



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 03:29 AM EDT

PDB ID : 5VXS  
Title : Crystal Structure Analysis of human CLYBL in apo form  
Authors : Shen, H.  
Deposited on : 2017-05-24  
Resolution : 2.95 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

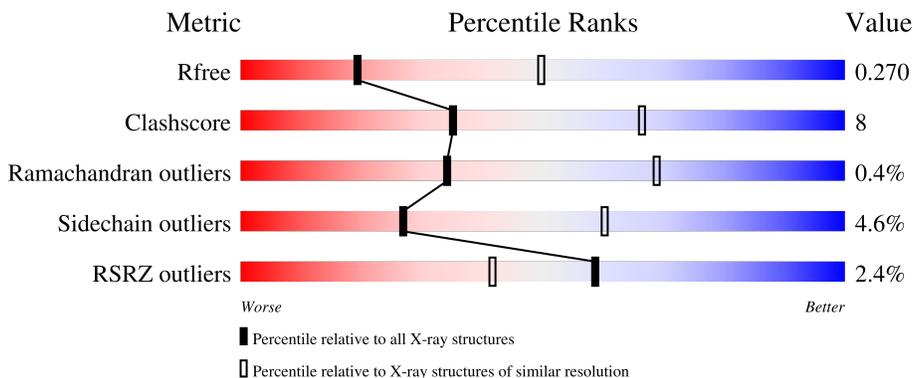
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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  $\leq 5\%$ . 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	325	 3% 63% 22% 15%
1	B	325	 % 69% 15% • 13%
1	C	325	 69% 21% • 8%
1	D	325	 6% 69% 16% • 12%
1	E	325	 % 70% 15% • 13%

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Mol	Chain	Length	Quality of chain
1	F	325	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '79%', a yellow segment labeled '13%', and a small grey segment at the end labeled '7%'.</p>

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 13462 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 Citrate lyase subunit beta-like protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	Total 2147	C 1372	N 365	O 402	S 8	0	0	0
1	B	283	Total 2200	C 1408	N 373	O 410	S 9	0	0	0
1	C	299	Total 2332	C 1491	N 396	O 435	S 10	0	0	0
1	D	285	Total 2218	C 1418	N 376	O 414	S 10	0	0	0
1	E	283	Total 2198	C 1404	N 373	O 412	S 9	0	0	0
1	F	301	Total 2341	C 1496	N 398	O 437	S 10	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP Q8N0X4
A	25	ALA	-	expression tag	UNP Q8N0X4
A	26	SER	-	expression tag	UNP Q8N0X4
A	27	LEU	-	expression tag	UNP Q8N0X4
A	28	ALA	-	expression tag	UNP Q8N0X4
A	29	ASN	-	expression tag	UNP Q8N0X4
A	341	LEU	-	expression tag	UNP Q8N0X4
A	342	GLU	-	expression tag	UNP Q8N0X4
A	343	HIS	-	expression tag	UNP Q8N0X4
A	344	HIS	-	expression tag	UNP Q8N0X4
A	345	HIS	-	expression tag	UNP Q8N0X4
A	346	HIS	-	expression tag	UNP Q8N0X4
A	347	HIS	-	expression tag	UNP Q8N0X4
A	348	HIS	-	expression tag	UNP Q8N0X4
B	24	MET	-	expression tag	UNP Q8N0X4
B	25	ALA	-	expression tag	UNP Q8N0X4
B	26	SER	-	expression tag	UNP Q8N0X4

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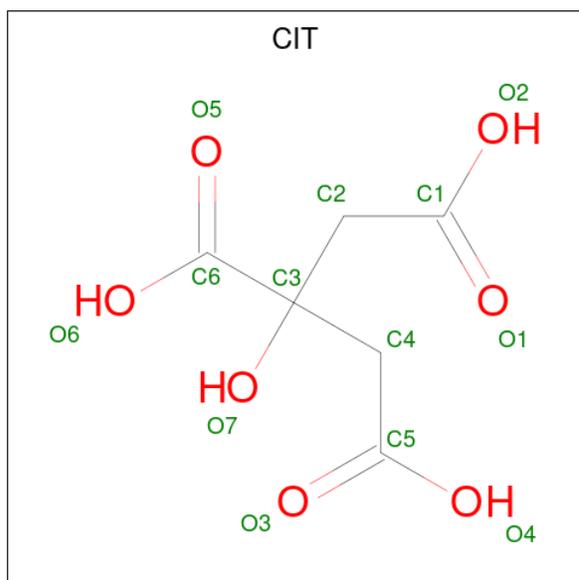
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	LEU	-	expression tag	UNP Q8N0X4
B	28	ALA	-	expression tag	UNP Q8N0X4
B	29	ASN	-	expression tag	UNP Q8N0X4
B	341	LEU	-	expression tag	UNP Q8N0X4
B	342	GLU	-	expression tag	UNP Q8N0X4
B	343	HIS	-	expression tag	UNP Q8N0X4
B	344	HIS	-	expression tag	UNP Q8N0X4
B	345	HIS	-	expression tag	UNP Q8N0X4
B	346	HIS	-	expression tag	UNP Q8N0X4
B	347	HIS	-	expression tag	UNP Q8N0X4
B	348	HIS	-	expression tag	UNP Q8N0X4
C	24	MET	-	expression tag	UNP Q8N0X4
C	25	ALA	-	expression tag	UNP Q8N0X4
C	26	SER	-	expression tag	UNP Q8N0X4
C	27	LEU	-	expression tag	UNP Q8N0X4
C	28	ALA	-	expression tag	UNP Q8N0X4
C	29	ASN	-	expression tag	UNP Q8N0X4
C	341	LEU	-	expression tag	UNP Q8N0X4
C	342	GLU	-	expression tag	UNP Q8N0X4
C	343	HIS	-	expression tag	UNP Q8N0X4
C	344	HIS	-	expression tag	UNP Q8N0X4
C	345	HIS	-	expression tag	UNP Q8N0X4
C	346	HIS	-	expression tag	UNP Q8N0X4
C	347	HIS	-	expression tag	UNP Q8N0X4
C	348	HIS	-	expression tag	UNP Q8N0X4
D	24	MET	-	expression tag	UNP Q8N0X4
D	25	ALA	-	expression tag	UNP Q8N0X4
D	26	SER	-	expression tag	UNP Q8N0X4
D	27	LEU	-	expression tag	UNP Q8N0X4
D	28	ALA	-	expression tag	UNP Q8N0X4
D	29	ASN	-	expression tag	UNP Q8N0X4
D	341	LEU	-	expression tag	UNP Q8N0X4
D	342	GLU	-	expression tag	UNP Q8N0X4
D	343	HIS	-	expression tag	UNP Q8N0X4
D	344	HIS	-	expression tag	UNP Q8N0X4
D	345	HIS	-	expression tag	UNP Q8N0X4
D	346	HIS	-	expression tag	UNP Q8N0X4
D	347	HIS	-	expression tag	UNP Q8N0X4
D	348	HIS	-	expression tag	UNP Q8N0X4
E	24	MET	-	expression tag	UNP Q8N0X4
E	25	ALA	-	expression tag	UNP Q8N0X4
E	26	SER	-	expression tag	UNP Q8N0X4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	27	LEU	-	expression tag	UNP Q8N0X4
E	28	ALA	-	expression tag	UNP Q8N0X4
E	29	ASN	-	expression tag	UNP Q8N0X4
E	341	LEU	-	expression tag	UNP Q8N0X4
E	342	GLU	-	expression tag	UNP Q8N0X4
E	343	HIS	-	expression tag	UNP Q8N0X4
E	344	HIS	-	expression tag	UNP Q8N0X4
E	345	HIS	-	expression tag	UNP Q8N0X4
E	346	HIS	-	expression tag	UNP Q8N0X4
E	347	HIS	-	expression tag	UNP Q8N0X4
E	348	HIS	-	expression tag	UNP Q8N0X4
F	24	MET	-	expression tag	UNP Q8N0X4
F	25	ALA	-	expression tag	UNP Q8N0X4
F	26	SER	-	expression tag	UNP Q8N0X4
F	27	LEU	-	expression tag	UNP Q8N0X4
F	28	ALA	-	expression tag	UNP Q8N0X4
F	29	ASN	-	expression tag	UNP Q8N0X4
F	341	LEU	-	expression tag	UNP Q8N0X4
F	342	GLU	-	expression tag	UNP Q8N0X4
F	343	HIS	-	expression tag	UNP Q8N0X4
F	344	HIS	-	expression tag	UNP Q8N0X4
F	345	HIS	-	expression tag	UNP Q8N0X4
F	346	HIS	-	expression tag	UNP Q8N0X4
F	347	HIS	-	expression tag	UNP Q8N0X4
F	348	HIS	-	expression tag	UNP Q8N0X4

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

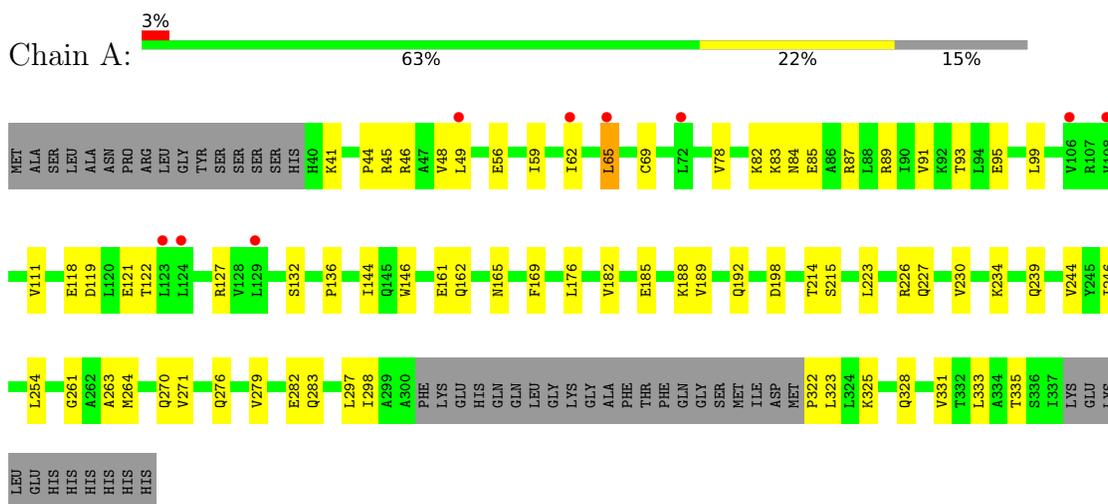


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
2	A	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

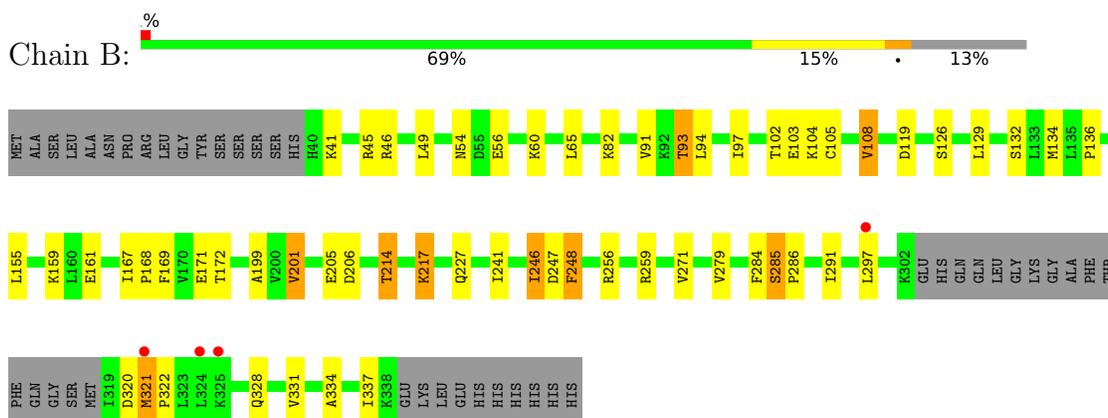
### 3 Residue-property plots [i](#)

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.

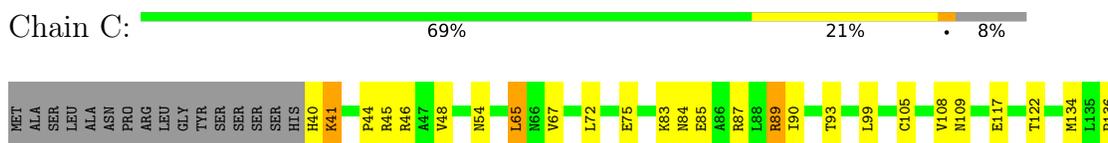
- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial

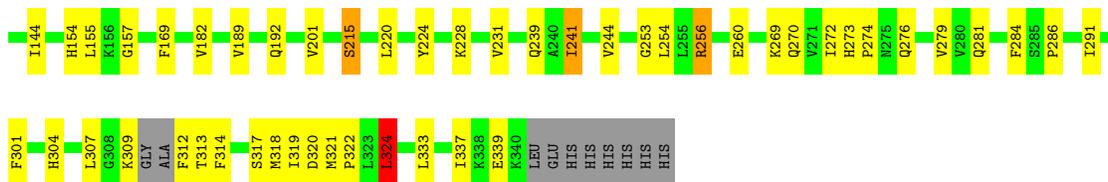


- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial

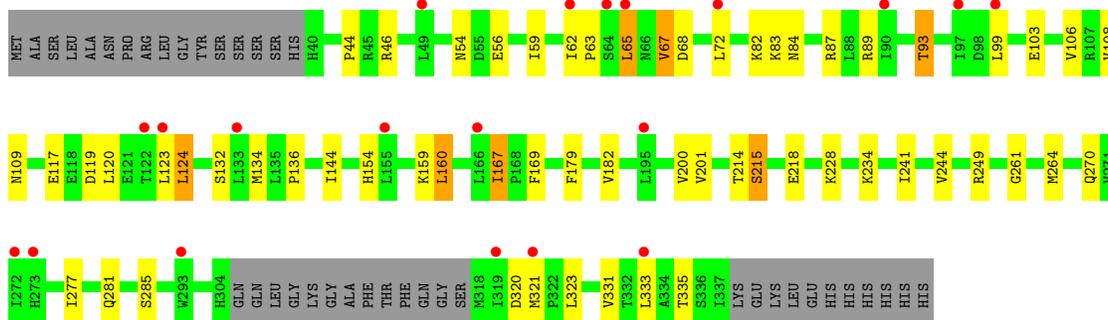


- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial

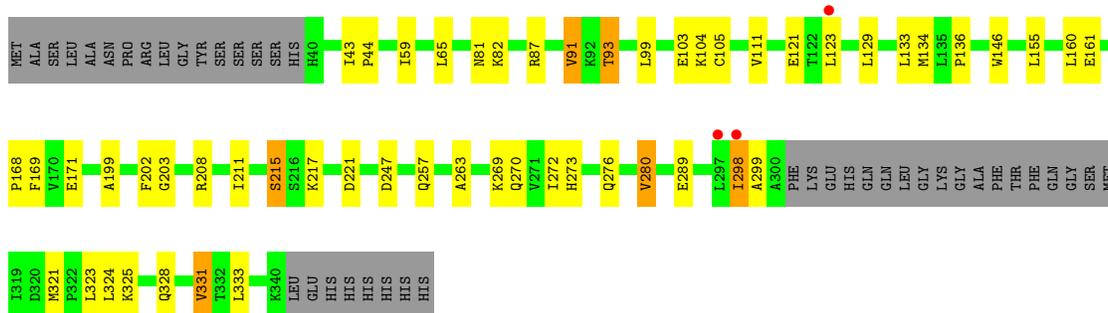




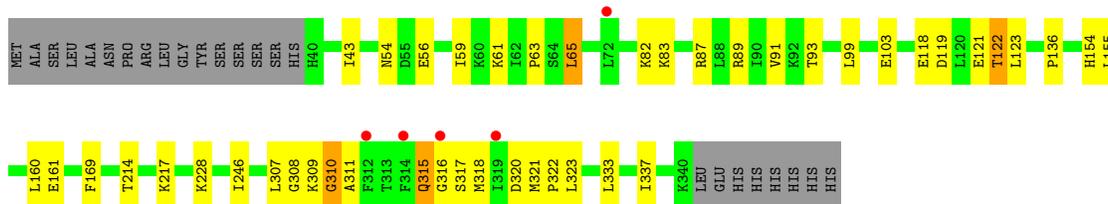
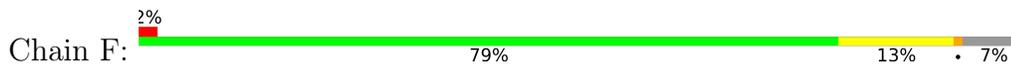
- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial



- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial



- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.63Å 154.63Å 156.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	133.91 – 2.95 133.91 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (133.91-2.95) 99.9 (133.91-2.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.205 , 0.272 0.204 , 0.270	Depositor DCC
$R_{free}$ test set	2309 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.4	Xtrriage
Anisotropy	0.234	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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	0.44	0/2182	0.60	0/2948
1	B	0.47	0/2236	0.64	0/3019
1	C	0.49	0/2371	0.63	1/3197 (0.0%)
1	D	0.46	0/2255	0.64	2/3045 (0.1%)
1	E	0.46	0/2233	0.65	1/3015 (0.0%)
1	F	0.48	0/2381	0.65	1/3212 (0.0%)
All	All	0.47	0/13658	0.64	5/18436 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	LEU	CA-CB-CG	6.61	130.49	115.30
1	F	123	LEU	CA-CB-CG	6.07	129.26	115.30
1	D	160	LEU	CA-CB-CG	5.87	128.79	115.30
1	E	161	GLU	C-N-CA	5.73	136.02	121.70
1	D	123	LEU	CA-CB-CG	5.31	127.51	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2147	0	2214	40	0
1	B	2200	0	2272	36	0
1	C	2332	0	2397	59	0
1	D	2218	0	2281	36	0
1	E	2198	0	2269	32	0
1	F	2341	0	2406	28	0
2	A	13	0	5	1	0
2	F	13	0	5	4	0
All	All	13462	0	13849	223	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 8.

All (223) 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:B:217:LYS:HE3	1:B:247:ASP:HB2	1.68	0.76
1:D:56:GLU:HA	1:D:59:ILE:HB	1.66	0.75
1:D:46:ARG:HD3	1:D:333:LEU:HD11	1.72	0.72
1:C:256:ARG:NH2	1:C:260:GLU:OE1	2.24	0.71
1:D:72:LEU:HB2	1:D:106:VAL:HG22	1.75	0.69
1:D:228:LYS:NZ	2:F:401:CIT:H41	2.08	0.68
1:D:46:ARG:HB2	1:D:281:GLN:OE1	1.94	0.68
1:C:84:ASN:HD22	1:D:249:ARG:HD2	1.57	0.68
1:A:59:ILE:HD11	1:A:93:THR:HG21	1.78	0.65
1:A:188:LYS:O	1:A:192:GLN:NE2	2.28	0.65
1:C:201:VAL:HG22	1:C:241:ILE:HG12	1.80	0.64
1:F:315:GLN:NE2	1:F:317:SER:OG	2.31	0.63
1:B:284:PHE:O	1:B:285:SER:OG	2.15	0.62
1:E:217:LYS:NZ	1:E:247:ASP:HB2	2.14	0.62
1:B:286:PRO:HB2	1:B:291:ILE:HG13	1.80	0.61
1:F:155:LEU:HD11	1:F:160:LEU:HD11	1.80	0.61
1:B:91:VAL:HG22	1:B:126:SER:HB2	1.81	0.61
1:F:136:PRO:HA	1:F:169:PHE:HB2	1.83	0.61
1:F:228:LYS:NZ	2:F:401:CIT:H21	2.15	0.61
1:B:328:GLN:O	1:B:331:VAL:HG22	2.01	0.61
1:E:136:PRO:HA	1:E:169:PHE:HB2	1.82	0.60
1:C:189:VAL:HA	1:C:192:GLN:HE21	1.66	0.60
1:F:121:GLU:OE1	1:F:154:HIS:ND1	2.35	0.59
1:D:320:ASP:OD1	1:D:320:ASP:N	2.33	0.59
1:B:136:PRO:HA	1:B:169:PHE:HB2	1.85	0.59
1:C:307:LEU:HD12	1:C:309:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:MET:HB3	1:B:322:PRO:HD3	1.86	0.58
1:C:201:VAL:HG13	1:C:241:ILE:HD11	1.85	0.58
1:E:298:ILE:HG13	1:E:299:ALA:N	2.19	0.58
1:C:45:ARG:HH11	1:C:239:GLN:HE22	1.53	0.57
1:C:40:HIS:HA	1:C:41:LYS:HZ2	1.70	0.57
1:C:48:VAL:HG21	1:C:241:ILE:HD13	1.87	0.57
1:C:75:GLU:O	1:C:83:LYS:NZ	2.37	0.56
1:A:322:PRO:HA	1:A:325:LYS:HE2	1.88	0.56
1:E:44:PRO:HB3	1:E:333:LEU:HD13	1.87	0.56
1:A:136:PRO:HA	1:A:169:PHE:HB2	1.87	0.56
1:C:136:PRO:HA	1:C:169:PHE:HB2	1.87	0.56
1:E:81:ASN:O	1:E:82:LYS:HG2	2.05	0.55
1:C:72:LEU:HB3	1:C:90:ILE:HG12	1.86	0.55
1:E:257:GLN:HE21	1:E:269:LYS:NZ	2.05	0.55
1:D:228:LYS:HZ1	2:F:401:CIT:H41	1.70	0.55
1:E:99:LEU:HB2	1:E:104:LYS:HE3	1.88	0.55
1:F:320:ASP:CG	1:F:322:PRO:HD2	2.28	0.54
1:F:87:ARG:O	1:F:91:VAL:HG12	2.08	0.54
1:A:226:ARG:NH2	1:A:264:MET:HE1	2.23	0.53
1:B:201:VAL:HB	1:B:241:ILE:HB	1.89	0.53
1:D:261:GLY:HA2	1:D:264:MET:HE2	1.91	0.53
1:C:241:ILE:O	1:C:241:ILE:HG13	2.08	0.53
1:A:56:GLU:HG3	1:A:89:ARG:NE	2.23	0.53
1:A:41:LYS:HE3	1:A:162:GLN:HE21	1.74	0.53
1:B:108:VAL:HG12	1:B:119:ASP:HB3	1.91	0.52
1:B:256:ARG:HA	1:B:259:ARG:HG2	1.90	0.52
1:B:248:PHE:H	1:B:248:PHE:HD1	1.58	0.52
1:F:56:GLU:HB2	1:F:89:ARG:NH1	2.24	0.52
1:F:63:PRO:HG3	1:F:99:LEU:HA	1.90	0.52
1:C:41:LYS:NZ	1:C:41:LYS:H	2.08	0.52
1:C:307:LEU:HB2	1:C:309:LYS:HG3	1.91	0.52
1:D:108:VAL:HG23	1:D:109:ASN:O	2.10	0.52
1:C:45:ARG:HH11	1:C:239:GLN:NE2	2.07	0.51
1:E:111:VAL:HG13	1:E:146:TRP:CE3	2.45	0.51
1:A:254:LEU:HD12	1:A:276:GLN:HE21	1.75	0.51
1:B:167:ILE:HG12	1:B:199:ALA:HB3	1.93	0.51
1:F:161:GLU:N	1:F:161:GLU:OE1	2.43	0.51
1:C:254:LEU:HD21	1:C:276:GLN:HB3	1.92	0.50
1:D:103:GLU:OE2	1:D:132:SER:OG	2.27	0.50
1:D:215:SER:O	1:D:215:SER:OG	2.28	0.50
1:E:217:LYS:HZ1	1:E:247:ASP:HB2	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:LEU:O	1:F:337:ILE:HG12	2.10	0.50
1:A:244:VAL:HG22	1:A:270:GLN:HB2	1.92	0.50
1:D:83:LYS:HG3	1:D:84:ASN:N	2.26	0.50
1:A:95:GLU:HG2	1:A:127:ARG:HB3	1.94	0.50
1:B:320:ASP:OD1	1:B:321:MET:N	2.43	0.50
1:D:136:PRO:HA	1:D:169:PHE:HB2	1.93	0.50
1:E:202:PHE:O	1:E:270:GLN:NE2	2.43	0.50
1:C:89:ARG:O	1:C:93:THR:N	2.44	0.50
1:A:328:GLN:O	1:A:331:VAL:HG22	2.12	0.50
1:D:68:ASP:H	1:D:281:GLN:HE22	1.60	0.50
1:C:304:HIS:CE1	1:C:312:PHE:HB2	2.47	0.49
1:C:41:LYS:H	1:C:41:LYS:HZ3	1.59	0.49
1:C:244:VAL:HG11	1:C:272:ILE:HD12	1.95	0.49
1:E:272:ILE:HG23	1:E:273:HIS:ND1	2.28	0.49
1:A:46:ARG:HD3	1:A:333:LEU:HD11	1.95	0.49
1:A:48:VAL:HG22	1:A:69:CYS:SG	2.53	0.49
1:C:215:SER:O	1:C:215:SER:OG	2.31	0.49
1:C:320:ASP:CG	1:C:322:PRO:HD2	2.33	0.49
1:A:89:ARG:NH1	1:A:89:ARG:HB2	2.28	0.48
1:A:176:LEU:HD23	1:C:231:VAL:HG11	1.95	0.48
1:D:228:LYS:HZ2	2:F:401:CIT:H41	1.79	0.48
1:E:168:PRO:HD2	1:E:199:ALA:O	2.14	0.48
1:B:227:GLN:HE21	1:C:224:TYR:HB3	1.78	0.48
1:A:44:PRO:HB3	1:A:333:LEU:HD13	1.95	0.48
1:A:87:ARG:NH2	1:A:118:GLU:HB3	2.28	0.48
1:E:276:GLN:O	1:E:280:VAL:HG13	2.14	0.47
1:C:87:ARG:HB3	1:C:122:THR:HG21	1.96	0.47
1:B:286:PRO:HB2	1:B:291:ILE:CG1	2.42	0.47
1:C:46:ARG:HG2	1:C:284:PHE:O	2.15	0.47
1:E:43:ILE:HD13	1:E:103:GLU:OE2	2.15	0.47
1:F:309:LYS:HG3	1:F:310:GLY:H	1.79	0.47
1:B:171:GLU:HG2	1:B:206:ASP:HB2	1.97	0.47
1:C:67:VAL:HA	1:C:281:GLN:OE1	2.15	0.47
1:D:117:GLU:HG2	1:D:154:HIS:NE2	2.30	0.47
1:E:208:ARG:HD2	1:E:215:SER:HA	1.97	0.47
1:A:62:ILE:HB	1:A:99:LEU:HD22	1.96	0.47
1:C:54:ASN:HB2	1:C:85:GLU:OE1	2.15	0.47
1:C:319:ILE:N	1:C:319:ILE:HD12	2.30	0.47
1:D:331:VAL:O	1:D:335:THR:HG23	2.14	0.47
1:F:54:ASN:HD22	1:F:82:LYS:HB3	1.80	0.47
1:E:257:GLN:HG2	1:E:269:LYS:HZ3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLU:HG2	1:C:154:HIS:NE2	2.30	0.46
1:D:244:VAL:HG22	1:D:270:GLN:HB2	1.96	0.46
1:B:168:PRO:HD2	1:B:199:ALA:O	2.16	0.46
1:D:65:LEU:HB2	1:D:67:VAL:HG22	1.98	0.46
1:E:105:CYS:SG	1:E:134:MET:HG3	2.56	0.46
1:E:263:ALA:HA	1:F:214:THR:HG23	1.97	0.46
1:A:87:ARG:NE	1:A:119:ASP:OD1	2.48	0.46
1:B:105:CYS:SG	1:B:134:MET:HG3	2.56	0.46
1:D:46:ARG:NE	1:D:285:SER:OG	2.49	0.45
1:F:118:GLU:O	1:F:122:THR:HG23	2.16	0.45
1:C:144:ILE:HG13	1:C:182:VAL:HG13	1.97	0.45
1:D:89:ARG:O	1:D:93:THR:OG1	2.31	0.45
1:A:261:GLY:HA2	1:A:264:MET:HE2	1.98	0.45
1:D:84:ASN:HA	1:D:87:ARG:HG2	1.98	0.45
1:F:87:ARG:NE	1:F:119:ASP:OD1	2.50	0.45
1:A:331:VAL:O	1:A:335:THR:HG23	2.17	0.45
1:E:325:LYS:HA	1:E:328:GLN:HG2	1.99	0.45
1:F:307:LEU:HB3	1:F:308:GLY:H	1.65	0.45
1:D:62:ILE:HB	1:D:99:LEU:HD22	1.99	0.45
1:D:134:MET:HG2	1:D:167:ILE:HG12	1.99	0.45
1:D:234:LYS:HG3	1:E:211:ILE:HA	1.99	0.45
1:F:323:LEU:HD23	1:F:323:LEU:HA	1.86	0.45
1:C:220:LEU:O	1:C:220:LEU:HG	2.17	0.45
1:A:254:LEU:HD11	1:A:276:GLN:HB3	1.99	0.44
1:A:111:VAL:HG13	1:A:146:TRP:CE3	2.52	0.44
1:A:226:ARG:CZ	1:A:264:MET:HE1	2.48	0.44
1:B:56:GLU:HG2	1:B:60:LYS:HE3	2.00	0.44
1:B:93:THR:HA	1:B:97:ILE:HD13	1.98	0.44
1:C:244:VAL:HG11	1:C:272:ILE:CD1	2.47	0.44
1:F:43:ILE:HG21	1:F:103:GLU:OE2	2.17	0.44
1:A:185:GLU:O	1:A:189:VAL:HG22	2.17	0.44
1:B:82:LYS:HA	1:B:82:LYS:HD2	1.66	0.44
1:C:65:LEU:H	1:C:65:LEU:HG	1.66	0.44
1:B:105:CYS:SG	1:B:132:SER:HB2	2.58	0.44
1:C:253:GLY:O	1:C:256:ARG:N	2.51	0.44
1:F:61:LYS:O	1:F:61:LYS:HG2	2.18	0.44
1:D:72:LEU:HD12	1:D:106:VAL:HG22	2.00	0.44
1:F:217:LYS:HB3	1:F:217:LYS:HE2	1.86	0.44
1:B:334:ALA:O	1:B:337:ILE:HG22	2.18	0.44
1:C:99:LEU:HD12	1:C:99:LEU:HA	1.71	0.43
1:A:230:VAL:O	1:A:234:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:HH11	1:B:45:ARG:HD3	1.68	0.43
1:A:144:ILE:HG13	1:A:182:VAL:HG13	2.00	0.43
1:C:108:VAL:HG23	1:C:109:ASN:O	2.18	0.43
1:C:40:HIS:HA	1:C:41:LYS:NZ	2.32	0.43
1:C:273:HIS:HA	1:C:274:PRO:HD3	1.87	0.43
1:E:217:LYS:HZ2	1:E:247:ASP:HB2	1.82	0.43
1:F:59:ILE:HD13	1:F:93:THR:HG21	1.99	0.43
1:B:227:GLN:HE22	1:C:224:TYR:H	1.66	0.43
1:B:246:ILE:HD13	1:B:246:ILE:HA	1.70	0.43
1:C:201:VAL:HA	1:C:241:ILE:HG13	2.00	0.43
1:C:105:CYS:SG	1:C:134:MET:HG3	2.58	0.43
1:A:49:LEU:HD12	1:A:271:VAL:O	2.19	0.43
2:A:401:CIT:H41	1:C:228:LYS:NZ	2.33	0.43
1:B:227:GLN:NE2	1:C:224:TYR:H	2.16	0.43
1:E:155:LEU:HD11	1:E:160:LEU:HD11	2.01	0.43
1:C:44:PRO:HB3	1:C:333:LEU:HD13	2.01	0.43
1:F:59:ILE:HG21	1:F:93:THR:HG21	2.01	0.43
1:A:65:LEU:H	1:A:65:LEU:HG	1.64	0.43
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.93	0.43
1:A:322:PRO:O	1:A:325:LYS:HG2	2.18	0.42
1:C:269:LYS:HB2	1:C:284:PHE:CE2	2.54	0.42
1:C:314:PHE:HB3	1:C:319:ILE:HD11	2.01	0.42
1:D:67:VAL:HG13	1:D:277:ILE:HD13	2.01	0.42
1:B:103:GLU:HG2	1:B:104:LYS:N	2.34	0.42
1:E:208:ARG:CD	1:E:215:SER:HA	2.49	0.42
1:E:129:LEU:HA	1:E:129:LEU:HD23	1.76	0.42
1:C:301:PHE:CZ	1:C:324:LEU:HD11	2.54	0.42
1:D:54:ASN:HD22	1:D:82:LYS:HB3	1.84	0.42
1:C:313:THR:HG22	1:C:318:MET:HG2	2.02	0.42
1:E:87:ARG:O	1:E:91:VAL:HG13	2.19	0.42
1:D:63:PRO:HG3	1:D:99:LEU:HA	2.02	0.42
1:D:144:ILE:HG13	1:D:182:VAL:HG13	2.01	0.42
1:E:215:SER:O	1:E:215:SER:OG	2.32	0.42
1:A:261:GLY:HA2	1:A:264:MET:CE	2.50	0.42
1:A:132:SER:OG	1:A:165:ASN:HB2	2.20	0.42
1:B:155:LEU:HD23	1:B:155:LEU:HA	1.74	0.42
1:D:159:LYS:HA	1:D:159:LYS:HD2	1.94	0.42
1:A:263:ALA:HA	1:B:214:THR:HG23	2.02	0.41
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.92	0.41
1:C:286:PRO:HG2	1:C:291:ILE:HD11	2.02	0.41
1:C:337:ILE:C	1:C:339:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:VAL:HG12	1:E:123:LEU:HD23	2.00	0.41
1:B:46:ARG:HH11	1:B:285:SER:HB3	1.85	0.41
1:C:54:ASN:HB3	1:C:85:GLU:HG3	2.03	0.41
1:D:44:PRO:O	1:D:68:ASP:HB3	2.20	0.41
1:E:99:LEU:HD12	1:E:104:LYS:HD2	2.02	0.41
1:A:95:GLU:O	1:A:127:ARG:NH1	2.48	0.41
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.91	0.41
1:C:46:ARG:NH1	1:C:337:ILE:HD11	2.36	0.41
1:E:59:ILE:HG21	1:E:93:THR:HG21	2.02	0.41
1:A:165:ASN:HD22	1:A:198:ASP:HB2	1.85	0.41
1:B:49:LEU:HA	1:B:271:VAL:O	2.21	0.41
1:C:304:HIS:HD2	1:C:309:LYS:HD3	1.86	0.41
1:C:320:ASP:OD1	1:C:322:PRO:HD2	2.21	0.41
1:E:133:LEU:HD23	1:E:133:LEU:HA	1.83	0.41
1:D:179:PHE:CZ	1:D:200:VAL:HG21	2.56	0.41
1:A:279:VAL:O	1:A:283:GLN:HG2	2.21	0.41
1:F:83:LYS:O	1:F:87:ARG:HG3	2.20	0.41
1:B:54:ASN:HD22	1:B:82:LYS:HB3	1.86	0.41
1:B:320:ASP:CG	1:B:321:MET:H	2.24	0.41
1:C:241:ILE:HD12	1:C:270:GLN:HG3	2.02	0.41
1:F:311:ALA:HB1	1:F:318:MET:HE3	2.03	0.41
1:A:223:LEU:HD21	1:A:227:GLN:NE2	2.36	0.41
1:E:171:GLU:CG	1:E:203:GLY:HA3	2.51	0.41
1:C:201:VAL:HG22	1:C:241:ILE:CG1	2.48	0.40
1:F:246:ILE:HD13	1:F:246:ILE:HA	1.95	0.40
1:A:45:ARG:HB2	1:A:239:GLN:OE1	2.21	0.40
1:D:201:VAL:HG22	1:D:241:ILE:HB	2.02	0.40
1:F:65:LEU:H	1:F:65:LEU:HG	1.48	0.40
1:E:328:GLN:O	1:E:331:VAL:HG12	2.21	0.40
1:F:315:GLN:H	1:F:315:GLN:HG3	1.64	0.40
1:D:120:LEU:O	1:D:124:LEU:HG	2.21	0.40
1:A:83:LYS:HG3	1:A:84:ASN:N	2.37	0.40
1:B:129:LEU:HD23	1:B:129:LEU:HA	1.81	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	273/325 (84%)	266 (97%)	6 (2%)	1 (0%)	34	69
1	B	279/325 (86%)	268 (96%)	8 (3%)	3 (1%)	14	46
1	C	295/325 (91%)	286 (97%)	8 (3%)	1 (0%)	41	73
1	D	281/325 (86%)	269 (96%)	12 (4%)	0	100	100
1	E	279/325 (86%)	270 (97%)	9 (3%)	0	100	100
1	F	299/325 (92%)	283 (95%)	14 (5%)	2 (1%)	22	56
All	All	1706/1950 (88%)	1642 (96%)	57 (3%)	7 (0%)	34	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	GLU
1	A	161	GLU
1	F	316	GLY
1	B	321	MET
1	C	157	GLY
1	B	285	SER
1	F	310	GLY

### 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	235/276 (85%)	222 (94%)	13 (6%)	21	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	241/276 (87%)	226 (94%)	15 (6%)	18	48
1	C	255/276 (92%)	245 (96%)	10 (4%)	32	65
1	D	243/276 (88%)	231 (95%)	12 (5%)	25	58
1	E	241/276 (87%)	228 (95%)	13 (5%)	22	54
1	F	255/276 (92%)	251 (98%)	4 (2%)	62	84
All	All	1470/1656 (89%)	1403 (95%)	67 (5%)	27	60

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	78	VAL
1	A	82	LYS
1	A	85	GLU
1	A	91	VAL
1	A	121	GLU
1	A	122	THR
1	A	214	THR
1	A	215	SER
1	A	246	ILE
1	A	282	GLU
1	A	297	LEU
1	A	298	ILE
1	B	41	LYS
1	B	65	LEU
1	B	93	THR
1	B	102	THR
1	B	108	VAL
1	B	159	LYS
1	B	172	THR
1	B	201	VAL
1	B	205	GLU
1	B	214	THR
1	B	217	LYS
1	B	246	ILE
1	B	248	PHE
1	B	279	VAL
1	B	297	LEU
1	C	41	LYS
1	C	65	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	89	ARG
1	C	215	SER
1	C	241	ILE
1	C	256	ARG
1	C	279	VAL
1	C	317	SER
1	C	321	MET
1	C	324	LEU
1	D	65	LEU
1	D	67	VAL
1	D	93	THR
1	D	119	ASP
1	D	124	LEU
1	D	160	LEU
1	D	167	ILE
1	D	214	THR
1	D	215	SER
1	D	218	GLU
1	D	321	MET
1	D	323	LEU
1	E	65	LEU
1	E	91	VAL
1	E	93	THR
1	E	121	GLU
1	E	215	SER
1	E	221	ASP
1	E	280	VAL
1	E	289	GLU
1	E	298	ILE
1	E	321	MET
1	E	323	LEU
1	E	324	LEU
1	E	331	VAL
1	F	65	LEU
1	F	122	THR
1	F	315	GLN
1	F	321	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	125	GLN

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Mol	Chain	Res	Type
1	A	162	GLN
1	A	165	ASN
1	A	276	GLN
1	A	281	GLN
1	A	329	ASN
1	B	125	GLN
1	B	227	GLN
1	B	326	GLN
1	C	84	ASN
1	C	192	GLN
1	C	239	GLN
1	C	304	HIS
1	D	165	ASN
1	D	257	GLN
1	D	270	GLN
1	E	257	GLN
1	E	326	GLN
1	F	84	ASN
1	F	273	HIS
1	F	306	GLN
1	F	315	GLN

### 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](#)

2 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	A	401	-	12,12,12	1.17	0	17,17,17	1.92	4 (23%)
2	CIT	F	401	-	12,12,12	1.40	1 (8%)	17,17,17	1.94	4 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	401	-	-	10/16/16/16	-
2	CIT	F	401	-	-	6/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	CIT	C3-C6	3.20	1.56	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CIT	O6-C6-C3	4.81	121.41	113.05
2	F	401	CIT	O6-C6-C3	4.57	120.98	113.05
2	F	401	CIT	C2-C3-C6	3.26	117.11	110.11
2	F	401	CIT	O6-C6-O5	-2.90	114.60	123.82
2	A	401	CIT	O4-C5-O3	-2.71	116.55	123.30
2	A	401	CIT	O4-C5-C4	2.61	122.72	114.35
2	A	401	CIT	O5-C6-C3	-2.31	118.98	122.25
2	F	401	CIT	C4-C3-C2	-2.00	103.94	109.16

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CIT	C1-C2-C3-O7
2	A	401	CIT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	F	401	CIT	O7-C3-C6-O5
2	F	401	CIT	O7-C3-C6-O6
2	F	401	CIT	C4-C3-C6-O5
2	F	401	CIT	C4-C3-C6-O6
2	A	401	CIT	C1-C2-C3-C6
2	A	401	CIT	C6-C3-C4-C5
2	A	401	CIT	C2-C3-C4-C5
2	A	401	CIT	O7-C3-C4-C5
2	A	401	CIT	C2-C3-C6-O6
2	A	401	CIT	C4-C3-C6-O5
2	A	401	CIT	C4-C3-C6-O6
2	F	401	CIT	C2-C3-C6-O5
2	F	401	CIT	C2-C3-C6-O6
2	A	401	CIT	C2-C3-C6-O5

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CIT	1	0
2	F	401	CIT	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/325 (85%)	0.17	9 (3%) 47 31	48, 87, 122, 129	0
1	B	283/325 (87%)	0.09	4 (1%) 75 59	48, 77, 129, 136	0
1	C	299/325 (92%)	0.02	0 100 100	45, 72, 98, 105	0
1	D	285/325 (87%)	0.30	20 (7%) 16 9	50, 99, 127, 144	0
1	E	283/325 (87%)	-0.08	3 (1%) 80 65	51, 73, 106, 130	0
1	F	301/325 (92%)	0.06	5 (1%) 70 53	43, 67, 112, 130	0
All	All	1728/1950 (88%)	0.09	41 (2%) 59 42	43, 77, 122, 144	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	123	LEU	4.4
1	A	129	LEU	4.1
1	B	321	MET	4.0
1	D	293	TRP	3.8
1	D	49	LEU	3.4
1	D	321	MET	3.3
1	D	122	THR	3.3
1	D	155	LEU	2.8
1	F	319	ILE	2.8
1	A	65	LEU	2.8
1	D	133	LEU	2.7
1	B	325	LYS	2.7
1	D	62	ILE	2.7
1	A	106	VAL	2.6
1	D	65	LEU	2.6
1	A	123	LEU	2.6
1	F	316	GLY	2.5
1	D	99	LEU	2.5
1	D	195	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	2.5
1	B	297	LEU	2.5
1	E	123	LEU	2.5
1	D	166	LEU	2.5
1	F	72	LEU	2.4
1	D	273	HIS	2.4
1	E	297	LEU	2.4
1	D	97	ILE	2.3
1	A	108	VAL	2.3
1	A	62	ILE	2.3
1	D	272	ILE	2.3
1	A	124	LEU	2.2
1	D	333	LEU	2.2
1	D	319	ILE	2.2
1	B	324	LEU	2.2
1	D	72	LEU	2.2
1	F	312	PHE	2.2
1	F	314	PHE	2.2
1	D	64	SER	2.2
1	E	298	ILE	2.1
1	D	90	ILE	2.0
1	A	49	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	CIT	A	401	13/13	0.82	0.20	65,86,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	F	401	13/13	0.89	0.12	74,87,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.