



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:04 PM UTC

PDB ID : 5VXS / pdb_00005vxs
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

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

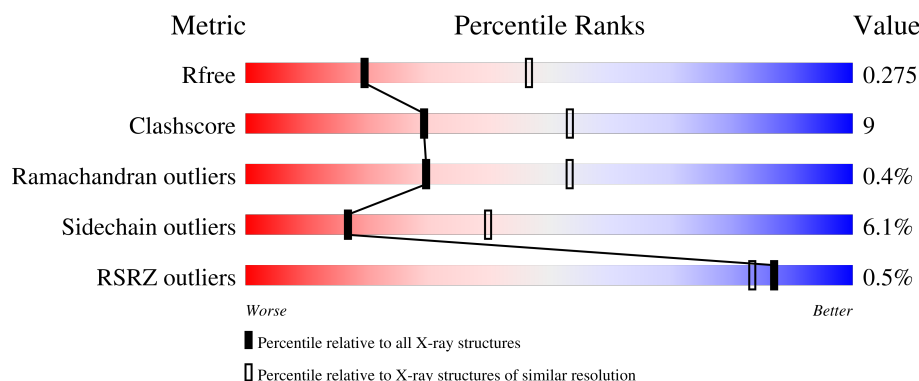
1 Overall quality at a glance

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	325	% 62% 22% • 15%
1	B	325	% 67% 17% • 13%
1	C	325	68% 21% • 8%
1	D	325	% 68% 17% • 12%
1	E	325	70% 16% • 13%

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Mol	Chain	Length	Quality of chain
1	F	325	76% 14% • 7%

2 Entry composition

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

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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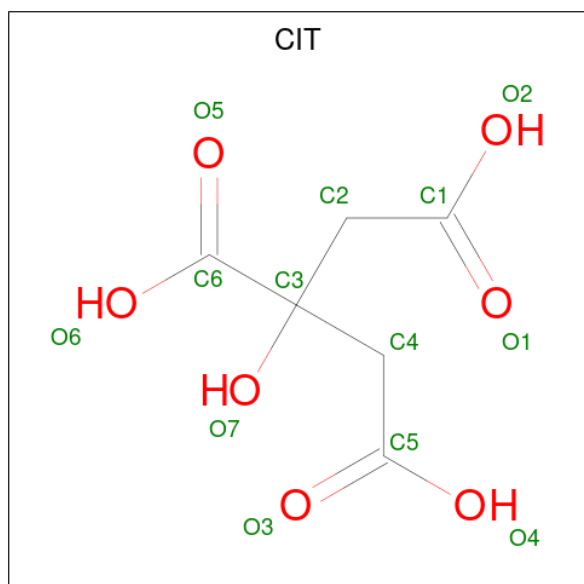
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	LEU	-	expression tag	UNP Q8N0X4
B	28	ALA	-	expression tag	UNP Q8N0X4
B	29	ASN	-	expression tag	UNP Q8N0X4
B	341	LEU	-	expression tag	UNP Q8N0X4
B	342	GLU	-	expression tag	UNP Q8N0X4
B	343	HIS	-	expression tag	UNP Q8N0X4
B	344	HIS	-	expression tag	UNP 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 (CCD ID: CIT) (formula: $C_6H_8O_7$).

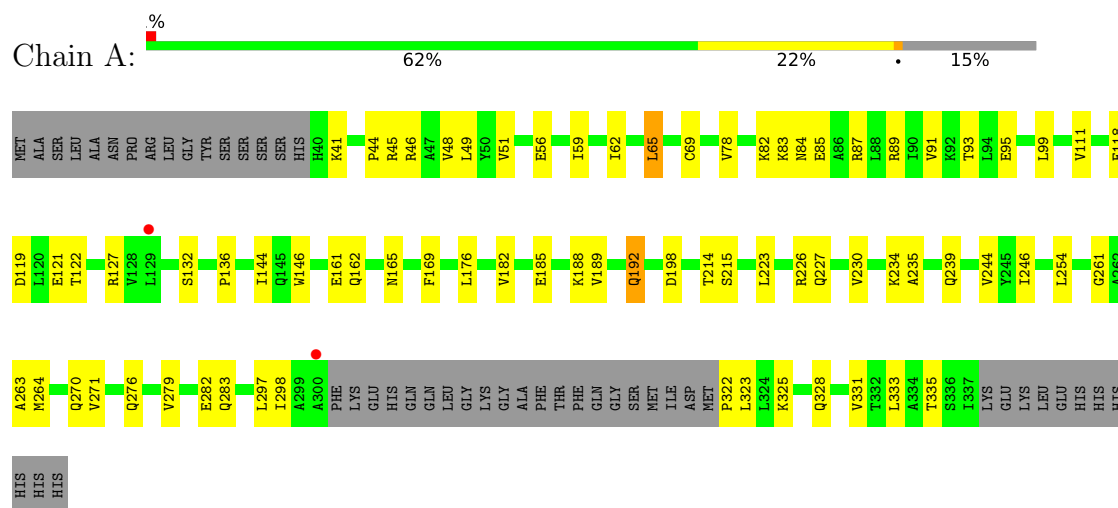


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

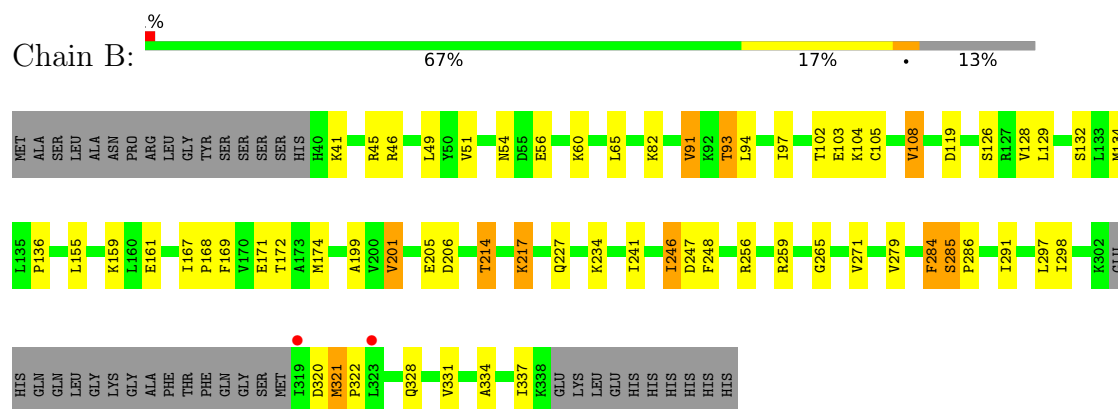
3 Residue-property plots

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.

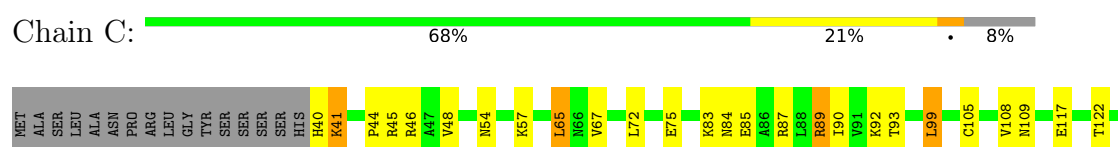
- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial

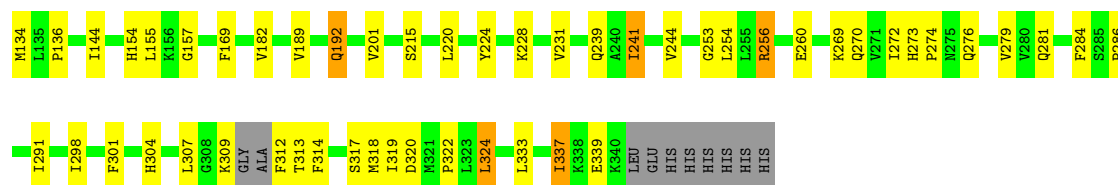


- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial

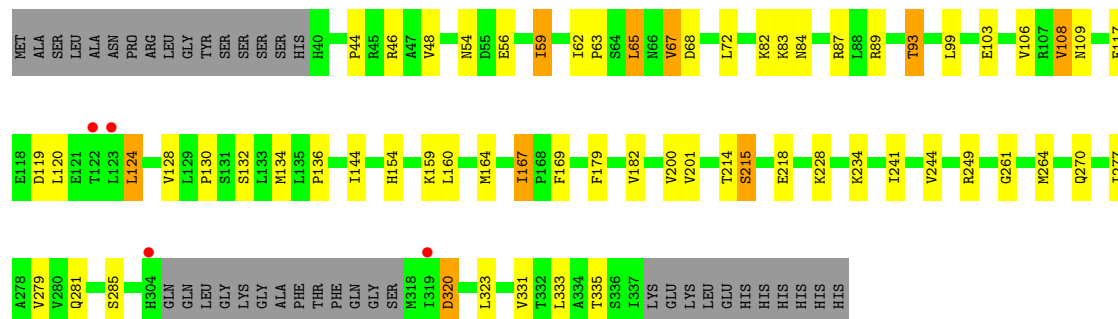


- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial

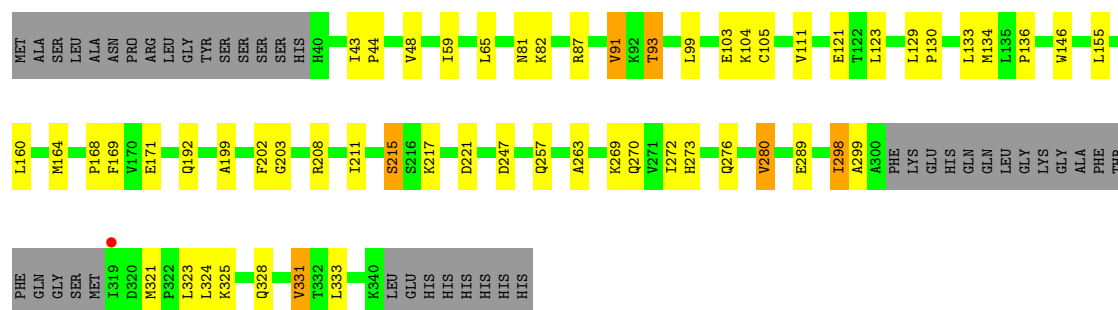




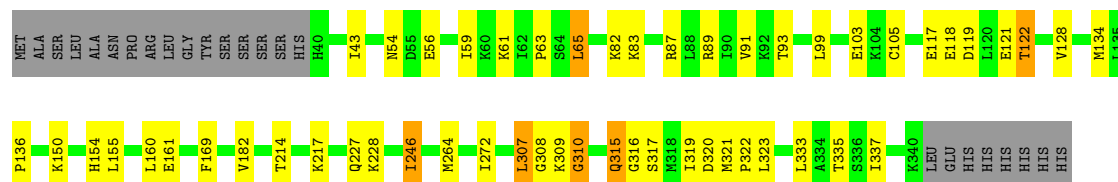
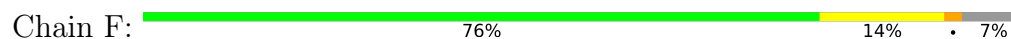
- Molecule 1: Citrate lyase subunit beta-like protein, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 100.0 (133.91-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.205 , 0.272 0.209 , 0.275	Depositor DCC
R_{free} test set	2309 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13462	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage'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.*

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	0.37	0/2182	0.58	0/2948
1	B	0.41	0/2236	0.62	1/3019 (0.0%)
1	C	0.44	0/2371	0.64	0/3197
1	D	0.39	0/2255	0.61	0/3045
1	E	0.41	0/2233	0.66	0/3015
1	F	0.43	0/2381	0.65	0/3212
All	All	0.41	0/13658	0.63	1/18436 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	PHE	N-CA-C	-6.20	100.25	109.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2147	0	2214	41	0
1	B	2200	0	2272	38	0
1	C	2332	0	2397	60	0
1	D	2218	0	2281	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2198	0	2269	32	0
1	F	2341	0	2406	32	0
2	A	13	0	5	1	0
2	F	13	0	5	5	0
All	All	13462	0	13849	234	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 9.

All (234) 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:D:261:GLY:HA2	1:D:264:MET:HE2	1.84	0.59
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:F:320:ASP:CG	1:F:322:PRO:HD2	2.28	0.59
1:C:307:LEU:HD12	1:C:309:LYS:HD2	1.84	0.58
1:B:321:MET:HB3	1:B:322:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:235:ALA:HB1	1:B:174:MET:HE2	1.89	0.55
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:134:MET:HE2	1:D:167:ILE:HD11	1.91	0.53
1:C:320:ASP:CG	1:C:322:PRO:HD2	2.33	0.53
1:C:241:ILE:O	1:C:241:ILE:HG13	2.08	0.53
1:D:48:VAL:HG11	1:D:134:MET:HE1	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:LYS:HZ1	1:E:247:ASP:HB2	1.74	0.50
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:257:GLN:HG2	1:E:269:LYS:HZ3	1.76	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: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:B:234:LYS:NZ	1:B:265:GLY:O	2.36	0.48
1:E:130:PRO:HD2	1:E:164:MET:HE1	1.95	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:D:89:ARG:O	1:D:93:THR:OG1	2.31	0.47
1:F:228:LYS:HZ1	2:F:401:CIT:H21	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:337:ILE:C	1:C:339:GLU:H	2.23	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:F:227:GLN:HG2	1:F:264:MET:HE3	1.97	0.46
1:B:320:ASP:CG	1:B:321:MET:H	2.24	0.45
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: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:C:105:CYS:SG	1:C:134:MET:HE3	2.57	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:D:103:GLU:CD	1:D:132:SER:HG	2.23	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:F:117:GLU:CD	1:F:150:LYS:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:MET:HE2	1:F:264:MET:HB3	1.56	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
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:48:VAL:HG11	1:C:134:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:HG13	1:D:182:VAL:HG13	2.01	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: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:C:241:ILE:HD12	1:C:270:GLN:HG3	2.02	0.41
1:F:105:CYS:SG	1:F:134:MET:HE3	2.61	0.41
1:A:223:LEU:HD21	1:A:227:GLN:NE2	2.36	0.41
1:D:130:PRO:HD2	1:D:164:MET:HE1	2.03	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%)	30	53
1	B	279/325 (86%)	268 (96%)	8 (3%)	3 (1%)	11	29
1	C	295/325 (91%)	286 (97%)	8 (3%)	1 (0%)	36	59
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%)	18	40
All	All	1706/1950 (88%)	1642 (96%)	57 (3%)	7 (0%)	30	53

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%)	220 (94%)	15 (6%)	16	38
1	B	241/276 (87%)	223 (92%)	18 (8%)	12	31
1	C	255/276 (92%)	240 (94%)	15 (6%)	18	41
1	D	243/276 (88%)	227 (93%)	16 (7%)	15	37
1	E	241/276 (87%)	226 (94%)	15 (6%)	16	39
1	F	255/276 (92%)	244 (96%)	11 (4%)	26	52
All	All	1470/1656 (89%)	1380 (94%)	90 (6%)	17	40

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
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	192	GLN
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	51	VAL
1	B	65	LEU
1	B	91	VAL
1	B	93	THR
1	B	102	THR
1	B	108	VAL
1	B	128	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

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Mol	Chain	Res	Type
1	B	279	VAL
1	B	297	LEU
1	B	298	ILE
1	C	41	LYS
1	C	57	LYS
1	C	65	LEU
1	C	89	ARG
1	C	92	LYS
1	C	99	LEU
1	C	192	GLN
1	C	215	SER
1	C	241	ILE
1	C	256	ARG
1	C	279	VAL
1	C	298	ILE
1	C	317	SER
1	C	324	LEU
1	C	337	ILE
1	D	59	ILE
1	D	65	LEU
1	D	67	VAL
1	D	93	THR
1	D	108	VAL
1	D	119	ASP
1	D	124	LEU
1	D	128	VAL
1	D	160	LEU
1	D	167	ILE
1	D	214	THR
1	D	215	SER
1	D	218	GLU
1	D	279	VAL
1	D	320	ASP
1	D	323	LEU
1	E	48	VAL
1	E	65	LEU
1	E	91	VAL
1	E	93	THR
1	E	121	GLU
1	E	192	GLN
1	E	215	SER
1	E	221	ASP

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Mol	Chain	Res	Type
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	128	VAL
1	F	182	VAL
1	F	246	ILE
1	F	272	ILE
1	F	307	LEU
1	F	315	GLN
1	F	319	ILE
1	F	321	MET
1	F	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	162	GLN
1	A	165	ASN
1	A	276	GLN
1	B	125	GLN
1	B	227	GLN
1	B	326	GLN
1	B	328	GLN
1	C	84	ASN
1	C	192	GLN
1	C	239	GLN
1	C	270	GLN
1	C	304	HIS
1	D	257	GLN
1	D	270	GLN
1	D	273	HIS
1	D	326	GLN
1	E	40	HIS
1	E	109	ASN
1	E	257	GLN

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Mol	Chain	Res	Type
1	E	326	GLN
1	F	84	ASN
1	F	125	GLN
1	F	192	GLN
1	F	273	HIS
1	F	305	GLN
1	F	306	GLN
1	F	315	GLN
1	F	329	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](#)

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	1.19	0	17,17,17	1.78	3 (17%)
2	CIT	F	401	-	12,12,12	1.43	1 (8%)	17,17,17	1.85	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. '-' 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	3.15	1.56	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CIT	O6-C6-C3	4.31	121.41	113.14
2	F	401	CIT	O6-C6-C3	4.09	120.98	113.14
2	F	401	CIT	C2-C3-C6	3.20	117.11	110.03
2	F	401	CIT	O6-C6-O5	-2.89	114.60	123.86
2	A	401	CIT	O4-C5-C4	2.64	122.72	114.35
2	A	401	CIT	O4-C5-O3	-2.64	116.55	123.33
2	F	401	CIT	C4-C3-C2	-2.09	103.94	109.31

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
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	O7-C3-C4-C5
2	A	401	CIT	C2-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	A	401	CIT	C2-C3-C6-O5
2	F	401	CIT	C2-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
2	F	401	CIT	C2-C3-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CIT	1	0
2	F	401	CIT	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	277/325 (85%)	-0.22	2 (0%) 84 80	48, 87, 122, 129	0
1	B	283/325 (87%)	-0.22	2 (0%) 84 80	48, 77, 129, 136	0
1	C	299/325 (92%)	-0.50	0 100 100	45, 72, 98, 105	0
1	D	285/325 (87%)	-0.00	4 (1%) 73 67	50, 99, 127, 144	0
1	E	283/325 (87%)	-0.47	1 (0%) 88 86	51, 73, 106, 130	0
1	F	301/325 (92%)	-0.51	0 100 100	43, 67, 112, 130	0
All	All	1728/1950 (88%)	-0.32	9 (0%) 87 83	43, 77, 122, 144	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	319	ILE	3.9
1	A	300	ALA	3.6
1	D	304	HIS	3.5
1	B	319	ILE	3.4
1	B	323	LEU	2.9
1	A	129	LEU	2.5
1	D	319	ILE	2.5
1	D	123	LEU	2.4
1	D	122	THR	2.3

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 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(Å ²)	Q<0.9
2	CIT	A	401	13/13	0.80	0.11	65,86,94,95	0
2	CIT	F	401	13/13	0.87	0.08	74,87,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.