



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:40 PM UTC

PDB ID : 4GM2 / pdb_00004gm2
Title : The crystal structure of a peptidase from plasmodium falciparum
Authors : El Bakkouri, M.; Jung, P.; Wernimont, A.K.; Calmettes, C.; Hui, R.; Houry, W.A.; Structural Genomics Consortium (SGC)
Deposited on : 2012-08-15
Resolution : 2.80 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:

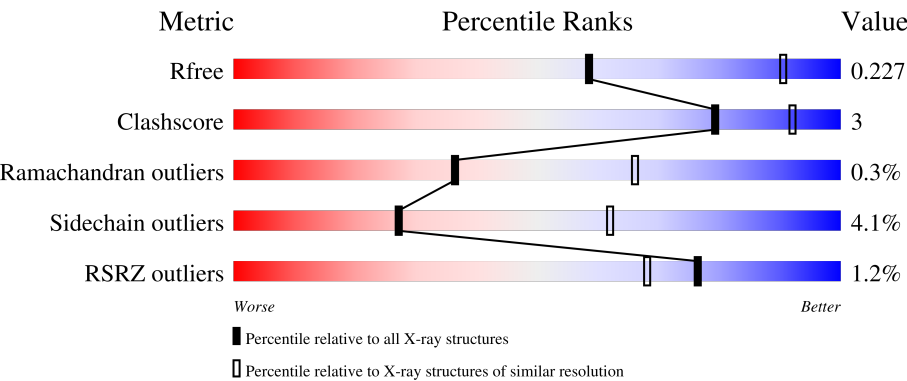
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	205	79%10%11%
1	B	205	2%74%7%20%
1	C	205	2%72%9%19%
1	D	205	2%73%6%20%
1	E	205	78%11%11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	205	75% 7% 17%
1	G	205	% 72% 11% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9611 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1453	931	236	282	4			
1	B	165	Total	C	N	O	S	0	0	0
			1313	845	214	251	3			
1	C	167	Total	C	N	O	S	0	0	0
			1323	849	214	256	4			
1	D	163	Total	C	N	O	S	0	0	0
			1295	832	211	248	4			
1	E	183	Total	C	N	O	S	0	0	0
			1439	926	232	277	4			
1	F	170	Total	C	N	O	S	0	0	0
			1359	875	219	261	4			
1	G	171	Total	C	N	O	S	0	0	0
			1360	872	223	261	4			

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	initiating methionine	UNP Q8IL98
A	41	GLY	-	expression tag	UNP Q8IL98
A	42	SER	-	expression tag	UNP Q8IL98
A	43	SER	-	expression tag	UNP Q8IL98
A	44	HIS	-	expression tag	UNP Q8IL98
A	45	HIS	-	expression tag	UNP Q8IL98
A	46	HIS	-	expression tag	UNP Q8IL98
A	47	HIS	-	expression tag	UNP Q8IL98
A	48	HIS	-	expression tag	UNP Q8IL98
A	49	HIS	-	expression tag	UNP Q8IL98
A	50	SER	-	expression tag	UNP Q8IL98
A	51	SER	-	expression tag	UNP Q8IL98
A	52	GLY	-	expression tag	UNP Q8IL98
A	53	ARG	-	expression tag	UNP Q8IL98
A	54	GLU	-	expression tag	UNP Q8IL98

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ASN	-	expression tag	UNP Q8IL98
A	56	LEU	-	expression tag	UNP Q8IL98
A	57	TYR	-	expression tag	UNP Q8IL98
A	58	PHE	-	expression tag	UNP Q8IL98
A	59	GLN	-	expression tag	UNP Q8IL98
A	60	GLY	-	expression tag	UNP Q8IL98
B	40	MET	-	initiating methionine	UNP Q8IL98
B	41	GLY	-	expression tag	UNP Q8IL98
B	42	SER	-	expression tag	UNP Q8IL98
B	43	SER	-	expression tag	UNP Q8IL98
B	44	HIS	-	expression tag	UNP Q8IL98
B	45	HIS	-	expression tag	UNP Q8IL98
B	46	HIS	-	expression tag	UNP Q8IL98
B	47	HIS	-	expression tag	UNP Q8IL98
B	48	HIS	-	expression tag	UNP Q8IL98
B	49	HIS	-	expression tag	UNP Q8IL98
B	50	SER	-	expression tag	UNP Q8IL98
B	51	SER	-	expression tag	UNP Q8IL98
B	52	GLY	-	expression tag	UNP Q8IL98
B	53	ARG	-	expression tag	UNP Q8IL98
B	54	GLU	-	expression tag	UNP Q8IL98
B	55	ASN	-	expression tag	UNP Q8IL98
B	56	LEU	-	expression tag	UNP Q8IL98
B	57	TYR	-	expression tag	UNP Q8IL98
B	58	PHE	-	expression tag	UNP Q8IL98
B	59	GLN	-	expression tag	UNP Q8IL98
B	60	GLY	-	expression tag	UNP Q8IL98
C	40	MET	-	initiating methionine	UNP Q8IL98
C	41	GLY	-	expression tag	UNP Q8IL98
C	42	SER	-	expression tag	UNP Q8IL98
C	43	SER	-	expression tag	UNP Q8IL98
C	44	HIS	-	expression tag	UNP Q8IL98
C	45	HIS	-	expression tag	UNP Q8IL98
C	46	HIS	-	expression tag	UNP Q8IL98
C	47	HIS	-	expression tag	UNP Q8IL98
C	48	HIS	-	expression tag	UNP Q8IL98
C	49	HIS	-	expression tag	UNP Q8IL98
C	50	SER	-	expression tag	UNP Q8IL98
C	51	SER	-	expression tag	UNP Q8IL98
C	52	GLY	-	expression tag	UNP Q8IL98
C	53	ARG	-	expression tag	UNP Q8IL98
C	54	GLU	-	expression tag	UNP Q8IL98

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	55	ASN	-	expression tag	UNP Q8IL98
C	56	LEU	-	expression tag	UNP Q8IL98
C	57	TYR	-	expression tag	UNP Q8IL98
C	58	PHE	-	expression tag	UNP Q8IL98
C	59	GLN	-	expression tag	UNP Q8IL98
C	60	GLY	-	expression tag	UNP Q8IL98
D	40	MET	-	initiating methionine	UNP Q8IL98
D	41	GLY	-	expression tag	UNP Q8IL98
D	42	SER	-	expression tag	UNP Q8IL98
D	43	SER	-	expression tag	UNP Q8IL98
D	44	HIS	-	expression tag	UNP Q8IL98
D	45	HIS	-	expression tag	UNP Q8IL98
D	46	HIS	-	expression tag	UNP Q8IL98
D	47	HIS	-	expression tag	UNP Q8IL98
D	48	HIS	-	expression tag	UNP Q8IL98
D	49	HIS	-	expression tag	UNP Q8IL98
D	50	SER	-	expression tag	UNP Q8IL98
D	51	SER	-	expression tag	UNP Q8IL98
D	52	GLY	-	expression tag	UNP Q8IL98
D	53	ARG	-	expression tag	UNP Q8IL98
D	54	GLU	-	expression tag	UNP Q8IL98
D	55	ASN	-	expression tag	UNP Q8IL98
D	56	LEU	-	expression tag	UNP Q8IL98
D	57	TYR	-	expression tag	UNP Q8IL98
D	58	PHE	-	expression tag	UNP Q8IL98
D	59	GLN	-	expression tag	UNP Q8IL98
D	60	GLY	-	expression tag	UNP Q8IL98
E	40	MET	-	initiating methionine	UNP Q8IL98
E	41	GLY	-	expression tag	UNP Q8IL98
E	42	SER	-	expression tag	UNP Q8IL98
E	43	SER	-	expression tag	UNP Q8IL98
E	44	HIS	-	expression tag	UNP Q8IL98
E	45	HIS	-	expression tag	UNP Q8IL98
E	46	HIS	-	expression tag	UNP Q8IL98
E	47	HIS	-	expression tag	UNP Q8IL98
E	48	HIS	-	expression tag	UNP Q8IL98
E	49	HIS	-	expression tag	UNP Q8IL98
E	50	SER	-	expression tag	UNP Q8IL98
E	51	SER	-	expression tag	UNP Q8IL98
E	52	GLY	-	expression tag	UNP Q8IL98
E	53	ARG	-	expression tag	UNP Q8IL98
E	54	GLU	-	expression tag	UNP Q8IL98

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	55	ASN	-	expression tag	UNP Q8IL98
E	56	LEU	-	expression tag	UNP Q8IL98
E	57	TYR	-	expression tag	UNP Q8IL98
E	58	PHE	-	expression tag	UNP Q8IL98
E	59	GLN	-	expression tag	UNP Q8IL98
E	60	GLY	-	expression tag	UNP Q8IL98
F	40	MET	-	initiating methionine	UNP Q8IL98
F	41	GLY	-	expression tag	UNP Q8IL98
F	42	SER	-	expression tag	UNP Q8IL98
F	43	SER	-	expression tag	UNP Q8IL98
F	44	HIS	-	expression tag	UNP Q8IL98
F	45	HIS	-	expression tag	UNP Q8IL98
F	46	HIS	-	expression tag	UNP Q8IL98
F	47	HIS	-	expression tag	UNP Q8IL98
F	48	HIS	-	expression tag	UNP Q8IL98
F	49	HIS	-	expression tag	UNP Q8IL98
F	50	SER	-	expression tag	UNP Q8IL98
F	51	SER	-	expression tag	UNP Q8IL98
F	52	GLY	-	expression tag	UNP Q8IL98
F	53	ARG	-	expression tag	UNP Q8IL98
F	54	GLU	-	expression tag	UNP Q8IL98
F	55	ASN	-	expression tag	UNP Q8IL98
F	56	LEU	-	expression tag	UNP Q8IL98
F	57	TYR	-	expression tag	UNP Q8IL98
F	58	PHE	-	expression tag	UNP Q8IL98
F	59	GLN	-	expression tag	UNP Q8IL98
F	60	GLY	-	expression tag	UNP Q8IL98
G	40	MET	-	initiating methionine	UNP Q8IL98
G	41	GLY	-	expression tag	UNP Q8IL98
G	42	SER	-	expression tag	UNP Q8IL98
G	43	SER	-	expression tag	UNP Q8IL98
G	44	HIS	-	expression tag	UNP Q8IL98
G	45	HIS	-	expression tag	UNP Q8IL98
G	46	HIS	-	expression tag	UNP Q8IL98
G	47	HIS	-	expression tag	UNP Q8IL98
G	48	HIS	-	expression tag	UNP Q8IL98
G	49	HIS	-	expression tag	UNP Q8IL98
G	50	SER	-	expression tag	UNP Q8IL98
G	51	SER	-	expression tag	UNP Q8IL98
G	52	GLY	-	expression tag	UNP Q8IL98
G	53	ARG	-	expression tag	UNP Q8IL98
G	54	GLU	-	expression tag	UNP Q8IL98

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	55	ASN	-	expression tag	UNP Q8IL98
G	56	LEU	-	expression tag	UNP Q8IL98
G	57	TYR	-	expression tag	UNP Q8IL98
G	58	PHE	-	expression tag	UNP Q8IL98
G	59	GLN	-	expression tag	UNP Q8IL98
G	60	GLY	-	expression tag	UNP Q8IL98

- Molecule 2 is water.

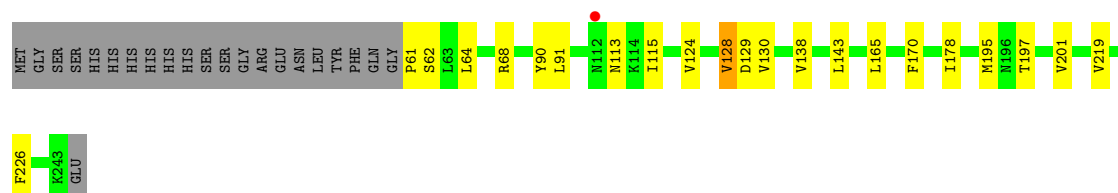
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	10	Total O 10 10	0	0
2	C	11	Total O 11 11	0	0
2	D	5	Total O 5 5	0	0
2	E	5	Total O 5 5	0	0
2	F	9	Total O 9 9	0	0
2	G	12	Total O 12 12	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

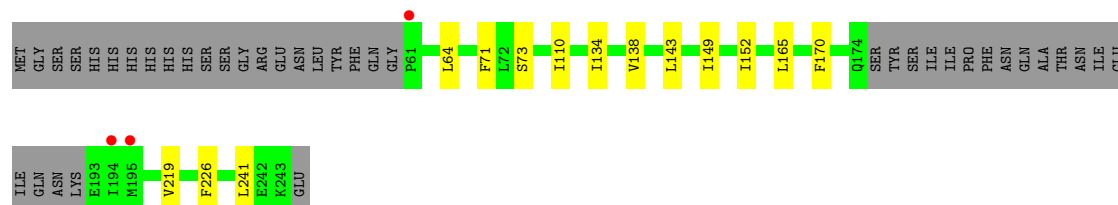
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A: 



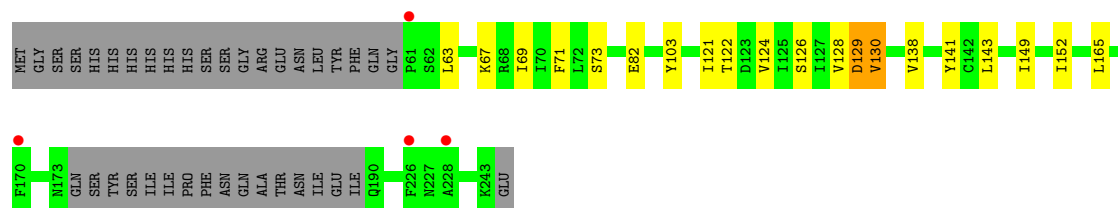
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

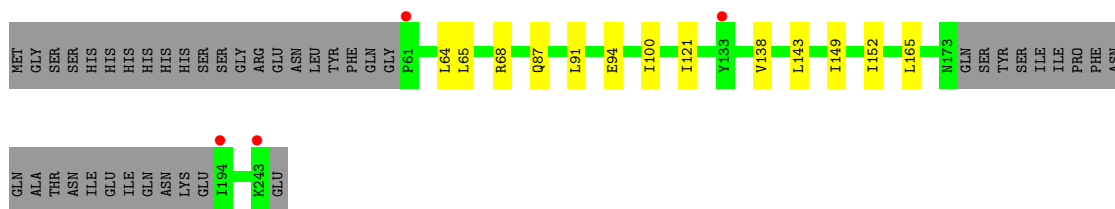
Chain C: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

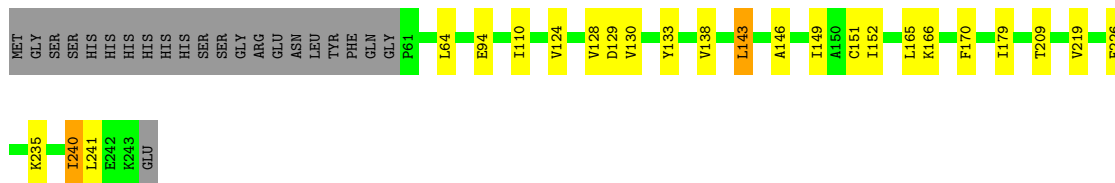
Chain D: 





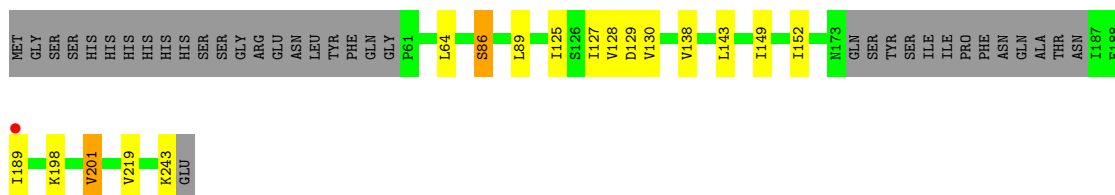
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E: 78% 11% • 11%



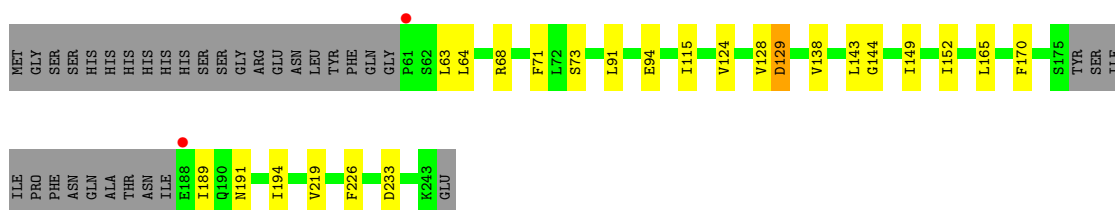
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F: 75% 7% • 17%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G: 72% 11% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.90Å 102.16Å 96.41Å 90.00° 114.53° 90.00°	Depositor
Resolution (Å)	48.79 – 2.80 48.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.79-2.80) 99.5 (48.79-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.229 0.198 , 0.227	Depositor DCC
R_{free} test set	2006 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9611	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/1475	0.78	0/1995
1	B	0.48	0/1333	0.76	0/1799
1	C	0.49	0/1343	0.78	0/1813
1	D	0.48	0/1315	0.75	0/1774
1	E	0.47	0/1463	0.77	0/1979
1	F	0.46	0/1379	0.76	0/1859
1	G	0.49	0/1380	0.77	0/1859
All	All	0.47	0/9688	0.77	0/13078

There are no bond length outliers.

There are no bond angle outliers.

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	1453	0	1472	10	0
1	B	1313	0	1343	6	0
1	C	1323	0	1340	11	0
1	D	1295	0	1320	5	0
1	E	1439	0	1450	12	0
1	F	1359	0	1399	8	0
1	G	1360	0	1392	9	0
2	A	17	0	0	0	0
2	B	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	11	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	9	0	0	0	0
2	G	12	0	0	0	0
All	All	9611	0	9716	51	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 3.

All (51) 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:A:124:VAL:O	1:A:128:VAL:HG12	1.86	0.76
1:E:240:ILE:HG13	1:E:241:LEU:H	1.59	0.67
1:A:129:ASP:HB3	1:G:165:LEU:HD13	1.77	0.65
1:G:124:VAL:O	1:G:128:VAL:HG12	1.97	0.64
1:B:165:LEU:HD13	1:E:129:ASP:HB3	1.80	0.63
1:E:170:PHE:HB2	1:E:226:PHE:HB2	1.81	0.62
1:G:170:PHE:HB2	1:G:226:PHE:HB2	1.80	0.62
1:B:170:PHE:HB2	1:B:226:PHE:HB2	1.82	0.61
1:C:165:LEU:HD13	1:F:129:ASP:HB3	1.84	0.59
1:C:124:VAL:O	1:C:128:VAL:HG12	2.03	0.58
1:A:195:MET:HA	1:A:195:MET:HE2	1.89	0.55
1:E:166:LYS:HA	1:E:240:ILE:HD11	1.90	0.54
1:C:126:SER:O	1:C:130:VAL:HG12	2.09	0.53
1:D:68:ARG:HG2	1:D:91:LEU:HD22	1.90	0.53
1:B:241:LEU:HD13	1:E:133:TYR:CE1	2.44	0.53
1:E:149:ILE:HA	1:E:152:ILE:HD12	1.92	0.52
1:A:165:LEU:HD13	1:C:129:ASP:HB3	1.91	0.52
1:C:165:LEU:HD11	1:F:130:VAL:HG12	1.93	0.51
1:D:165:LEU:HD13	1:G:129:ASP:HB3	1.93	0.51
1:G:149:ILE:HA	1:G:152:ILE:HD12	1.93	0.51
1:D:149:ILE:HA	1:D:152:ILE:HD12	1.93	0.50
1:C:67:LYS:HB2	1:C:69:ILE:HD12	1.93	0.50
1:B:149:ILE:HA	1:B:152:ILE:HD12	1.92	0.49
1:E:124:VAL:O	1:E:128:VAL:HG13	2.14	0.48
1:E:143:LEU:HA	1:E:165:LEU:HD12	1.95	0.48
1:C:71:PHE:HE2	1:F:86:SER:HA	1.79	0.48
1:E:240:ILE:HG13	1:E:241:LEU:N	2.28	0.47
1:F:149:ILE:HA	1:F:152:ILE:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:PHE:CZ	1:G:73:SER:HB3	2.52	0.45
1:A:68:ARG:HG2	1:A:91:LEU:HD22	1.98	0.45
1:A:115:ILE:HD13	1:A:178:ILE:HG12	1.99	0.44
1:C:71:PHE:CZ	1:C:73:SER:HB3	2.52	0.44
1:B:134:ILE:O	1:F:243:LYS:HE3	2.17	0.44
1:C:149:ILE:HA	1:C:152:ILE:HD12	2.00	0.43
1:F:125:ILE:O	1:F:128:VAL:HG12	2.19	0.43
1:F:198:LYS:O	1:F:201:VAL:HG12	2.19	0.43
1:G:191:ASN:HA	1:G:194:ILE:HD12	2.01	0.42
1:B:71:PHE:CZ	1:B:73:SER:HB3	2.55	0.42
1:D:100:ILE:HB	1:D:138:VAL:HG12	2.01	0.42
1:A:197:THR:O	1:A:201:VAL:HG12	2.20	0.42
1:F:127:ILE:O	1:F:130:VAL:HG22	2.19	0.42
1:C:103:TYR:CD2	1:C:141:TYR:HB2	2.56	0.41
1:A:170:PHE:HB2	1:A:226:PHE:HB2	2.02	0.41
1:E:146:ALA:O	1:E:151:CYS:HB2	2.20	0.41
1:E:209:THR:HA	1:E:235:LYS:HB3	2.02	0.41
1:A:90:TYR:CE1	1:G:63:LEU:HG	2.56	0.41
1:D:65:LEU:HD11	1:D:87:GLN:HG2	2.02	0.41
1:E:130:VAL:HA	1:E:133:TYR:HB3	2.03	0.41
1:G:68:ARG:HG2	1:G:91:LEU:HD22	2.03	0.40
1:C:121:ILE:O	1:C:124:VAL:HG12	2.22	0.40
1:A:61:PRO:HB2	1:A:62:SER:H	1.65	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	181/205 (88%)	173 (96%)	7 (4%)	1 (1%)	21 51
1	B	161/205 (78%)	155 (96%)	6 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	163/205 (80%)	157 (96%)	6 (4%)	0	100	100
1	D	159/205 (78%)	152 (96%)	7 (4%)	0	100	100
1	E	181/205 (88%)	170 (94%)	10 (6%)	1 (1%)	21	51
1	F	166/205 (81%)	161 (97%)	5 (3%)	0	100	100
1	G	167/205 (82%)	161 (96%)	4 (2%)	2 (1%)	10	34
All	All	1178/1435 (82%)	1129 (96%)	45 (4%)	4 (0%)	36	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	189	ILE
1	E	240	ILE
1	A	113	ASN
1	G	144	GLY

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	167/190 (88%)	161 (96%)	6 (4%)	31	66
1	B	151/190 (80%)	146 (97%)	5 (3%)	33	69
1	C	152/190 (80%)	145 (95%)	7 (5%)	24	58
1	D	149/190 (78%)	145 (97%)	4 (3%)	39	74
1	E	163/190 (86%)	156 (96%)	7 (4%)	26	60
1	F	158/190 (83%)	150 (95%)	8 (5%)	21	54
1	G	157/190 (83%)	149 (95%)	8 (5%)	21	54
All	All	1097/1330 (82%)	1052 (96%)	45 (4%)	27	62

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	128	VAL
1	A	130	VAL
1	A	138	VAL
1	A	143	LEU
1	A	219	VAL
1	B	64	LEU
1	B	110	ILE
1	B	138	VAL
1	B	143	LEU
1	B	219	VAL
1	C	63	LEU
1	C	82	GLU
1	C	122	THR
1	C	129	ASP
1	C	130	VAL
1	C	138	VAL
1	C	143	LEU
1	D	64	LEU
1	D	94	GLU
1	D	121	ILE
1	D	143	LEU
1	E	64	LEU
1	E	94	GLU
1	E	110	ILE
1	E	138	VAL
1	E	143	LEU
1	E	179	ILE
1	E	219	VAL
1	F	64	LEU
1	F	86	SER
1	F	89	LEU
1	F	138	VAL
1	F	143	LEU
1	F	189	ILE
1	F	201	VAL
1	F	219	VAL
1	G	64	LEU
1	G	94	GLU
1	G	115	ILE
1	G	129	ASP
1	G	138	VAL
1	G	143	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	219	VAL
1	G	233	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	183	GLN
1	B	87	GLN
1	B	174	GLN
1	B	239	HIS
1	C	87	GLN
1	C	119	ASN
1	C	190	GLN
1	D	83	GLN
1	E	87	GLN
1	F	79	HIS
1	F	190	GLN
1	F	191	ASN
1	G	87	GLN
1	G	112	ASN
1	G	119	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	183/205 (89%)	-0.46	1 (0%) 87 82	58, 79, 116, 127	0
1	B	165/205 (80%)	-0.20	3 (1%) 67 58	64, 99, 162, 190	0
1	C	167/205 (81%)	-0.33	4 (2%) 59 49	61, 84, 147, 204	0
1	D	163/205 (79%)	-0.17	4 (2%) 58 48	77, 115, 180, 198	0
1	E	183/205 (89%)	-0.21	0 100 100	70, 104, 142, 171	0
1	F	170/205 (82%)	-0.32	1 (0%) 85 80	61, 97, 166, 223	0
1	G	171/205 (83%)	-0.44	2 (1%) 76 68	62, 88, 139, 213	0
All	All	1202/1435 (83%)	-0.31	15 (1%) 76 68	58, 95, 159, 223	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	TYR	2.8
1	G	188	GLU	2.8
1	C	170	PHE	2.7
1	B	61	PRO	2.6
1	D	61	PRO	2.6
1	D	243	LYS	2.5
1	B	194	ILE	2.5
1	C	228	ALA	2.5
1	D	194	ILE	2.4
1	A	112	ASN	2.4
1	C	61	PRO	2.1
1	B	195	MET	2.1
1	F	189	ILE	2.1
1	G	61	PRO	2.0
1	C	226	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.