



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2022 – 01:11 pm BST

PDB ID : 7Z3H  
Title : Crystal structure of Iba57 from Chaetomium thermophilum  
Authors : Altegoer, F.; Mrusek, D.; Bange, G.  
Deposited on : 2022-03-02  
Resolution : 2.40 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.30  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.30

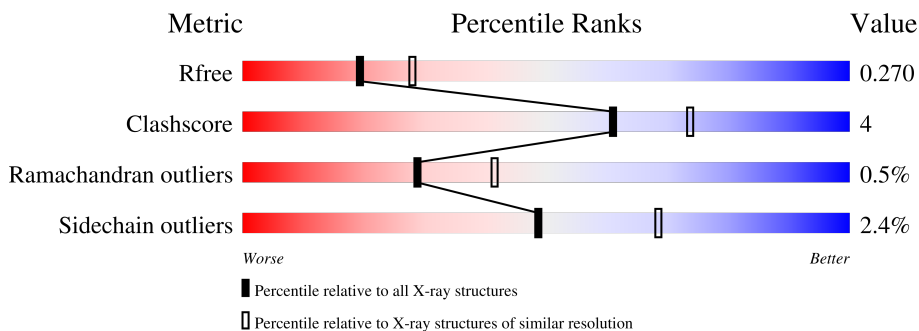
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	432	
1	B	432	
1	C	432	
1	D	432	
1	E	432	
1	F	432	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17142 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 Transferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	2862	1809	511	529	13	0	0	0
1	B	363	2801	1770	499	519	13	0	0	0
1	C	363	2800	1771	499	517	13	0	0	0
1	D	365	2819	1782	502	522	13	0	0	0
1	E	361	2785	1760	496	516	13	0	0	0
1	F	359	2768	1752	491	512	13	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	MET	-	initiating methionine	UNP G0SHN3
A	46	GLY	-	expression tag	UNP G0SHN3
A	47	SER	-	expression tag	UNP G0SHN3
A	48	SER	-	expression tag	UNP G0SHN3
A	49	HIS	-	expression tag	UNP G0SHN3
A	50	HIS	-	expression tag	UNP G0SHN3
A	51	HIS	-	expression tag	UNP G0SHN3
A	52	HIS	-	expression tag	UNP G0SHN3
A	53	HIS	-	expression tag	UNP G0SHN3
A	54	HIS	-	expression tag	UNP G0SHN3
A	55	SER	-	expression tag	UNP G0SHN3
A	56	GLN	-	expression tag	UNP G0SHN3
A	57	ASP	-	expression tag	UNP G0SHN3
A	58	PRO	-	expression tag	UNP G0SHN3
A	59	ASN	-	expression tag	UNP G0SHN3
A	60	SER	-	expression tag	UNP G0SHN3
B	45	MET	-	initiating methionine	UNP G0SHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	46	GLY	-	expression tag	UNP G0SHN3
B	47	SER	-	expression tag	UNP G0SHN3
B	48	SER	-	expression tag	UNP G0SHN3
B	49	HIS	-	expression tag	UNP G0SHN3
B	50	HIS	-	expression tag	UNP G0SHN3
B	51	HIS	-	expression tag	UNP G0SHN3
B	52	HIS	-	expression tag	UNP G0SHN3
B	53	HIS	-	expression tag	UNP G0SHN3
B	54	HIS	-	expression tag	UNP G0SHN3
B	55	SER	-	expression tag	UNP G0SHN3
B	56	GLN	-	expression tag	UNP G0SHN3
B	57	ASP	-	expression tag	UNP G0SHN3
B	58	PRO	-	expression tag	UNP G0SHN3
B	59	ASN	-	expression tag	UNP G0SHN3
B	60	SER	-	expression tag	UNP G0SHN3
C	45	MET	-	initiating methionine	UNP G0SHN3
C	46	GLY	-	expression tag	UNP G0SHN3
C	47	SER	-	expression tag	UNP G0SHN3
C	48	SER	-	expression tag	UNP G0SHN3
C	49	HIS	-	expression tag	UNP G0SHN3
C	50	HIS	-	expression tag	UNP G0SHN3
C	51	HIS	-	expression tag	UNP G0SHN3
C	52	HIS	-	expression tag	UNP G0SHN3
C	53	HIS	-	expression tag	UNP G0SHN3
C	54	HIS	-	expression tag	UNP G0SHN3
C	55	SER	-	expression tag	UNP G0SHN3
C	56	GLN	-	expression tag	UNP G0SHN3
C	57	ASP	-	expression tag	UNP G0SHN3
C	58	PRO	-	expression tag	UNP G0SHN3
C	59	ASN	-	expression tag	UNP G0SHN3
C	60	SER	-	expression tag	UNP G0SHN3
D	45	MET	-	initiating methionine	UNP G0SHN3
D	46	GLY	-	expression tag	UNP G0SHN3
D	47	SER	-	expression tag	UNP G0SHN3
D	48	SER	-	expression tag	UNP G0SHN3
D	49	HIS	-	expression tag	UNP G0SHN3
D	50	HIS	-	expression tag	UNP G0SHN3
D	51	HIS	-	expression tag	UNP G0SHN3
D	52	HIS	-	expression tag	UNP G0SHN3
D	53	HIS	-	expression tag	UNP G0SHN3
D	54	HIS	-	expression tag	UNP G0SHN3
D	55	SER	-	expression tag	UNP G0SHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	56	GLN	-	expression tag	UNP G0SHN3
D	57	ASP	-	expression tag	UNP G0SHN3
D	58	PRO	-	expression tag	UNP G0SHN3
D	59	ASN	-	expression tag	UNP G0SHN3
D	60	SER	-	expression tag	UNP G0SHN3
E	45	MET	-	initiating methionine	UNP G0SHN3
E	46	GLY	-	expression tag	UNP G0SHN3
E	47	SER	-	expression tag	UNP G0SHN3
E	48	SER	-	expression tag	UNP G0SHN3
E	49	HIS	-	expression tag	UNP G0SHN3
E	50	HIS	-	expression tag	UNP G0SHN3
E	51	HIS	-	expression tag	UNP G0SHN3
E	52	HIS	-	expression tag	UNP G0SHN3
E	53	HIS	-	expression tag	UNP G0SHN3
E	54	HIS	-	expression tag	UNP G0SHN3
E	55	SER	-	expression tag	UNP G0SHN3
E	56	GLN	-	expression tag	UNP G0SHN3
E	57	ASP	-	expression tag	UNP G0SHN3
E	58	PRO	-	expression tag	UNP G0SHN3
E	59	ASN	-	expression tag	UNP G0SHN3
E	60	SER	-	expression tag	UNP G0SHN3
F	45	MET	-	initiating methionine	UNP G0SHN3
F	46	GLY	-	expression tag	UNP G0SHN3
F	47	SER	-	expression tag	UNP G0SHN3
F	48	SER	-	expression tag	UNP G0SHN3
F	49	HIS	-	expression tag	UNP G0SHN3
F	50	HIS	-	expression tag	UNP G0SHN3
F	51	HIS	-	expression tag	UNP G0SHN3
F	52	HIS	-	expression tag	UNP G0SHN3
F	53	HIS	-	expression tag	UNP G0SHN3
F	54	HIS	-	expression tag	UNP G0SHN3
F	55	SER	-	expression tag	UNP G0SHN3
F	56	GLN	-	expression tag	UNP G0SHN3
F	57	ASP	-	expression tag	UNP G0SHN3
F	58	PRO	-	expression tag	UNP G0SHN3
F	59	ASN	-	expression tag	UNP G0SHN3
F	60	SER	-	expression tag	UNP G0SHN3

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0

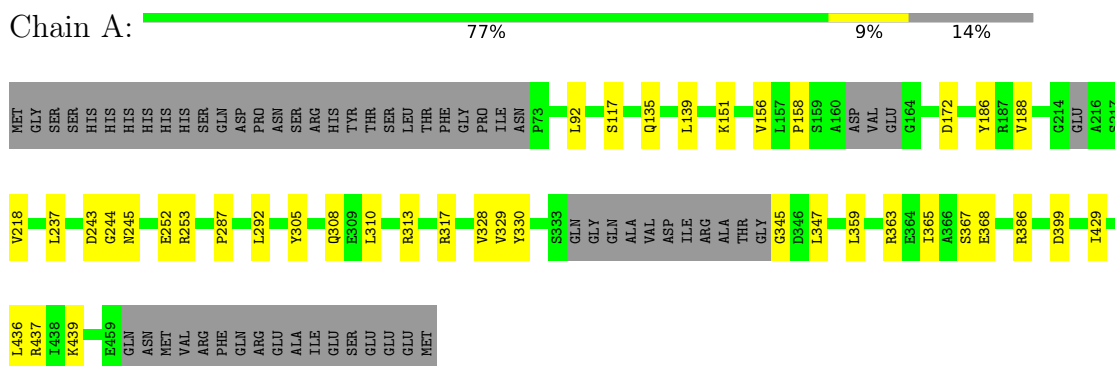
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	32	Total O 32 32	0	0
3	C	50	Total O 50 50	0	0
3	D	31	Total O 31 31	0	0
3	E	41	Total O 41 41	0	0
3	F	36	Total O 36 36	0	0

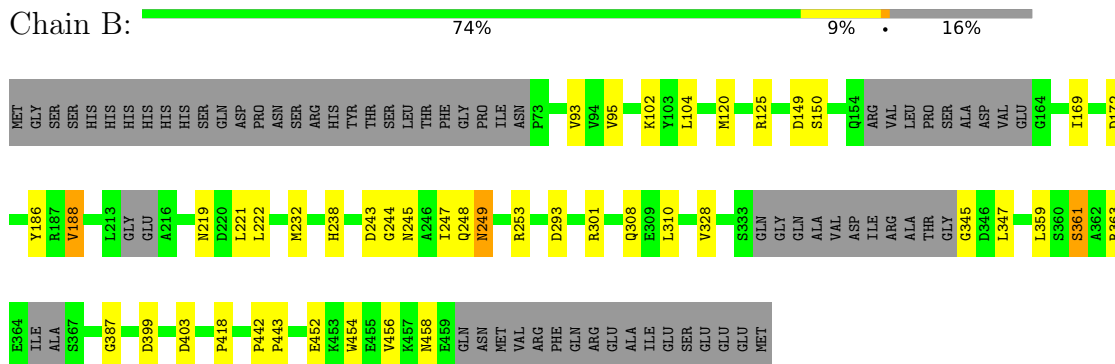
### 3 Residue-property plots [i](#)

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. 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. 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.

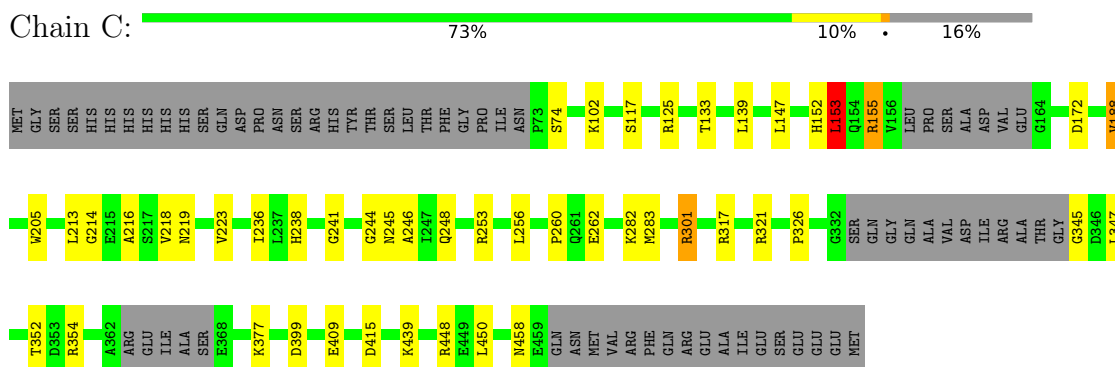
- Molecule 1: Transferase-like protein



- Molecule 1: Transferase-like protein

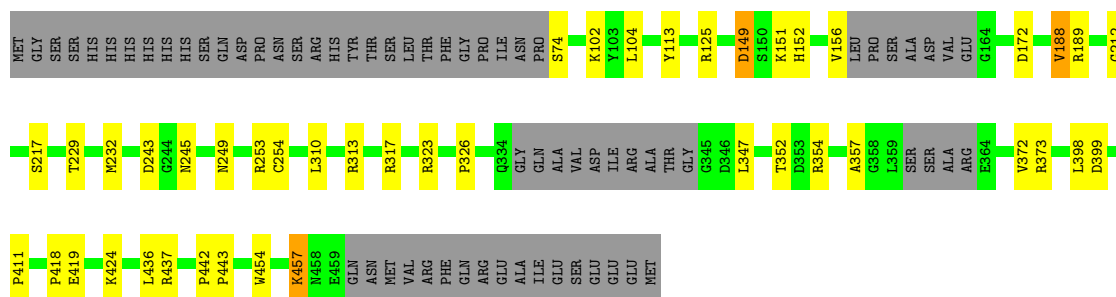


- Molecule 1: Transferase-like protein



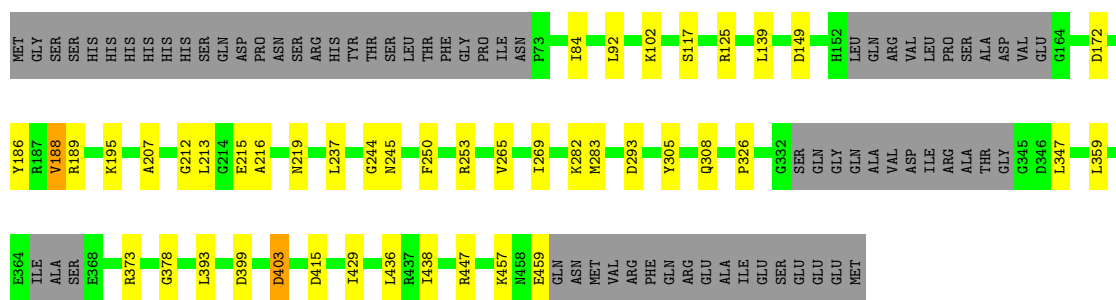
● Molecule 1: Transferase-like protein

Chain D:  74% 9% 16%



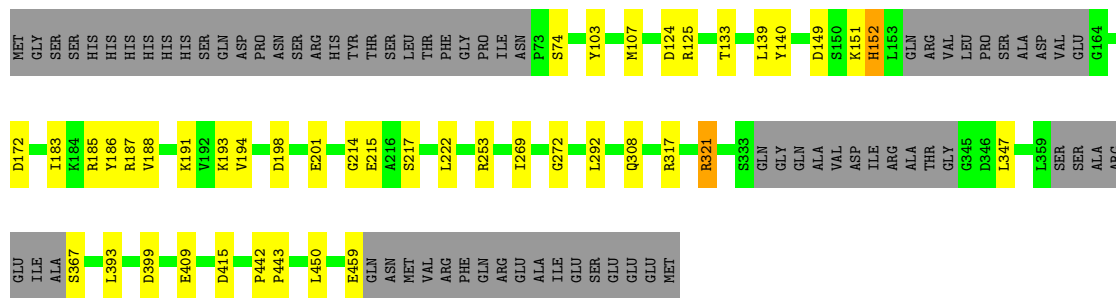
● Molecule 1: Transferase-like protein

Chain E:  73% 10% 16%



● Molecule 1: Transferase-like protein

Chain F:  73% 9% 17%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.53Å 134.18Å 107.01Å 90.00° 97.59° 90.00°	Depositor
Resolution (Å)	47.34 – 2.40 47.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.34-2.40) 99.6 (47.84-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.238 , 0.274 0.234 , 0.270	Depositor DCC
$R_{free}$ test set	5246 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

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	0.26	0/2919	0.54	0/3956
1	B	0.26	0/2856	0.55	0/3868
1	C	0.27	0/2856	0.55	1/3870 (0.0%)
1	D	0.28	0/2874	0.55	0/3894
1	E	0.26	0/2841	0.55	0/3849
1	F	0.26	0/2824	0.55	0/3827
All	All	0.27	0/17170	0.55	1/23264 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	LEU	CA-CB-CG	5.39	127.70	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	D	149	ASP	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2862	0	2882	29	0
1	B	2801	0	2812	23	0
1	C	2800	0	2815	32	0
1	D	2819	0	2832	29	0
1	E	2785	0	2793	29	0
1	F	2768	0	2780	29	0
2	A	13	0	5	1	0
2	B	13	0	5	1	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	1	0
2	F	13	0	5	2	0
3	A	39	0	0	0	0
3	B	32	0	0	0	0
3	C	50	0	0	2	0
3	D	31	0	0	0	0
3	E	41	0	0	1	0
3	F	36	0	0	2	0
All	All	17142	0	16944	151	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 4.

All (151) 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:D:253:ARG:HD2	1:E:253:ARG:HD2	1.52	0.90
1:F:139:LEU:HD11	2:F:501:CIT:H22	1.66	0.76
1:F:125:ARG:HB3	1:F:222:LEU:HD21	1.68	0.75
1:E:459:GLU:OE1	1:F:317:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:CIT:O6	1:E:189:ARG:NH1	2.25	0.70
1:A:139:LEU:HD11	2:A:501:CIT:H22	1.72	0.70
1:C:458:ASN:ND2	1:D:317:ARG:HG2	2.07	0.69
1:D:125:ARG:HD3	1:D:217:SER:HB2	1.72	0.69
1:A:317:ARG:HH12	1:F:459:GLU:HB3	1.59	0.67
1:E:457:LYS:NZ	3:E:601:HOH:O	2.26	0.67
1:E:139:LEU:HD11	2:E:501:CIT:H41	1.76	0.67
1:E:215:GLU:HG3	1:E:253:ARG:HH22	1.61	0.65
1:A:367:SER:HB3	1:A:368:GLU:HG2	1.77	0.65
1:F:125:ARG:HH11	1:F:215:GLU:HG2	1.61	0.64
1:F:367:SER:N	3:F:603:HOH:O	2.31	0.63
1:A:359:LEU:HD21	1:A:363:ARG:HG2	1.79	0.63
1:C:352:THR:HG22	1:C:354:ARG:H	1.64	0.62
1:A:305:TYR:CE2	1:A:308:GLN:HG3	2.35	0.62
1:F:198:ASP:HB2	1:F:201:GLU:HG3	1.83	0.60
1:C:301:ARG:NH1	3:C:601:HOH:O	2.34	0.59
1:B:458:ASN:HD21	1:C:317:ARG:HG2	1.68	0.59
1:D:125:ARG:NH2	1:E:212:GLY:H	1.99	0.59
1:B:238:HIS:HB2	1:B:247:ILE:HD11	1.85	0.58
1:A:313:ARG:HD2	1:F:415:ASP:O	2.04	0.57
1:B:458:ASN:ND2	1:C:317:ARG:HG2	2.19	0.57
1:A:399:ASP:N	1:A:399:ASP:OD1	2.38	0.56
1:B:125:ARG:HB3	1:B:222:LEU:HD21	1.88	0.56
1:B:359:LEU:HD21	1:B:363:ARG:CD	2.36	0.56
1:F:103:TYR:CZ	1:F:107:MET:HE1	2.42	0.55
1:E:429:ILE:HG23	1:E:438:ILE:HD11	1.89	0.55
1:E:215:GLU:HG3	1:E:253:ARG:NH2	2.22	0.54
1:C:214:GLY:HA3	1:F:214:GLY:HA3	1.89	0.54
1:D:310:LEU:HD13	1:D:313:ARG:HH12	1.72	0.54
1:E:282:LYS:HG2	1:E:283:MET:HG3	1.89	0.54
1:E:399:ASP:OD1	1:E:399:ASP:N	2.42	0.53
1:B:399:ASP:OD1	1:B:399:ASP:N	2.41	0.53
1:C:458:ASN:HD21	1:D:317:ARG:HG2	1.73	0.53
1:C:345:GLY:O	1:C:347:LEU:N	2.41	0.52
1:C:246:ALA:O	1:C:248:GLN:N	2.41	0.52
1:C:133:THR:HG22	1:C:139:LEU:HD13	1.92	0.51
1:A:365:ILE:O	1:A:367:SER:N	2.44	0.51
1:F:140:TYR:OH	2:F:501:CIT:O2	2.19	0.51
1:F:149:ASP:O	1:F:151:LYS:N	2.44	0.51
1:B:328:VAL:HG22	1:B:347:LEU:HD11	1.93	0.51
1:F:272:GLY:O	3:F:601:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLY:O	1:B:347:LEU:N	2.43	0.50
1:D:399:ASP:N	1:D:399:ASP:OD1	2.42	0.50
1:B:149:ASP:OD2	1:B:150:SER:N	2.45	0.50
1:E:265:VAL:O	1:E:269:ILE:HG12	2.12	0.49
1:A:92:LEU:HD11	1:A:237:LEU:HD22	1.94	0.49
1:D:149:ASP:O	1:D:151:LYS:N	2.45	0.49
1:F:269:ILE:HD12	1:F:393:LEU:HG	1.94	0.49
1:C:213:LEU:HD21	1:C:256:LEU:HD11	1.94	0.49
1:E:84:ILE:HG13	1:E:207:ALA:HB2	1.94	0.49
1:C:321:ARG:HD3	1:C:409:GLU:OE1	2.13	0.49
1:C:399:ASP:OD1	1:C:399:ASP:N	2.43	0.48
1:A:310:LEU:HD12	1:A:313:ARG:HH21	1.79	0.48
1:A:345:GLY:O	1:A:347:LEU:N	2.44	0.48
1:C:448:ARG:NH1	3:C:602:HOH:O	2.37	0.48
1:F:193:LYS:HA	1:F:193:LYS:HD2	1.76	0.48
1:F:399:ASP:N	1:F:399:ASP:OD1	2.41	0.48
1:D:418:PRO:HD3	1:D:454:TRP:CZ3	2.49	0.48
1:A:317:ARG:NH1	1:F:459:GLU:HB3	2.26	0.48
1:A:244:GLY:C	1:A:245:ASN:HD22	2.17	0.47
1:A:156:VAL:O	1:A:158:PRO:HD3	2.13	0.47
1:D:457:LYS:HE3	1:D:457:LYS:HB2	1.65	0.47
1:D:189:ARG:HH21	1:F:185:ARG:CZ	2.28	0.47
1:B:248:GLN:H	1:B:248:GLN:CD	2.13	0.47
1:A:359:LEU:HD11	1:A:363:ARG:NH2	2.30	0.46
1:B:245:ASN:O	1:B:249:ASN:HB2	2.14	0.46
1:D:212:GLY:HA3	1:E:125:ARG:NH2	2.31	0.46
1:E:403:ASP:HB3	1:E:447:ARG:HH12	1.80	0.46
1:A:305:TYR:CZ	1:A:308:GLN:HG3	2.51	0.46
1:B:95:VAL:HG11	1:B:104:LEU:HD11	1.98	0.46
1:B:418:PRO:HD3	1:B:454:TRP:CZ3	2.51	0.46
1:E:244:GLY:O	1:E:245:ASN:HB2	2.15	0.46
1:C:155:ARG:N	1:C:155:ARG:HD2	2.31	0.46
1:D:245:ASN:OD1	1:D:249:ASN:ND2	2.48	0.46
1:D:229:THR:OG1	1:D:232:MET:HG2	2.16	0.45
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.81	0.45
1:F:193:LYS:HE3	1:F:194:VAL:H	1.81	0.45
1:D:253:ARG:NH2	1:D:254:CYS:SG	2.89	0.45
1:C:238:HIS:NE2	1:C:241:GLY:O	2.41	0.45
1:C:326:PRO:HB2	1:C:347:LEU:HD22	1.99	0.45
1:A:287:PRO:HB3	1:A:292:LEU:HD12	1.98	0.45
1:E:213:LEU:HD12	1:E:250:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:HG22	1:B:169:ILE:HB	1.99	0.44
1:D:152:HIS:O	1:D:156:VAL:HG13	2.17	0.44
1:B:243:ASP:OD1	1:B:244:GLY:N	2.49	0.44
1:C:214:GLY:HA3	1:F:214:GLY:CA	2.47	0.44
1:D:372:VAL:HG12	1:D:373:ARG:O	2.18	0.44
1:A:429:ILE:HD12	1:A:436:LEU:HD22	1.99	0.44
1:C:216:ALA:HA	1:C:223:VAL:HB	1.99	0.44
1:F:133:THR:HG22	1:F:139:LEU:HD13	1.99	0.43
1:A:347:LEU:HD12	1:A:347:LEU:HA	1.73	0.43
1:E:102:LYS:HA	1:E:102:LYS:HD2	1.67	0.43
1:A:328:VAL:CG2	1:A:347:LEU:HD11	2.49	0.43
1:D:352:THR:OG1	1:D:354:ARG:NH1	2.51	0.43
1:E:326:PRO:HB2	1:E:347:LEU:HD22	2.01	0.43
1:D:102:LYS:HD3	1:D:113:TYR:OH	2.18	0.43
1:F:321:ARG:NH1	1:F:409:GLU:OE1	2.52	0.43
1:D:347:LEU:HD12	1:D:347:LEU:HA	1.82	0.43
1:D:424:LYS:HA	1:D:424:LYS:HD2	1.94	0.43
1:F:347:LEU:HD12	1:F:347:LEU:HA	1.73	0.43
1:E:373:ARG:HH12	1:E:378:GLY:HA3	1.83	0.43
1:E:293:ASP:OD1	1:E:293:ASP:N	2.52	0.43
1:E:429:ILE:HG12	1:E:436:LEU:HD22	2.00	0.42
1:C:253:ARG:HG3	1:F:253:ARG:NH2	2.34	0.42
1:C:153:LEU:HD22	1:C:153:LEU:O	2.19	0.42
1:A:245:ASN:HD22	1:A:245:ASN:N	2.16	0.42
1:A:253:ARG:HD2	1:B:253:ARG:HD3	2.01	0.42
1:B:188:VAL:HG21	1:E:186:TYR:CD1	2.55	0.42
1:C:244:GLY:O	1:C:245:ASN:HB2	2.19	0.42
1:A:186:TYR:CD1	1:C:188:VAL:HG21	2.55	0.42
1:B:186:TYR:CD1	1:E:188:VAL:HG21	2.55	0.42
1:B:293:ASP:OD1	1:B:293:ASP:N	2.53	0.42
1:C:415:ASP:OD2	1:C:415:ASP:N	2.42	0.42
1:A:436:LEU:HD23	1:A:437:ARG:N	2.35	0.42
1:D:436:LEU:O	1:D:437:ARG:NH1	2.50	0.42
1:F:450:LEU:HD23	1:F:450:LEU:HA	1.92	0.42
1:C:139:LEU:HD12	1:C:283:MET:HG2	2.01	0.42
1:E:92:LEU:HD11	1:E:237:LEU:HD22	2.02	0.41
1:B:361:SER:HB3	1:B:387:GLY:HA3	2.02	0.41
1:C:205:TRP:HB2	1:C:236:ILE:HB	2.02	0.41
1:A:330:TYR:HE1	1:A:439:LYS:HB2	1.85	0.41
1:A:151:LYS:HD3	1:A:151:LYS:HA	1.75	0.41
1:B:442:PRO:HA	1:B:443:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ILE:HD12	1:E:393:LEU:HG	2.03	0.41
1:A:329:VAL:HG13	1:A:436:LEU:HD21	2.02	0.41
1:B:452:GLU:O	1:B:456:VAL:HG13	2.21	0.41
1:D:323:ARG:HD2	1:D:398:LEU:HD11	2.02	0.41
1:F:183:ILE:O	1:F:187:ARG:HG3	2.21	0.41
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.93	0.41
1:C:125:ARG:HD2	1:C:216:ALA:HB1	2.03	0.40
1:D:104:LEU:HD23	1:D:104:LEU:HA	1.95	0.40
1:E:213:LEU:HD12	1:E:250:PHE:CZ	2.56	0.40
1:A:243:ASP:OD1	1:A:243:ASP:N	2.52	0.40
1:A:310:LEU:HD12	1:A:313:ARG:NH2	2.37	0.40
1:C:102:LYS:HA	1:C:102:LYS:HD2	1.85	0.40
1:C:260:PRO:HB2	1:C:262:GLU:OE1	2.21	0.40
1:C:282:LYS:HG2	1:C:283:MET:HG3	2.03	0.40
1:D:442:PRO:HA	1:D:443:PRO:HD3	1.96	0.40
1:D:243:ASP:N	1:D:243:ASP:OD1	2.53	0.40
1:E:415:ASP:N	1:E:415:ASP:OD1	2.53	0.40
1:C:450:LEU:HD23	1:C:450:LEU:HA	1.91	0.40
1:D:188:VAL:HG21	1:F:186:TYR:CD1	2.57	0.40
1:D:326:PRO:HB2	1:D:347:LEU:HD23	2.03	0.40
1:D:411:PRO:O	1:D:419:GLU:HG3	2.20	0.40
1:E:305:TYR:CE1	1:E:308:GLN:HG3	2.56	0.40
1:F:152:HIS:ND1	1:F:152:HIS:N	2.69	0.40
1:F:442:PRO:HA	1:F:443:PRO:HD3	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	364/432 (84%)	349 (96%)	14 (4%)	1 (0%)	41 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	353/432 (82%)	340 (96%)	11 (3%)	2 (1%)	25	36
1	C	355/432 (82%)	341 (96%)	12 (3%)	2 (1%)	25	36
1	D	357/432 (83%)	346 (97%)	9 (2%)	2 (1%)	25	36
1	E	353/432 (82%)	337 (96%)	14 (4%)	2 (1%)	25	36
1	F	351/432 (81%)	339 (97%)	11 (3%)	1 (0%)	41	55
All	All	2133/2592 (82%)	2052 (96%)	71 (3%)	10 (0%)	29	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	ASN
1	C	219	ASN
1	D	357	ALA
1	E	216	ALA
1	A	188	VAL
1	D	188	VAL
1	F	188	VAL
1	B	188	VAL
1	C	188	VAL
1	E	188	VAL

### 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	306/359 (85%)	301 (98%)	5 (2%)	62	79
1	B	300/359 (84%)	290 (97%)	10 (3%)	38	57
1	C	299/359 (83%)	289 (97%)	10 (3%)	38	57
1	D	301/359 (84%)	298 (99%)	3 (1%)	76	88
1	E	297/359 (83%)	290 (98%)	7 (2%)	49	68
1	F	296/359 (82%)	287 (97%)	9 (3%)	41	61
All	All	1799/2154 (84%)	1755 (98%)	44 (2%)	49	68



All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	135	GLN
1	A	172	ASP
1	A	252	GLU
1	A	386	ARG
1	B	102	LYS
1	B	120	MET
1	B	172	ASP
1	B	232	MET
1	B	249	ASN
1	B	301	ARG
1	B	308	GLN
1	B	310	LEU
1	B	361	SER
1	B	403	ASP
1	C	74	SER
1	C	117	SER
1	C	152	HIS
1	C	153	LEU
1	C	155	ARG
1	C	172	ASP
1	C	218	VAL
1	C	301	ARG
1	C	377	LYS
1	C	439	LYS
1	D	74	SER
1	D	172	ASP
1	D	457	LYS
1	E	117	SER
1	E	149	ASP
1	E	172	ASP
1	E	195	LYS
1	E	219	ASN
1	E	359	LEU
1	E	403	ASP
1	F	74	SER
1	F	124	ASP
1	F	152	HIS
1	F	172	ASP
1	F	191	LYS
1	F	217	SER
1	F	292	LEU

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Mol	Chain	Res	Type
1	F	308	GLN
1	F	321	ARG

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

Mol	Chain	Res	Type
1	A	245	ASN
1	B	458	ASN
1	C	458	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CIT	C	501	-	12,12,12	1.04	0	17,17,17	1.76	3 (17%)
2	CIT	D	501	-	12,12,12	1.02	0	17,17,17	1.51	3 (17%)
2	CIT	B	501	-	12,12,12	1.09	0	17,17,17	1.60	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CIT	A	501	-	12,12,12	1.06	0	17,17,17	1.52	2 (11%)
2	CIT	F	501	-	12,12,12	1.07	0	17,17,17	1.46	2 (11%)
2	CIT	E	501	-	12,12,12	1.04	0	17,17,17	1.61	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	C	501	-	-	7/16/16/16	-
2	CIT	D	501	-	-	8/16/16/16	-
2	CIT	B	501	-	-	4/16/16/16	-
2	CIT	A	501	-	-	1/16/16/16	-
2	CIT	F	501	-	-	0/16/16/16	-
2	CIT	E	501	-	-	5/16/16/16	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	CIT	O6-C6-C3	4.47	120.81	113.05
2	E	501	CIT	O6-C6-C3	4.38	120.66	113.05
2	A	501	CIT	O6-C6-C3	4.19	120.33	113.05
2	D	501	CIT	O6-C6-C3	3.97	119.94	113.05
2	F	501	CIT	O6-C6-C3	3.82	119.69	113.05
2	B	501	CIT	O6-C6-C3	3.77	119.59	113.05
2	C	501	CIT	C3-C4-C5	-2.86	106.90	113.81
2	A	501	CIT	C3-C4-C5	-2.21	108.45	113.81
2	D	501	CIT	O4-C5-C4	2.14	121.23	114.35
2	C	501	CIT	O4-C5-C4	2.10	121.09	114.35
2	D	501	CIT	O2-C1-O1	-2.09	118.09	123.30
2	F	501	CIT	O4-C5-C4	2.07	121.01	114.35
2	B	501	CIT	O2-C1-C2	2.00	120.79	114.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	CIT	C1-C2-C3-O7
2	C	501	CIT	O7-C3-C6-O5
2	C	501	CIT	O7-C3-C6-O6
2	C	501	CIT	C4-C3-C6-O5
2	C	501	CIT	C4-C3-C6-O6
2	C	501	CIT	C1-C2-C3-C4
2	C	501	CIT	C1-C2-C3-C6
2	D	501	CIT	C2-C3-C6-O5
2	D	501	CIT	O7-C3-C6-O5
2	D	501	CIT	C2-C3-C6-O6
2	D	501	CIT	C4-C3-C6-O6
2	E	501	CIT	C2-C3-C6-O6
2	E	501	CIT	C4-C3-C6-O5
2	E	501	CIT	C4-C3-C6-O6
2	B	501	CIT	C6-C3-C4-C5
2	D	501	CIT	C4-C3-C6-O5
2	E	501	CIT	C2-C3-C6-O5
2	B	501	CIT	O7-C3-C4-C5
2	D	501	CIT	O7-C3-C6-O6
2	E	501	CIT	O7-C3-C6-O6
2	A	501	CIT	C1-C2-C3-C6
2	D	501	CIT	C3-C4-C5-O4
2	D	501	CIT	C3-C4-C5-O3
2	B	501	CIT	C3-C4-C5-O3
2	B	501	CIT	C3-C4-C5-O4

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	CIT	1	0
2	A	501	CIT	1	0
2	F	501	CIT	2	0
2	E	501	CIT	1	0

## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.