1:D:342:ILE:HG13	1:D:411:ILE:HD11	1.92	0.51
1:C:353:ARG:HG2	1:D:356:VAL:HG13	1.93	0.50
1:B:339:HIS:CD2	1:B:388:LEU:HD12	2.46	0.50
1:C:414:ASN:HB3	1:C:417:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TYR:CZ	1:A:412:ASN:HB2	2.48	0.49
1:F:339:HIS:HA	1:F:412:ASN:HD21	1.78	0.48
1:A:366:ILE:HD11	1:A:369:PHE:HB2	1.96	0.48
1:B:340:TYR:HB3	1:B:411:ILE:HD12	1.96	0.48
1:H:339:HIS:HB3	1:H:410:TYR:HE1	1.80	0.47
1:G:339:HIS:HA	1:G:412:ASN:HD21	1.79	0.46
1:A:339:HIS:HA	1:A:412:ASN:HD21	1.80	0.46
1:H:356:VAL:HA	1:H:360:LEU:HB2	1.96	0.46
1:H:342:ILE:HB	1:H:409:ILE:HB	1.98	0.46
1:H:394:LEU:HD11	1:H:398:LYS:HE3	1.97	0.46
1:H:356:VAL:HA	1:H:360:LEU:HD12	1.97	0.45
1:C:411:ILE:HG23	1:C:417:LEU:HB3	1.99	0.45
1:E:353:ARG:HA	1:F:356:VAL:HG11	1.98	0.45
1:F:340:TYR:HB3	1:F:411:ILE:HD12	1.99	0.45
1:E:339:HIS:CD2	1:E:394:LEU:HD13	2.52	0.45
1:D:394:LEU:HD11	1:D:398:LYS:HE3	1.99	0.45
1:F:410:TYR:CE2	1:F:412:ASN:HB2	2.53	0.44
1:F:338:LYS:HG2	1:F:387:GLN:HG3	2.01	0.43
1:G:411:ILE:HG23	1:G:417:LEU:HB3	2.00	0.43
1:B:360:LEU:HD23	1:B:360:LEU:HA	1.90	0.43
1:F:411:ILE:HD13	1:F:421:LEU:HD23	2.01	0.42
1:H:373:LYS:HA	1:H:373:LYS:HD3	1.85	0.42
1:F:355:PHE:HZ	1:F:386:ILE:HD11	1.85	0.42
1:G:413:GLU:HG3	1:G:414:ASN:N	2.35	0.42
1:B:339:HIS:HD2	1:B:388:LEU:HD12	1.83	0.42
1:C:339:HIS:HA	1:C:412:ASN:HD21	1.85	0.42
1:G:414:ASN:ND2	1:G:417:LEU:HG	2.35	0.42
1:B:412:ASN:OD1	1:B:412:ASN:N	2.53	0.41
1:E:352:LEU:HD23	1:F:366:ILE:HD12	2.02	0.41
1:E:338:LYS:HB2	1:E:338:LYS:HE3	1.88	0.41
1:G:356:VAL:O	1:G:360:LEU:HB3	2.20	0.41
1:D:410:TYR:CD2	1:D:413:GLU:HG3	2.56	0.41
1:E:339:HIS:ND1	1:E:410:TYR:OH	2.54	0.41
1:H:355:PHE:O	1:H:359:VAL:HG22	2.21	0.41
1:B:410:TYR:HD2	1:B:413:GLU:HG3	1.87	0.40
1:B:394:LEU:HG	1:B:398:LYS:HE3	2.03	0.40
1:D:414:ASN:HB3	1:D:417:LEU:HB2	2.04	0.40
1:H:360:LEU:HD23	1:H:360:LEU:HA	1.97	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	81/107 (76%)	79 (98%)	2 (2%)	0	100	100
1	B	74/107 (69%)	72 (97%)	2 (3%)	0	100	100
1	C	81/107 (76%)	80 (99%)	1 (1%)	0	100	100
1	D	78/107 (73%)	75 (96%)	3 (4%)	0	100	100
1	E	81/107 (76%)	77 (95%)	4 (5%)	0	100	100
1	F	76/107 (71%)	75 (99%)	1 (1%)	0	100	100
1	G	77/107 (72%)	75 (97%)	2 (3%)	0	100	100
1	H	79/107 (74%)	76 (96%)	3 (4%)	0	100	100
All	All	627/856 (73%)	609 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	76/99 (77%)	74 (97%)	2 (3%)	41	75
1	B	71/99 (72%)	68 (96%)	3 (4%)	25	58
1	C	74/99 (75%)	72 (97%)	2 (3%)	40	74
1	D	74/99 (75%)	71 (96%)	3 (4%)	26	59
1	E	75/99 (76%)	75 (100%)	0	100	100
1	F	74/99 (75%)	73 (99%)	1 (1%)	62	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	76/99 (77%)	72 (95%)	4 (5%)	19 49
1	H	75/99 (76%)	71 (95%)	4 (5%)	19 49
All	All	595/792 (75%)	576 (97%)	19 (3%)	34 68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	PHE
1	A	377	GLN
1	B	412	ASN
1	B	420	LEU
1	B	421	LEU
1	C	345	PHE
1	C	408	ASN
1	D	345	PHE
1	D	356	VAL
1	D	388	LEU
1	F	345	PHE
1	H	345	PHE
1	H	359	VAL
1	H	373	LYS
1	H	391	HIS
1	G	371	TYR
1	G	388	LEU
1	G	391	HIS
1	G	392	ASP

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

Mol	Chain	Res	Type
1	B	339	HIS
1	H	347	GLN
1	G	414	ASN

5.3.3 RNA

There are no RNA molecules 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 oligosaccharides 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, 95^{th} 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	85/107 (79%)	-0.01	0	100	100	62, 82, 127, 160	0
1	B	78/107 (72%)	-0.23	0	100	100	60, 86, 118, 133	0
1	C	85/107 (79%)	-0.02	0	100	100	67, 90, 129, 170	0
1	D	82/107 (76%)	0.16	0	100	100	68, 89, 132, 141	0
1	E	85/107 (79%)	-0.21	0	100	100	53, 78, 120, 139	0
1	F	80/107 (74%)	0.07	0	100	100	64, 97, 148, 177	0
1	G	81/107 (75%)	0.10	0	100	100	70, 96, 135, 153	0
1	H	83/107 (77%)	-0.04	0	100	100	56, 91, 132, 155	0
All	All	659/856 (76%)	-0.02	0	100	100	53, 90, 132, 177	0

There are no RSRZ outliers to report.

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 monosaccharides 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.