



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:19 am BST

PDB ID : 2GUZ
Title : Structure of the Tim14-Tim16 complex of the mitochondrial protein import motor
Authors : Mokranjac, D.; Bourenkov, G.; Hell, K.; Neupert, W.; Groll, M.
Deposited on : 2006-05-02
Resolution : 2.00 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 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)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

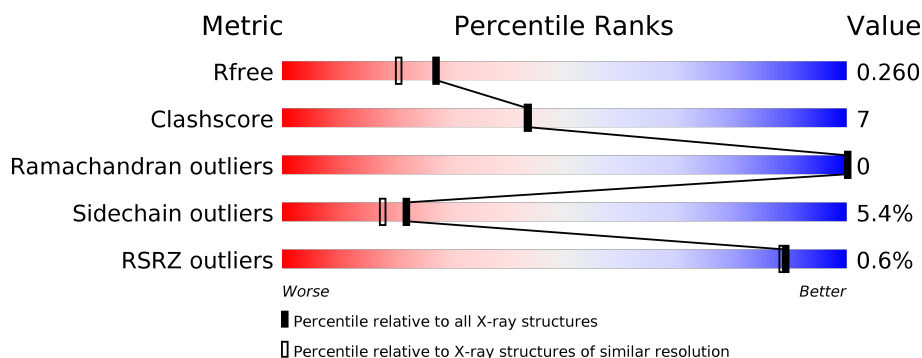
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	71	
1	C	71	
1	E	71	
1	G	71	
1	I	71	
1	K	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	71	 75% 23% .
1	O	71	 % 86% 10% .
2	B	65	 75% 20% . .
2	D	65	 78% 15% 6%
2	F	65	 77% 18% 5%
2	H	65	 69% 29% .
2	J	65	 74% 22% 5%
2	L	65	 85% 15%
2	N	65	 3% 68% 28% 5%
2	P	65	 2% 86% 12% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9819 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 Mitochondrial import inner membrane translocase subunit TIM14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	71	Total	C	N	O	S	6	0	0
			560	357	100	101	2			
1	C	71	Total	C	N	O	S	12	1	0
			562	359	100	101	2			
1	E	71	Total	C	N	O	S	13	1	0
			562	359	100	101	2			
1	G	71	Total	C	N	O	S	0	1	0
			562	359	100	101	2			
1	I	71	Total	C	N	O	S	10	1	0
			562	359	100	101	2			
1	K	71	Total	C	N	O	S	17	1	0
			562	359	100	101	2			
1	M	71	Total	C	N	O	S	12	0	0
			559	357	100	100	2			
1	O	71	Total	C	N	O	S	11	0	0
			559	357	100	100	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	GLY	-	CLONING ARTIFACT	UNP Q07914
C	98	GLY	-	CLONING ARTIFACT	UNP Q07914
E	98	GLY	-	CLONING ARTIFACT	UNP Q07914
G	98	GLY	-	CLONING ARTIFACT	UNP Q07914
I	98	GLY	-	CLONING ARTIFACT	UNP Q07914
K	98	GLY	-	CLONING ARTIFACT	UNP Q07914
M	98	GLY	-	CLONING ARTIFACT	UNP Q07914
O	98	GLY	-	CLONING ARTIFACT	UNP Q07914

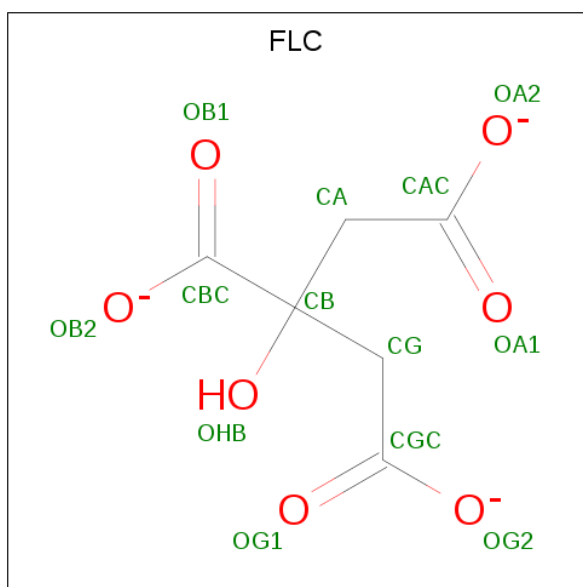
- Molecule 2 is a protein called Mitochondrial import inner membrane translocase subunit TIM16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	65	Total 551	C 346	N 97	O 105	S 3	13	1	0
2	D	65	Total 549	C 345	N 95	O 106	S 3	6	1	0
2	F	65	Total 543	C 341	N 94	O 105	S 3	0	0	0
2	H	65	Total 543	C 341	N 94	O 105	S 3	13	0	0
2	J	65	Total 543	C 341	N 94	O 105	S 3	8	0	0
2	L	65	Total 543	C 341	N 94	O 105	S 3	4	0	0
2	N	65	Total 543	C 341	N 94	O 105	S 3	24	0	0
2	P	65	Total 543	C 341	N 94	O 105	S 3	7	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	53	MET	-	CLONING ARTIFACT	UNP P42949
D	53	MET	-	CLONING ARTIFACT	UNP P42949
F	53	MET	-	CLONING ARTIFACT	UNP P42949
H	53	MET	-	CLONING ARTIFACT	UNP P42949
J	53	MET	-	CLONING ARTIFACT	UNP P42949
L	53	MET	-	CLONING ARTIFACT	UNP P42949
N	53	MET	-	CLONING ARTIFACT	UNP P42949
P	53	MET	-	CLONING ARTIFACT	UNP P42949

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		
3	J	1	Total	C	O	0	0
			13	6	7		
3	L	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	66	Total	O	0	0
			66	66		
4	C	54	Total	O	0	0
			54	54		
4	D	53	Total	O	0	0
			53	53		
4	E	77	Total	O	0	0
			77	77		
4	F	45	Total	O	0	0
			45	45		
4	G	64	Total	O	0	0
			64	64		
4	H	47	Total	O	0	0
			47	47		

Continued on next page...

Continued from previous page...

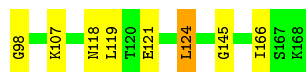
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	55	Total 55	O 55	0	0
4	J	54	Total 54	O 54	0	0
4	K	50	Total 50	O 50	0	0
4	L	37	Total 37	O 37	0	0
4	M	69	Total 69	O 69	0	0
4	N	56	Total 56	O 56	0	0
4	O	70	Total 70	O 70	0	0
4	P	51	Total 51	O 51	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: Mitochondrial import inner membrane translocase subunit TIM14

Chain A: 



- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM14

Chain C: 




- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM14

Chain E: 




- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM14

Chain G: 




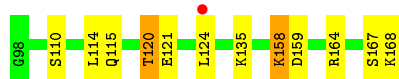
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM14

Chain I: 



- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM14

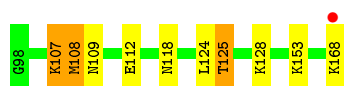
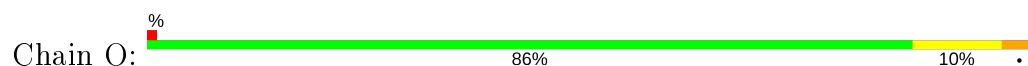
Chain K: 



- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM14



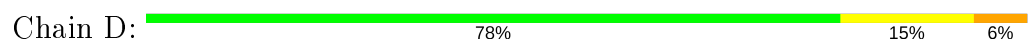
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM14



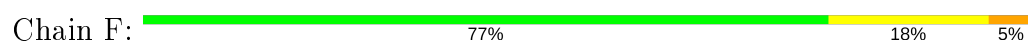
- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16



- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16



- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16



- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16

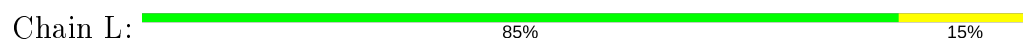


- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16

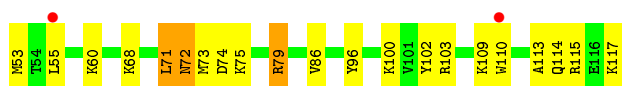




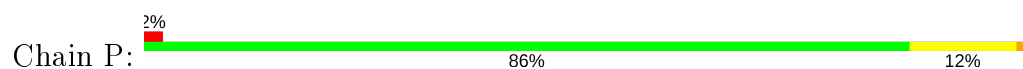
- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16



- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16



- Molecule 2: Mitochondrial import inner membrane translocase subunit TIM16



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.59Å 114.44Å 162.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 14.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.00) 90.1 (14.98-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.205 , 0.253 0.215 , 0.260	Depositor DCC
R_{free} test set	6848 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.217 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9819	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: FLC

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	1.03	1/568 (0.2%)	0.88	1/753 (0.1%)
1	C	1.07	2/573 (0.3%)	0.88	2/762 (0.3%)
1	E	1.01	1/573 (0.2%)	0.91	1/762 (0.1%)
1	G	0.98	0/573	0.90	1/762 (0.1%)
1	I	1.03	2/573 (0.3%)	0.95	4/762 (0.5%)
1	K	0.98	1/573 (0.2%)	0.87	1/762 (0.1%)
1	M	1.11	3/567 (0.5%)	0.97	2/753 (0.3%)
1	O	0.97	1/567 (0.2%)	0.87	1/753 (0.1%)
2	B	1.03	1/561 (0.2%)	1.05	4/746 (0.5%)
2	D	1.06	2/559 (0.4%)	1.01	3/744 (0.4%)
2	F	1.09	2/550 (0.4%)	0.95	1/732 (0.1%)
2	H	1.35	2/550 (0.4%)	1.00	4/732 (0.5%)
2	J	1.11	4/550 (0.7%)	0.95	2/732 (0.3%)
2	L	1.01	0/550	0.85	1/732 (0.1%)
2	N	1.63	5/550 (0.9%)	1.21	8/732 (1.1%)
2	P	1.12	2/550 (0.4%)	0.90	1/732 (0.1%)
All	All	1.11	29/8987 (0.3%)	0.95	37/11951 (0.3%)

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
2	N	1	0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	117	LYS	CA-CB	-26.67	0.95	1.53
2	H	65	GLU	CG-CD	-19.49	1.22	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	101	LYS	CG-CD	9.70	1.85	1.52
1	M	107	LYS	CB-CG	9.59	1.78	1.52
1	I	168	LYS	CG-CD	-9.36	1.20	1.52
2	J	117	LYS	CD-CE	9.09	1.74	1.51
1	C	163	LYS	CG-CD	-9.08	1.21	1.52
2	N	114	GLN	CB-CG	-8.77	1.28	1.52
2	N	60	LYS	CD-CE	-8.10	1.31	1.51
1	I	163	LYS	CG-CD	-7.90	1.25	1.52
1	E	107	LYS	CB-CG	7.69	1.73	1.52
1	C	107	LYS	CB-CG	-7.47	1.32	1.52
2	N	68	LYS	CA-CB	-6.97	1.38	1.53
2	N	115	ARG	CA-CB	-6.95	1.38	1.53
1	O	107	LYS	CB-CG	6.83	1.71	1.52
2	J	116	GLU	CG-CD	6.78	1.62	1.51
2	P	68	LYS	CG-CD	6.62	1.75	1.52
1	A	107	LYS	CB-CG	-6.24	1.35	1.52
1	M	163	LYS	CG-CD	-5.70	1.33	1.52
1	K	168	LYS	CA-CB	-5.69	1.41	1.53
2	F	109	LYS	CE-NZ	5.67	1.63	1.49
2	D	82	TYR	CE1-CZ	-5.55	1.31	1.38
2	B	100	LYS	CE-NZ	5.55	1.62	1.49
2	H	68	LYS	CB-CG	-5.53	1.37	1.52
2	J	68	LYS	CG-CD	-5.43	1.33	1.52
2	D	109	LYS	CE-NZ	5.43	1.62	1.49
2	P	82	TYR	CE1-CZ	-5.28	1.31	1.38
2	J	102	TYR	CE1-CZ	5.12	1.45	1.38
2	F	106	GLU	CD-OE1	-5.11	1.20	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	117	LYS	CA-C-O	10.09	141.28	120.10
2	B	117	LYS	CB-CA-C	9.67	129.74	110.40
1	I	168	LYS	CB-CG-CD	8.92	134.78	111.60
2	F	107	ARG	NE-CZ-NH1	-8.65	115.98	120.30
1	O	108	MET	CG-SD-CE	8.42	113.67	100.20
2	N	79	ARG	NE-CZ-NH1	-7.89	116.36	120.30
2	N	60	LYS	CG-CD-CE	7.64	134.81	111.90
2	N	117	LYS	CB-CA-C	7.64	125.67	110.40
1	C	107	LYS	CA-CB-CG	7.59	130.10	113.40
2	D	79	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	M	107	LYS	CA-CB-CG	-7.14	97.70	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	101	LYS	CB-CG-CD	-6.95	93.53	111.60
2	D	79	ARG	NE-CZ-NH1	-6.73	116.94	120.30
2	J	68	LYS	CB-CG-CD	6.61	128.78	111.60
1	C	163	LYS	CB-CG-CD	6.51	128.52	111.60
1	I	143	ASP	CB-CG-OD2	6.41	124.07	118.30
1	K	135	LYS	CB-CG-CD	6.17	127.65	111.60
2	P	68	LYS	CB-CG-CD	-6.14	95.64	111.60
1	I	163	LYS	CB-CG-CD	6.09	127.44	111.60
2	N	68	LYS	CB-CA-C	6.05	122.50	110.40
1	G	134	ARG	NE-CZ-NH2	6.03	123.32	120.30
2	H	53	MET	CA-CB-CG	6.01	123.52	113.30
2	N	114	GLN	CA-CB-CG	5.87	126.32	113.40
2	D	107	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	N	79	ARG	NE-CZ-NH2	5.75	123.18	120.30
2	H	65	GLU	CB-CG-CD	5.72	129.65	114.20
1	E	124	LEU	CB-CG-CD2	5.61	120.54	111.00
2	B	79[A]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	B	79[B]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	L	79	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	107	LYS	CA-CB-CG	5.28	125.01	113.40
2	B	86	VAL	CG1-CB-CG2	5.21	119.23	110.90
2	H	91	LYS	CB-CG-CD	5.20	125.11	111.60
2	J	79	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	I	135	LYS	CD-CE-NZ	5.10	123.43	111.70
2	H	68	LYS	CA-CB-CG	5.10	124.61	113.40
2	N	71	LEU	CB-CG-CD1	5.03	119.55	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	N	117	LYS	CA

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	560	0	596	7	0
1	C	562	0	601	3	0
1	E	562	0	601	3	0
1	G	562	0	601	8	0
1	I	562	0	601	6	0
1	K	562	0	601	8	0
1	M	559	0	596	12	0
1	O	559	0	596	7	0
2	B	551	0	550	12	0
2	D	549	0	545	11	0
2	F	543	0	537	11	0
2	H	543	0	537	9	0
2	J	543	0	537	10	0
2	L	543	0	537	6	0
2	N	543	0	537	15	0
2	P	543	0	537	3	0
3	F	26	0	10	1	0
3	J	13	0	5	0	0
3	L	13	0	5	0	0
4	A	73	0	0	1	0
4	B	66	0	0	1	0
4	C	54	0	0	2	0
4	D	53	0	0	2	0
4	E	77	0	0	2	0
4	F	45	0	0	4	0
4	G	64	0	0	0	0
4	H	47	0	0	1	0
4	I	55	0	0	2	0
4	J	54	0	0	0	0
4	K	50	0	0	6	0
4	L	37	0	0	3	0
4	M	69	0	0	3	0
4	N	56	0	0	6	0
4	O	70	0	0	1	0
4	P	51	0	0	1	0
All	All	9819	0	9130	117	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 7.

All (117) 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)
2:N:109:LYS:HB2	4:N:170:HOH:O	1.73	0.87
1:E:107:LYS:CB	4:E:241:HOH:O	2.22	0.87
1:E:107:LYS:HB2	4:E:241:HOH:O	1.74	0.85
1:M:125:THR:HG22	1:M:128:LYS:H	1.42	0.85
1:O:125:THR:HG22	1:O:128:LYS:H	1.42	0.84
4:B:131:HOH:O	1:M:125:THR:HG21	1.79	0.82
1:E:141:HIS:HD2	1:E:143:ASP:H	1.28	0.81
2:B:73:MET:HG2	2:F:73:MET:HG2	1.62	0.81
4:L:1038:HOH:O	2:N:102:TYR:CE1	2.35	0.80
2:D:73:MET:HG2	2:J:73:MET:HG2	1.65	0.79
1:I:125:THR:HG22	1:I:128:LYS:H	1.48	0.78
1:G:120:THR:HG23	4:K:182:HOH:O	1.85	0.76
2:B:73:MET:HE1	2:B:109:LYS:HG2	1.67	0.75
4:L:1038:HOH:O	2:N:102:TYR:HE1	1.70	0.73
1:I:125:THR:HG21	4:I:217:HOH:O	1.89	0.72
2:L:90:GLU:CD	4:L:1036:HOH:O	2.32	0.68
2:D:73:MET:CG	2:J:73:MET:HG2	2.24	0.67
2:D:73:MET:HE2	4:D:169:HOH:O	1.95	0.67
2:D:62:LEU:HD12	2:D:108:LEU:HD12	1.76	0.66
1:K:115:GLN:NE2	4:K:197:HOH:O	2.28	0.65
2:N:110:TRP:CG	4:N:168:HOH:O	2.50	0.64
1:A:119:LEU:HD13	1:A:124:LEU:HD23	1.80	0.64
2:J:107:ARG:NH1	2:J:111:GLU:OE2	2.30	0.64
1:M:118:ASN:HB3	4:M:199:HOH:O	1.98	0.64
1:M:141:HIS:HD2	1:M:143:ASP:H	1.46	0.64
1:A:124:LEU:HD13	1:A:166:ILE:HG23	1.80	0.63
1:M:121:GLU:OE2	4:M:231:HOH:O	2.15	0.62
1:M:108:MET:HB3	4:M:233:HOH:O	1.98	0.62
1:O:108:MET:CE	1:O:112:GLU:HB3	2.30	0.61
2:B:62:LEU:O	2:B:79[A]:ARG:CD	2.48	0.61
1:O:168:LYS:O	4:O:237:HOH:O	2.17	0.58
2:D:64:ILE:HD11	2:D:71:LEU:HG	1.85	0.58
2:B:62:LEU:O	2:B:79[A]:ARG:HD2	2.03	0.58
1:K:158:LYS:HE3	1:K:159:ASP:OD2	2.02	0.58
1:M:108:MET:HE3	1:M:112:GLU:OE1	2.03	0.58
1:K:120:THR:HG23	4:K:216:HOH:O	2.02	0.58
1:A:124:LEU:CD1	1:A:166:ILE:HG23	2.34	0.57
2:D:73:MET:CE	4:D:169:HOH:O	2.50	0.56
2:L:87:ASN:HD22	2:L:93:GLY:HA3	1.69	0.56
2:N:74:ASP:HB2	4:N:141:HOH:O	2.04	0.56
1:K:159:ASP:HB3	4:K:180:HOH:O	2.06	0.55
1:M:98:GLY:O	1:M:99:PHE:C	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:ASN:HD22	2:F:93:GLY:HA3	1.71	0.55
2:P:115:ARG:NH1	4:P:145:HOH:O	2.40	0.55
2:J:73:MET:HE2	2:J:112:LEU:HD23	1.90	0.54
2:H:71:LEU:HD12	2:H:76:ILE:HD11	1.89	0.54
2:J:55:LEU:HD21	2:J:111:GLU:HG2	1.91	0.53
2:H:62:LEU:HD12	2:H:108:LEU:HD12	1.91	0.53
2:H:77:ASN:ND2	2:H:109:LYS:HE2	2.24	0.52
1:G:122:ASN:HD21	1:K:114:LEU:HD13	1.75	0.52
1:A:121:GLU:HB3	1:C:164:ARG:HD2	1.92	0.52
1:A:98:GLY:N	3:F:1004:FLC:HOB	2.07	0.52
1:I:144:LYS:HG2	2:L:82:TYR:HB2	1.92	0.52
2:F:62:LEU:HD12	2:F:108:LEU:HD12	1.92	0.51
2:B:96:TYR:CZ	2:B:100:LYS:HE2	2.46	0.51
2:J:87:ASN:HD22	2:J:93:GLY:HA3	1.76	0.51
2:L:73:MET:HG2	2:N:73:MET:HG2	1.93	0.50
2:D:76:ILE:HD12	2:D:112:LEU:HD21	1.94	0.49
2:D:73:MET:CE	2:D:112:LEU:HD23	2.43	0.49
2:B:64:ILE:HG12	2:B:70:ASP:HB3	1.94	0.49
2:H:87:ASN:HD22	2:H:93:GLY:HA3	1.77	0.49
1:M:141:HIS:CD2	1:M:143:ASP:H	2.29	0.49
2:B:62:LEU:HD12	2:B:108:LEU:HD12	1.94	0.48
1:A:145:GLY:O	2:B:79[A]:ARG:NH1	2.45	0.48
1:G:167:SER:O	1:G:168:LYS:CB	2.61	0.48
1:G:167:SER:O	1:G:168:LYS:HB2	2.13	0.48
2:F:107:ARG:HD3	4:F:1019:HOH:O	2.13	0.47
2:N:110:TRP:CD1	4:N:168:HOH:O	2.67	0.47
2:B:73:MET:HG2	4:F:1047:HOH:O	2.14	0.47
1:M:141:HIS:CD2	1:M:142:PRO:HD2	2.49	0.47
2:D:71:LEU:HD21	2:D:108:LEU:HD22	1.96	0.47
2:F:71:LEU:CD2	2:F:112:LEU:HD11	2.44	0.47
1:I:103:GLY:HA2	2:J:100:LYS:HD2	1.97	0.47
1:C:111:LYS:HE2	4:C:205:HOH:O	2.13	0.47
1:C:119:LEU:O	4:C:184:HOH:O	2.21	0.47
2:L:62:LEU:HD12	2:L:108:LEU:HD12	1.96	0.47
2:P:73:MET:CE	2:P:112:LEU:HD23	2.45	0.46
2:F:88:ASP:OD1	2:F:90:GLU:HB2	2.15	0.46
1:I:130:LYS:HE2	2:N:110:TRP:CZ2	2.51	0.46
1:O:108:MET:HE2	1:O:109:ASN:O	2.15	0.46
2:D:107:ARG:NH1	2:D:111:GLU:OE2	2.46	0.45
1:M:108:MET:HE1	1:M:112:GLU:HG2	1.98	0.45
2:N:113:ALA:HA	4:N:172:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:THR:HG22	1:G:128:LYS:H	1.82	0.45
1:M:111:LYS:O	1:M:115:GLN:HG3	2.16	0.45
2:B:75:LYS:HZ1	2:B:79[B]:ARG:HH12	1.65	0.45
1:K:120:THR:HA	4:K:216:HOH:O	2.16	0.45
2:B:75:LYS:NZ	2:B:79[B]:ARG:NH1	2.65	0.45
1:G:122:ASN:O	1:K:121:GLU:HA	2.17	0.45
2:F:85:GLU:OE2	4:F:1039:HOH:O	2.21	0.44
2:B:73:MET:CE	2:B:77:ASN:OD1	2.66	0.44
1:A:118:ASN:ND2	4:A:180:HOH:O	2.51	0.44
2:D:71:LEU:HD23	2:D:76:ILE:HD11	1.99	0.43
1:O:125:THR:CG2	1:O:128:LYS:H	2.23	0.43
1:O:153:LYS:HA	1:O:153:LYS:HD2	1.85	0.43
2:J:71:LEU:CD1	2:J:76:ILE:HD11	2.48	0.43
2:F:73:MET:HE2	4:F:1047:HOH:O	2.17	0.43
2:N:96:TYR:CZ	2:N:100:LYS:HE2	2.52	0.43
2:H:88:ASP:OD1	2:H:90:GLU:HB2	2.19	0.43
2:F:71:LEU:CD2	2:F:112:LEU:CD1	2.96	0.43
2:J:71:LEU:HD12	2:J:76:ILE:HD11	2.01	0.42
1:I:133:HIS:O	1:I:137:MET:HB2	2.20	0.42
4:I:214:HOH:O	2:N:110:TRP:HA	2.19	0.42
2:N:79:ARG:HD3	4:N:129:HOH:O	2.19	0.42
1:G:104:PHE:CE1	2:H:100:LYS:HG2	2.55	0.42
2:H:85:GLU:HB3	4:H:162:HOH:O	2.20	0.41
2:N:53:MET:HE1	2:N:103:ARG:HB2	2.02	0.41
2:F:82:TYR:HB2	1:G:144:LYS:HG2	2.03	0.41
1:K:164:ARG:O	4:K:202:HOH:O	2.22	0.41
2:N:72:ASN:ND2	2:N:75:LYS:H	2.18	0.41
2:J:62:LEU:HD12	2:J:108:LEU:HD12	2.01	0.41
2:F:71:LEU:HD22	2:F:112:LEU:HD11	2.02	0.41
2:H:75:LYS:O	2:H:79:ARG:HG2	2.20	0.41
2:L:77:ASN:HD22	2:N:109:LYS:NZ	2.18	0.41
2:P:55:LEU:HD23	2:P:108:LEU:CD2	2.50	0.41
1:O:108:MET:HE1	1:O:112:GLU:HG2	2.03	0.40
2:H:108:LEU:HA	2:H:108:LEU:HD23	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	69/71 (97%)	69 (100%)	0	0	100	100
1	C	70/71 (99%)	69 (99%)	1 (1%)	0	100	100
1	E	70/71 (99%)	70 (100%)	0	0	100	100
1	G	70/71 (99%)	69 (99%)	1 (1%)	0	100	100
1	I	70/71 (99%)	70 (100%)	0	0	100	100
1	K	70/71 (99%)	69 (99%)	1 (1%)	0	100	100
1	M	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
1	O	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
2	B	64/65 (98%)	63 (98%)	1 (2%)	0	100	100
2	D	64/65 (98%)	64 (100%)	0	0	100	100
2	F	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
2	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
2	J	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
2	L	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
2	N	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
2	P	63/65 (97%)	63 (100%)	0	0	100	100
All	All	1063/1088 (98%)	1048 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	61/61 (100%)	60 (98%)	1 (2%)	62	67
1	C	62/61 (102%)	58 (94%)	4 (6%)	17	12
1	E	62/61 (102%)	61 (98%)	1 (2%)	62	67
1	G	62/61 (102%)	58 (94%)	4 (6%)	17	12
1	I	62/61 (102%)	60 (97%)	2 (3%)	39	38
1	K	62/61 (102%)	57 (92%)	5 (8%)	11	7
1	M	61/61 (100%)	57 (93%)	4 (7%)	16	12
1	O	61/61 (100%)	57 (93%)	4 (7%)	16	12
2	B	60/59 (102%)	55 (92%)	5 (8%)	11	7
2	D	60/59 (102%)	55 (92%)	5 (8%)	11	7
2	F	59/59 (100%)	56 (95%)	3 (5%)	24	19
2	H	59/59 (100%)	56 (95%)	3 (5%)	24	19
2	J	59/59 (100%)	56 (95%)	3 (5%)	24	19
2	L	59/59 (100%)	58 (98%)	1 (2%)	60	65
2	N	59/59 (100%)	55 (93%)	4 (7%)	16	11
2	P	59/59 (100%)	56 (95%)	3 (5%)	24	19
All	All	967/960 (101%)	915 (95%)	52 (5%)	22	18

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
2	B	55	LEU
2	B	71	LEU
2	B	86	VAL
2	B	100	LYS
2	B	112	LEU
1	C	107	LYS
1	C	124	LEU
1	C	127	LYS
1	C	158	LYS
2	D	53	MET
2	D	64	ILE
2	D	71	LEU
2	D	86	VAL
2	D	112	LEU
1	E	124	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	86	VAL
2	F	90	GLU
2	F	112	LEU
1	G	110	SER
1	G	124	LEU
1	G	125	THR
1	G	158	LYS
2	H	86	VAL
2	H	91	LYS
2	H	117	LYS
1	I	124	LEU
1	I	125	THR
2	J	55	LEU
2	J	71	LEU
2	J	112	LEU
1	K	110	SER
1	K	120	THR
1	K	124	LEU
1	K	158	LYS
1	K	167	SER
2	L	55	LEU
1	M	107	LYS
1	M	124	LEU
1	M	125	THR
1	M	147	SER
2	N	55	LEU
2	N	71	LEU
2	N	72	ASN
2	N	86	VAL
1	O	107	LYS
1	O	118	ASN
1	O	124	LEU
1	O	125	THR
2	P	63	ASN
2	P	86	VAL
2	P	112	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	122	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	63	ASN
2	B	78	ASN
1	C	118	ASN
2	D	63	ASN
2	D	72	ASN
2	D	77	ASN
2	D	81	ASN
1	E	140	ASN
1	E	141	HIS
2	F	63	ASN
2	F	81	ASN
2	F	87	ASN
1	G	118	ASN
1	G	122	ASN
1	G	140	ASN
2	H	63	ASN
2	H	77	ASN
2	H	78	ASN
2	H	81	ASN
2	H	87	ASN
2	H	98	GLN
1	I	118	ASN
1	I	140	ASN
2	J	63	ASN
2	J	77	ASN
2	J	81	ASN
2	J	87	ASN
1	K	118	ASN
1	K	140	ASN
2	L	63	ASN
2	L	77	ASN
2	L	78	ASN
2	L	81	ASN
2	L	87	ASN
2	L	98	GLN
1	M	118	ASN
1	M	140	ASN
1	M	141	HIS
2	N	63	ASN
2	N	72	ASN
2	N	78	ASN
2	N	81	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	87	ASN
2	N	98	GLN
1	O	118	ASN
1	O	122	ASN
2	P	63	ASN
2	P	77	ASN
2	P	78	ASN
2	P	81	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	FLC	F	1002	-	3,12,12	0.51	0	3,17,17	0.79	0
3	FLC	J	1001	-	3,12,12	1.78	2 (66%)	3,17,17	1.87	1 (33%)
3	FLC	L	1003	-	3,12,12	0.32	0	3,17,17	1.43	1 (33%)
3	FLC	F	1004	-	3,12,12	0.33	0	3,17,17	1.93	1 (33%)

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
3	FLC	F	1002	-	-	2/6/16/16	-
3	FLC	J	1001	-	-	2/6/16/16	-
3	FLC	L	1003	-	-	1/6/16/16	-
3	FLC	F	1004	-	-	0/6/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1001	FLC	CA-CB	-2.20	1.51	1.54
3	J	1001	FLC	CG-CB	-2.09	1.52	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1001	FLC	CB-CA-CAC	-2.77	110.55	114.98
3	F	1004	FLC	CG-CB-CA	2.47	115.93	109.33
3	L	1003	FLC	CB-CG-CGC	-2.20	111.45	114.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1002	FLC	CBC-CB-CG-CGC
3	J	1001	FLC	CAC-CA-CB-CBC
3	L	1003	FLC	CBC-CB-CG-CGC
3	F	1002	FLC	OHB-CB-CG-CGC
3	J	1001	FLC	CAC-CA-CB-OHB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1004	FLC	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	71/71 (100%)	-0.25	0 100 100	19, 32, 49, 55	3 (4%)
1	C	71/71 (100%)	-0.10	0 100 100	23, 38, 58, 74	4 (5%)
1	E	71/71 (100%)	-0.23	0 100 100	24, 33, 49, 70	5 (7%)
1	G	71/71 (100%)	-0.09	0 100 100	24, 34, 49, 73	0
1	I	71/71 (100%)	-0.16	1 (1%) 75 74	26, 35, 56, 76	4 (5%)
1	K	71/71 (100%)	-0.12	1 (1%) 75 74	24, 36, 63, 71	5 (7%)
1	M	71/71 (100%)	-0.23	0 100 100	24, 35, 51, 64	4 (5%)
1	O	71/71 (100%)	-0.15	1 (1%) 75 74	23, 36, 53, 77	3 (4%)
2	B	65/65 (100%)	-0.21	0 100 100	21, 30, 49, 72	5 (7%)
2	D	65/65 (100%)	-0.22	0 100 100	24, 33, 49, 75	2 (3%)
2	F	65/65 (100%)	-0.22	0 100 100	22, 30, 56, 73	0
2	H	65/65 (100%)	-0.22	0 100 100	24, 31, 57, 77	4 (6%)
2	J	65/65 (100%)	-0.23	0 100 100	23, 31, 58, 64	3 (4%)
2	L	65/65 (100%)	-0.17	0 100 100	24, 34, 59, 84	2 (3%)
2	N	65/65 (100%)	0.02	2 (3%) 49 48	22, 42, 69, 100	5 (7%)
2	P	65/65 (100%)	0.03	1 (1%) 73 72	24, 37, 72, 89	2 (3%)
All	All	1088/1088 (100%)	-0.16	6 (0%) 89 88	19, 34, 59, 100	51 (4%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	167	SER	3.5
1	K	124	LEU	3.2
2	P	55	LEU	3.0
2	N	110	TRP	3.0
1	O	168	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	55	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 carbohydrates 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(\AA^2)	Q<0.9
3	FLC	F	1004	13/13	0.55	0.29	77,96,99,100	0
3	FLC	L	1003	13/13	0.65	0.21	70,92,98,102	0
3	FLC	F	1002	13/13	0.90	0.15	31,49,62,70	0
3	FLC	J	1001	13/13	0.90	0.17	34,56,63,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.