



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:18 AM UTC

PDB ID : 7Z3H / pdb_00007z3h
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

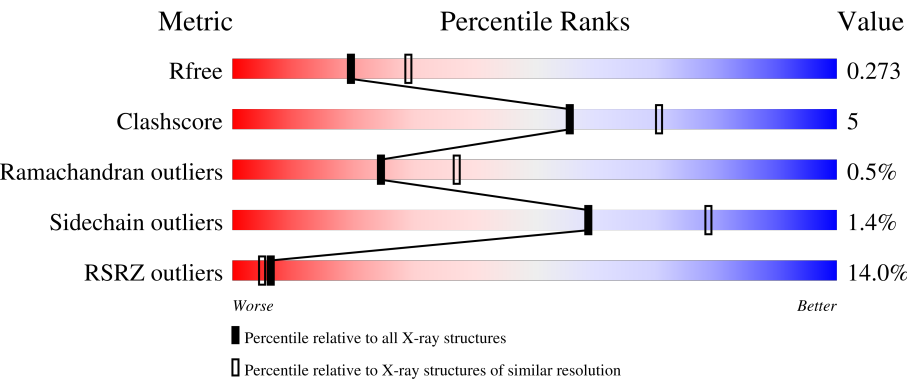
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	432	11% 77% 9% 14%
1	B	432	9% 75% 9% 16%
1	C	432	13% 74% 10% 16%
1	D	432	11% 74% 10% 16%
1	E	432	14% 73% 10% 16%

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Mol	Chain	Length	Quality of chain
1	F	432	

2 Entry composition

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

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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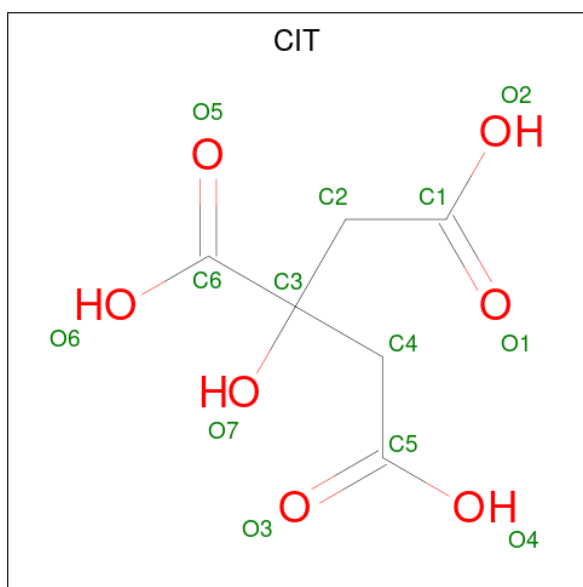
Chain	Residue	Modelled	Actual	Comment	Reference
B	46	GLY	-	expression tag	UNP G0SHN3
B	47	SER	-	expression tag	UNP G0SHN3
B	48	SER	-	expression tag	UNP G0SHN3
B	49	HIS	-	expression tag	UNP G0SHN3
B	50	HIS	-	expression tag	UNP G0SHN3
B	51	HIS	-	expression tag	UNP G0SHN3
B	52	HIS	-	expression tag	UNP G0SHN3
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 (CCD ID: CIT) (formula: C₆H₈O₇).



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

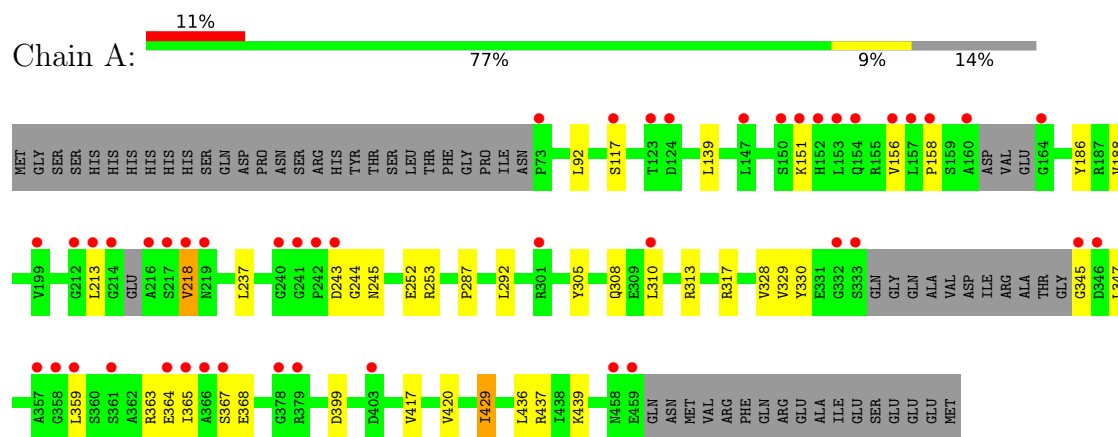
- Molecule 3 is water.

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

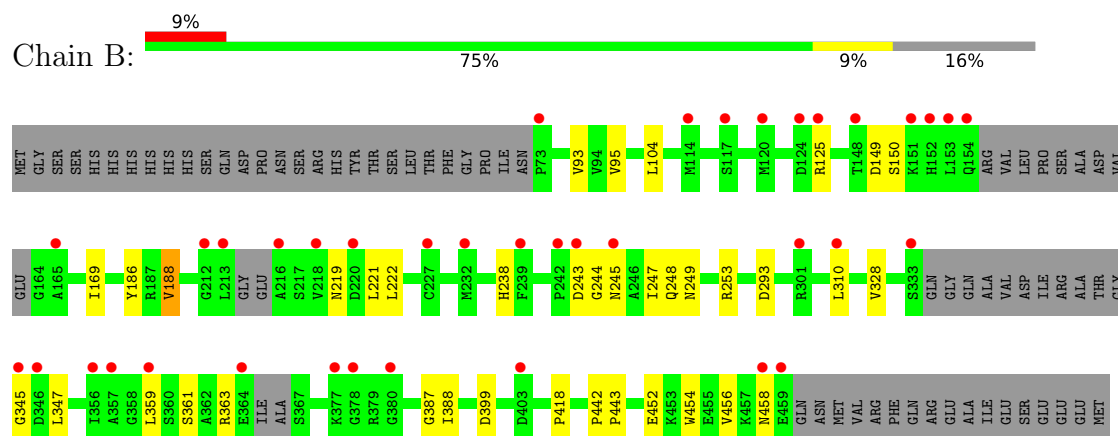
3 Residue-property plots [i](#)

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.

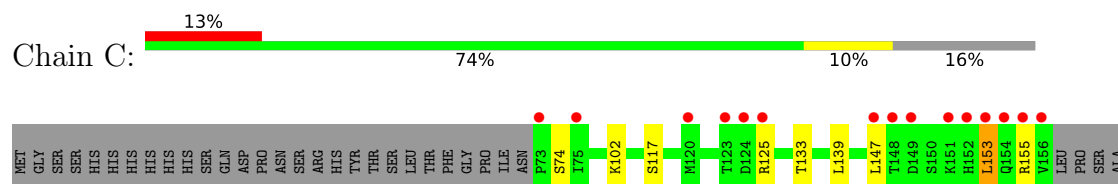
- Molecule 1: Transferase-like protein

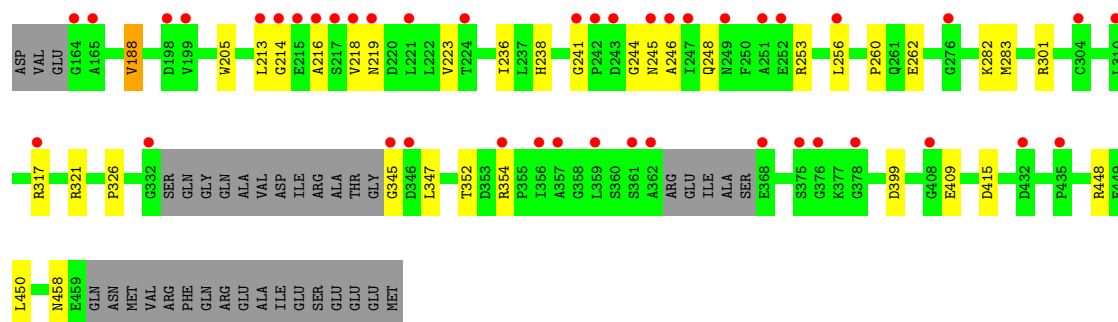


- Molecule 1: Transferase-like protein

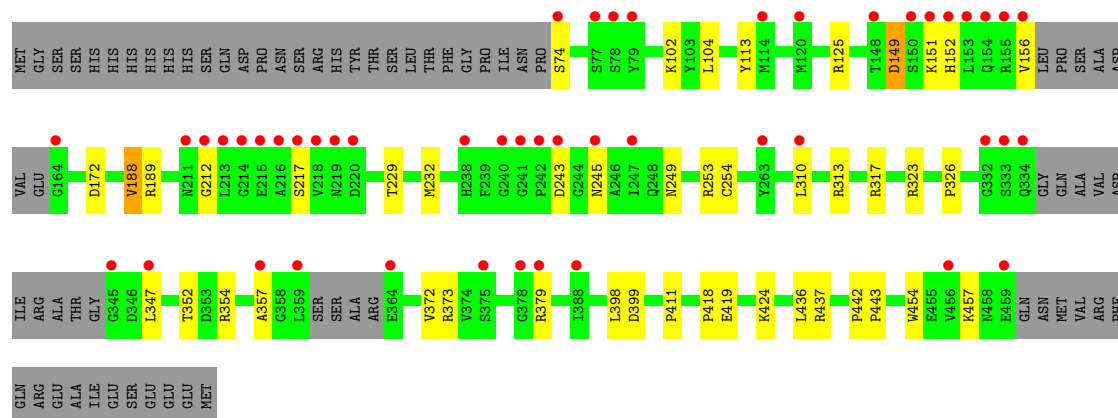
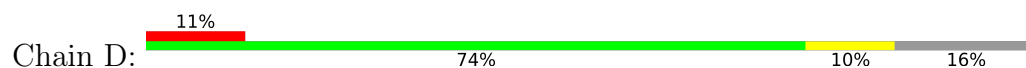


- Molecule 1: Transferase-like protein

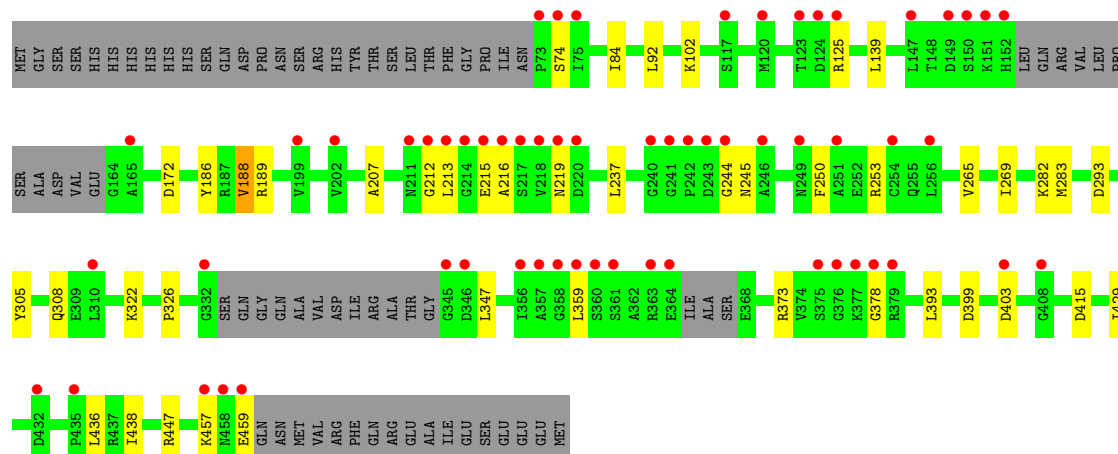
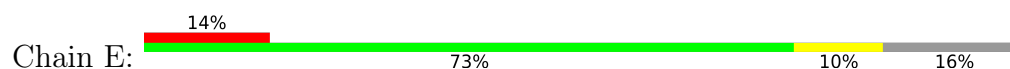




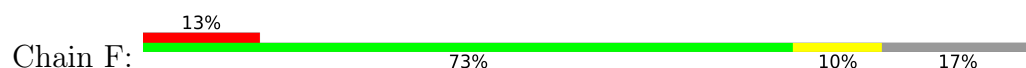
• Molecule 1: Transferase-like protein

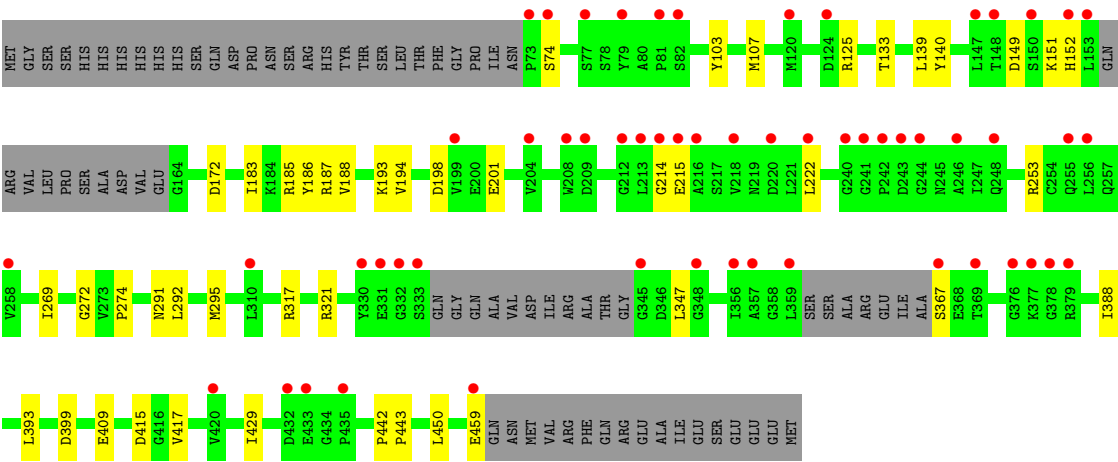


• Molecule 1: Transferase-like protein



• Molecule 1: Transferase-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.53Å 134.18Å 107.01Å 90.00° 97.59° 90.00°	Depositor
Resolution (Å)	47.34 – 2.40 47.34 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.34-2.40) 99.5 (47.34-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.238 , 0.274 0.238 , 0.273	Depositor DCC
R_{free} test set	5246 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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

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	0.14	0/2919	0.35	0/3956
1	B	0.13	0/2856	0.35	0/3868
1	C	0.14	0/2856	0.35	0/3870
1	D	0.15	0/2874	0.35	0/3894
1	E	0.13	0/2841	0.36	0/3849
1	F	0.14	0/2824	0.35	0/3827
All	All	0.14	0/17170	0.35	0/23264

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.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	VAL	Peptide
1	D	149	ASP	Peptide

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	2862	0	2882	30	0
1	B	2801	0	2812	24	0
1	C	2800	0	2815	32	0
1	D	2819	0	2832	29	0
1	E	2785	0	2793	30	0
1	F	2768	0	2780	33	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	2	0
3	F	36	0	0	2	0
All	All	17142	0	16944	158	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 5.

All (158) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:TYR:CZ	1:F:107:MET:HE1	2.32	0.64
1:E:457:LYS:NZ	3:E:601:HOH:O	2.26	0.63
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:F:274:PRO:HD2	1:F:295:MET:HE1	1.80	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:248:GLN:H	1:B:248:GLN:CD	2.13	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:291:ASN:HB2	1:F:295:MET:HE3	1.88	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:A:244:GLY:C	1:A:245:ASN:HD22	2.17	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:140:TYR:OH	2:F:501:CIT:O2	2.19	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:E:322:LYS:NZ	3:E:608:HOH:O	2.46	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: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: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:E:244:GLY:O	1:E:245:ASN:HB2	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:364:GLU:O	1:A:365:ILE:C	2.62	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:C:244:GLY:O	1:C:245:ASN:HB2	2.19	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
1:E:269:ILE:HD12	1:E:393:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:HG13	1:A:436:LEU:HD21	2.02	0.41
1:B:248:GLN:CD	1:B:248:GLN:N	2.79	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:103:TYR:CE2	1:F:107:MET:HE1	2.56	0.41
1:F:107:MET:HB2	1:F:107:MET:HE3	1.53	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%)	36	50
1	B	353/432 (82%)	340 (96%)	11 (3%)	2 (1%)	21	32
1	C	355/432 (82%)	341 (96%)	12 (3%)	2 (1%)	21	32
1	D	357/432 (83%)	346 (97%)	9 (2%)	2 (1%)	21	32
1	E	353/432 (82%)	337 (96%)	14 (4%)	2 (1%)	21	32
1	F	351/432 (81%)	339 (97%)	11 (3%)	1 (0%)	36	50
All	All	2133/2592 (82%)	2052 (96%)	71 (3%)	10 (0%)	24	37

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 ⓘ

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%)	299 (98%)	7 (2%)	44	66
1	B	300/359 (84%)	298 (99%)	2 (1%)	76	88
1	C	299/359 (83%)	295 (99%)	4 (1%)	61	80
1	D	301/359 (84%)	298 (99%)	3 (1%)	68	84
1	E	297/359 (83%)	293 (99%)	4 (1%)	61	80
1	F	296/359 (82%)	290 (98%)	6 (2%)	48	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1799/2154 (84%)	1773 (99%)	26 (1%)	59 79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	213	LEU
1	A	218	VAL
1	A	252	GLU
1	A	417	VAL
1	A	420	VAL
1	A	429	ILE
1	B	310	LEU
1	B	388	ILE
1	C	74	SER
1	C	117	SER
1	C	153	LEU
1	C	218	VAL
1	D	74	SER
1	D	172	ASP
1	D	379	ARG
1	E	74	SER
1	E	172	ASP
1	E	219	ASN
1	E	359	LEU
1	F	74	SER
1	F	172	ASP
1	F	292	LEU
1	F	388	ILE
1	F	417	VAL
1	F	429	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	B	152	HIS
1	B	458	ASN
1	C	135	GLN
1	C	248	GLN
1	C	316	HIS

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Mol	Chain	Res	Type
1	C	458	ASN
1	D	135	GLN
1	D	316	HIS
1	D	458	ASN
1	E	308	GLN
1	F	316	HIS
1	F	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 oligosaccharides 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	E	501	-	12,12,12	1.09	0	17,17,17	1.50	2 (11%)
2	CIT	F	501	-	12,12,12	1.12	0	17,17,17	1.38	2 (11%)
2	CIT	B	501	-	12,12,12	1.14	0	17,17,17	1.50	2 (11%)
2	CIT	C	501	-	12,12,12	1.10	0	17,17,17	1.64	3 (17%)
2	CIT	D	501	-	12,12,12	1.07	0	17,17,17	1.42	3 (17%)
2	CIT	A	501	-	12,12,12	1.12	0	17,17,17	1.42	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	E	501	-	-	4/16/16/16	-
2	CIT	F	501	-	-	0/16/16/16	-
2	CIT	B	501	-	-	4/16/16/16	-
2	CIT	C	501	-	-	7/16/16/16	-
2	CIT	D	501	-	-	8/16/16/16	-
2	CIT	A	501	-	-	1/16/16/16	-

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	4.00	120.81	113.14
2	E	501	CIT	O6-C6-C3	3.92	120.66	113.14
2	A	501	CIT	O6-C6-C3	3.75	120.33	113.14
2	D	501	CIT	O6-C6-C3	3.54	119.94	113.14
2	F	501	CIT	O6-C6-C3	3.41	119.69	113.14
2	B	501	CIT	O6-C6-C3	3.36	119.59	113.14
2	C	501	CIT	C3-C4-C5	-2.57	106.90	113.92
2	D	501	CIT	O4-C5-C4	2.17	121.23	114.35
2	C	501	CIT	O4-C5-C4	2.13	121.09	114.35
2	F	501	CIT	O4-C5-C4	2.10	121.00	114.35
2	D	501	CIT	O2-C1-O1	-2.04	118.09	123.33
2	B	501	CIT	O2-C1-C2	2.03	120.78	114.35
2	E	501	CIT	O4-C5-C4	2.03	120.77	114.35

There are no chirality outliers.

All (24) 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	D	501	CIT	C2-C3-C6-O5
2	C	501	CIT	C1-C2-C3-C6

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Mol	Chain	Res	Type	Atoms
2	D	501	CIT	O7-C3-C6-O5
2	D	501	CIT	C2-C3-C6-O6
2	D	501	CIT	C4-C3-C6-O5
2	D	501	CIT	C4-C3-C6-O6
2	B	501	CIT	C6-C3-C4-C5
2	D	501	CIT	O7-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	O7-C3-C4-C5
2	E	501	CIT	C2-C3-C6-O5
2	D	501	CIT	C3-C4-C5-O4
2	A	501	CIT	C1-C2-C3-C6
2	B	501	CIT	C3-C4-C5-O3
2	D	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	E	501	CIT	1	0
2	F	501	CIT	2	0
2	B	501	CIT	1	0
2	A	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

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	372/432 (86%)	0.83	46 (12%) 8 6	39, 55, 90, 110	0
1	B	363/432 (84%)	0.71	38 (10%) 11 8	38, 55, 87, 104	0
1	C	363/432 (84%)	0.99	58 (15%) 5 4	41, 60, 91, 110	0
1	D	365/432 (84%)	0.95	48 (13%) 7 5	41, 57, 92, 113	0
1	E	361/432 (83%)	0.96	60 (16%) 4 3	42, 58, 90, 107	0
1	F	359/432 (83%)	1.02	56 (15%) 5 4	45, 60, 94, 113	0
All	All	2183/2592 (84%)	0.91	306 (14%) 6 5	38, 57, 91, 113	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	ALA	7.0
1	F	153	LEU	6.2
1	A	365	ILE	6.1
1	C	153	LEU	5.8
1	F	345	GLY	5.6
1	A	156	VAL	5.5
1	E	216	ALA	5.5
1	B	216	ALA	5.2
1	C	246	ALA	5.2
1	A	214	GLY	5.2
1	D	241	GLY	5.0
1	D	153	LEU	5.0
1	C	216	ALA	4.9
1	E	214	GLY	4.9
1	B	357	ALA	4.7
1	E	241	GLY	4.6
1	A	357	ALA	4.5
1	A	218	VAL	4.5
1	E	152	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	157	LEU	4.5
1	F	213	LEU	4.5
1	A	154	GLN	4.4
1	A	216	ALA	4.3
1	D	74	SER	4.3
1	A	378	GLY	4.2
1	D	218	VAL	4.2
1	D	359	LEU	4.2
1	E	73	PRO	4.2
1	E	359	LEU	4.2
1	D	345	GLY	4.1
1	E	310	LEU	4.1
1	C	214	GLY	4.1
1	E	332	GLY	4.1
1	B	378	GLY	4.0
1	C	156	VAL	4.0
1	F	240	GLY	3.9
1	E	123	THR	3.9
1	D	242	PRO	3.9
1	E	240	GLY	3.9
1	D	154	GLN	3.8
1	B	364	GLU	3.8
1	E	218	VAL	3.8
1	C	378	GLY	3.8
1	E	345	GLY	3.8
1	B	154	GLN	3.8
1	C	332	GLY	3.7
1	D	357	ALA	3.7
1	F	378	GLY	3.7
1	A	73	PRO	3.7
1	A	241	GLY	3.7
1	D	332	GLY	3.7
1	F	82	SER	3.7
1	E	357	ALA	3.7
1	B	153	LEU	3.7
1	F	310	LEU	3.7
1	A	151	LYS	3.7
1	E	375	SER	3.6
1	E	215	GLU	3.6
1	E	219	ASN	3.6
1	E	249	ASN	3.6
1	F	214	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	124	ASP	3.6
1	A	240	GLY	3.5
1	D	213	LEU	3.5
1	F	212	GLY	3.5
1	C	148	THR	3.5
1	D	152	HIS	3.5
1	B	458	ASN	3.5
1	F	218	VAL	3.5
1	C	408	GLY	3.4
1	B	151	LYS	3.4
1	F	79	TYR	3.4
1	E	364	GLU	3.4
1	B	73	PRO	3.4
1	D	378	GLY	3.4
1	E	213	LEU	3.4
1	F	242	PRO	3.4
1	E	75	ILE	3.4
1	C	123	THR	3.3
1	C	213	LEU	3.3
1	E	199	VAL	3.3
1	D	240	GLY	3.3
1	A	152	HIS	3.3
1	C	357	ALA	3.3
1	D	156	VAL	3.3
1	A	147	LEU	3.2
1	A	403	ASP	3.2
1	B	213	LEU	3.2
1	D	212	GLY	3.2
1	E	246	ALA	3.2
1	E	361	SER	3.2
1	A	242	PRO	3.1
1	A	364	GLU	3.1
1	B	242	PRO	3.1
1	A	117	SER	3.1
1	D	375	SER	3.1
1	D	334	GLN	3.1
1	C	362	ALA	3.0
1	E	403	ASP	3.0
1	A	217	SER	3.0
1	C	164	GLY	3.0
1	E	165	ALA	3.0
1	F	435	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	164	GLY	3.0
1	B	152	HIS	3.0
1	F	243	ASP	3.0
1	B	345	GLY	3.0
1	C	215	GLU	3.0
1	E	379	ARG	3.0
1	E	151	LYS	3.0
1	C	375	SER	3.0
1	F	356	ILE	2.9
1	C	73	PRO	2.9
1	F	379	ARG	2.9
1	D	150	SER	2.9
1	A	158	PRO	2.9
1	A	150	SER	2.9
1	F	74	SER	2.9
1	A	310	LEU	2.9
1	D	215	GLU	2.9
1	C	152	HIS	2.9
1	F	199	VAL	2.9
1	B	346	ASP	2.9
1	C	245	ASN	2.8
1	B	227	CYS	2.8
1	C	310	LEU	2.8
1	F	152	HIS	2.8
1	C	252	GLU	2.8
1	C	125	ARG	2.8
1	C	198	ASP	2.8
1	C	243	ASP	2.8
1	F	81	PRO	2.8
1	C	359	LEU	2.8
1	F	216	ALA	2.8
1	D	243	ASP	2.8
1	F	332	GLY	2.7
1	C	249	ASN	2.7
1	D	216	ALA	2.7
1	F	215	GLU	2.7
1	E	149	ASP	2.7
1	A	345	GLY	2.7
1	C	247	ILE	2.7
1	D	148	THR	2.7
1	B	245	ASN	2.7
1	C	120	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	120	MET	2.7
1	E	125	ARG	2.7
1	F	433	GLU	2.7
1	F	248	GLN	2.7
1	E	243	ASP	2.7
1	C	356	ILE	2.7
1	F	73	PRO	2.7
1	C	151	LYS	2.7
1	C	361	SER	2.7
1	D	217	SER	2.7
1	F	150	SER	2.7
1	A	124	ASP	2.6
1	A	379	ARG	2.6
1	C	219	ASN	2.6
1	D	310	LEU	2.6
1	A	160	ALA	2.6
1	C	154	GLN	2.6
1	C	345	GLY	2.6
1	D	164	GLY	2.6
1	C	435	PRO	2.6
1	A	301	ARG	2.6
1	A	213	LEU	2.6
1	F	222	LEU	2.6
1	F	357	ALA	2.6
1	D	263	TYR	2.6
1	A	332	GLY	2.6
1	B	232	MET	2.6
1	F	120	MET	2.6
1	E	459	GLU	2.6
1	F	359	LEU	2.6
1	D	211	ASN	2.6
1	D	78	SER	2.6
1	E	217	SER	2.6
1	D	79	TYR	2.6
1	B	124	ASP	2.6
1	E	150	SER	2.6
1	F	333	SER	2.6
1	E	120	MET	2.5
1	E	212	GLY	2.5
1	F	348	GLY	2.5
1	B	356	ILE	2.5
1	B	310	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	254	CYS	2.5
1	C	224	THR	2.5
1	E	242	PRO	2.5
1	B	377	LYS	2.5
1	B	125	ARG	2.5
1	C	241	GLY	2.5
1	F	244	GLY	2.5
1	F	209	ASP	2.5
1	B	218	VAL	2.5
1	D	238	HIS	2.5
1	C	165	ALA	2.5
1	F	241	GLY	2.5
1	E	457	LYS	2.5
1	F	147	LEU	2.5
1	F	255	GLN	2.5
1	C	251	ALA	2.5
1	A	333	SER	2.5
1	D	114	MET	2.5
1	B	380	GLY	2.4
1	D	379	ARG	2.4
1	A	367	SER	2.4
1	B	220	ASP	2.4
1	E	244	GLY	2.4
1	D	220	ASP	2.4
1	E	220	ASP	2.4
1	A	153	LEU	2.4
1	D	219	ASN	2.4
1	C	354	ARG	2.4
1	E	124	ASP	2.4
1	C	218	VAL	2.4
1	F	420	VAL	2.4
1	C	155	ARG	2.3
1	F	124	ASP	2.3
1	F	204	VAL	2.3
1	A	219	ASN	2.3
1	D	214	GLY	2.3
1	E	378	GLY	2.3
1	B	359	LEU	2.3
1	C	75	ILE	2.3
1	C	432	ASP	2.3
1	F	330	TYR	2.3
1	B	212	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	2.3
1	F	246	ALA	2.3
1	F	376	GLY	2.3
1	C	217	SER	2.3
1	D	77	SER	2.3
1	F	77	SER	2.3
1	C	149	ASP	2.3
1	F	432	ASP	2.3
1	A	459	GLU	2.3
1	B	459	GLU	2.3
1	E	435	PRO	2.3
1	B	165	ALA	2.2
1	B	114	MET	2.2
1	B	120	MET	2.2
1	D	247	ILE	2.2
1	E	74	SER	2.2
1	E	360	SER	2.2
1	A	458	ASN	2.2
1	F	148	THR	2.2
1	C	376	GLY	2.2
1	E	376	GLY	2.2
1	C	147	LEU	2.2
1	E	147	LEU	2.2
1	B	333	SER	2.2
1	E	346	ASP	2.2
1	F	220	ASP	2.2
1	E	211	ASN	2.2
1	E	458	ASN	2.2
1	D	151	LYS	2.2
1	D	347	LEU	2.2
1	F	256	LEU	2.2
1	E	363	ARG	2.2
1	F	377	LYS	2.2
1	D	245	ASN	2.2
1	C	221	LEU	2.2
1	C	256	LEU	2.2
1	F	367	SER	2.2
1	E	432	ASP	2.2
1	B	301	ARG	2.2
1	D	155	ARG	2.2
1	C	242	PRO	2.2
1	E	358	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	368	GLU	2.1
1	F	331	GLU	2.1
1	B	117	SER	2.1
1	D	456	VAL	2.1
1	A	123	THR	2.1
1	D	364	GLU	2.1
1	F	459	GLU	2.1
1	A	243	ASP	2.1
1	A	361	SER	2.1
1	E	377	LYS	2.1
1	B	239	PHE	2.1
1	E	202	VAL	2.1
1	E	251	ALA	2.1
1	C	317	ARG	2.1
1	E	356	ILE	2.1
1	C	276	GLY	2.1
1	F	369	THR	2.1
1	A	346	ASP	2.1
1	B	403	ASP	2.1
1	A	199	VAL	2.0
1	F	258	VAL	2.0
1	A	359	LEU	2.0
1	E	256	LEU	2.0
1	E	408	GLY	2.0
1	B	148	THR	2.0
1	D	333	SER	2.0
1	E	117	SER	2.0
1	C	304	CYS	2.0
1	C	199	VAL	2.0
1	D	459	GLU	2.0
1	A	212	GLY	2.0
1	A	358	GLY	2.0
1	D	388	ILE	2.0
1	F	208	TRP	2.0
1	C	346	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	C	501	13/13	0.78	0.15	61,70,79,94	0
2	CIT	A	501	13/13	0.83	0.13	53,62,67,68	0
2	CIT	E	501	13/13	0.83	0.14	67,72,78,82	0
2	CIT	F	501	13/13	0.87	0.13	60,69,76,77	0
2	CIT	B	501	13/13	0.93	0.10	55,57,64,68	0
2	CIT	D	501	13/13	0.93	0.08	54,62,65,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.